

DEPARTMENT OF CHEMISTRY AND PHARMACY

PROFILE 2014







DEPARTMENT OF CHEMISTRY AND PHARMACY – MISSION AND VISION

Chemistry plays an integral role in today's scientific endeavors. It is situated at the heart of many scientific disciplines as science has become increasingly interdisciplinary. With a strong commitment to excellence in education and research we are dedicated to the fundamental chemical sciences as well as to exploring fundamental scientific problems at the interface between chemistry and other disciplines.

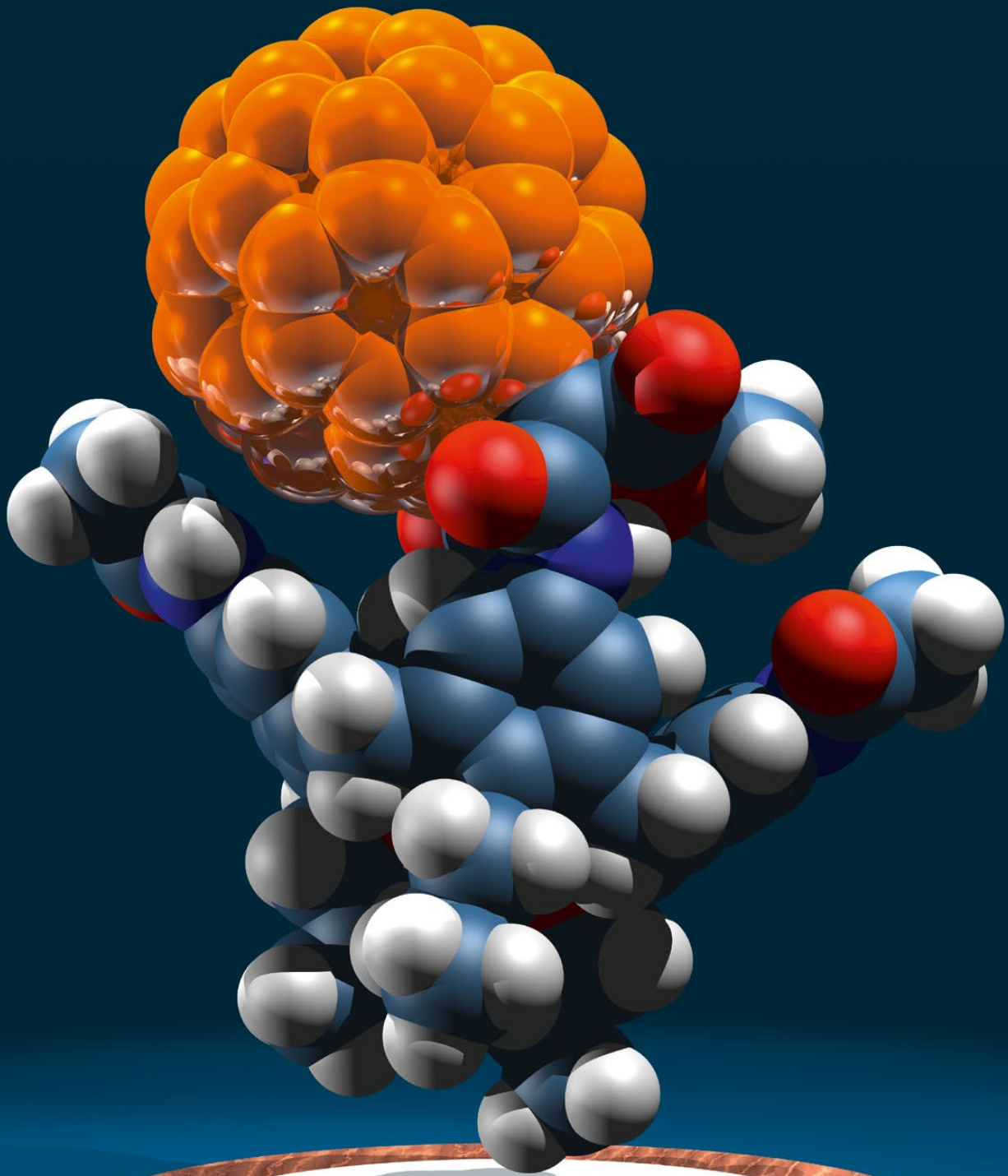
The Department of Chemistry and Pharmacy has a long standing tradition of excellence—because of our vast resources, cutting-edge facilities, and outstanding faculty—and is ranked among the best in the country. This is documented by the quality of its programs, the caliber of its faculty, and the excellence 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 from countries all over the world to study in specific research programs directed by the University of Erlangen-Nürnberg's chemistry professors.

The Department employs 28 professors pursuing research in all areas of chemistry and pharmacy. The foci of our renowned and well-funded research programs are molecular materials and 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 and several Collaborative Research Centers.

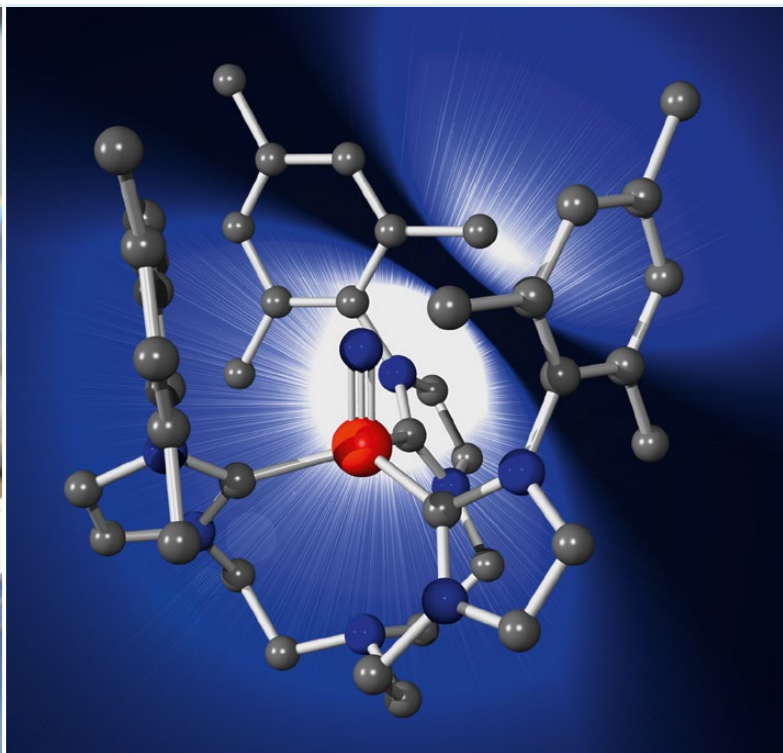
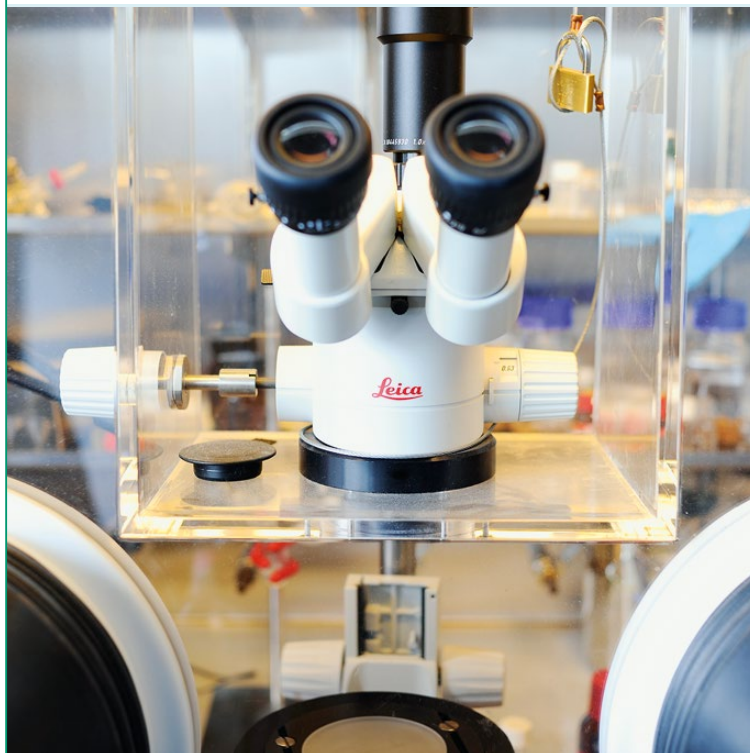
Our motto: "A dedication to promote excellence and innovation in chemistry through education and research."

Andreas Görling
Head of the Department of Chemistry and Pharmacy





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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, which are based on excellence in a wide range of research areas. For the fall/winter term of 2014/15, about 39,000 students are enrolled at the FAU. The latter places the FAU among the 12 largest universities in Germany. In 2013, the FAU raised 171 million euros in third-party funding for research. 576 professors and 3,400 academic staff members educate and train 39,085 students. Among the five FAU Faculties the Faculty of Sciences features five Departments, that are, **Biology, Mathematics, Geography and Geosciences, Physics** as well as **Chemistry and Pharmacy**.

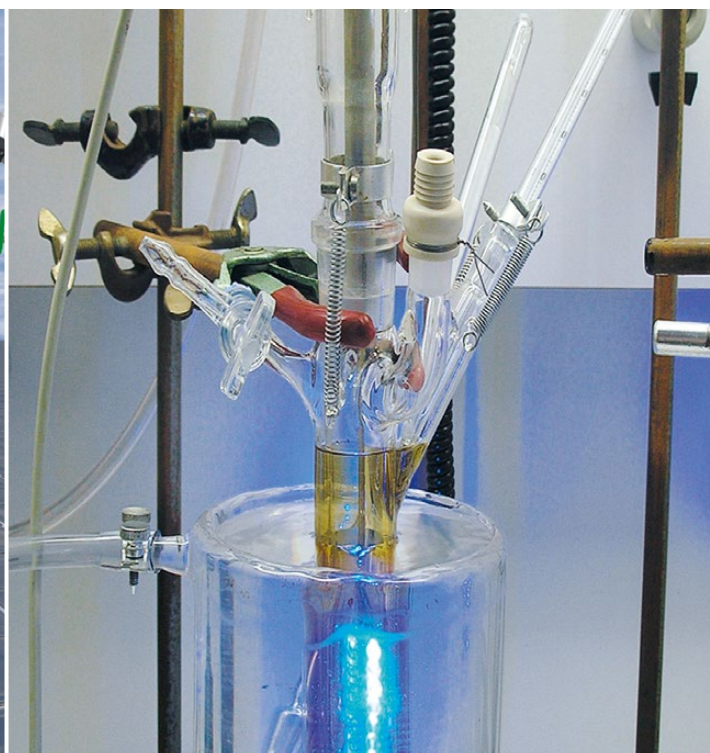
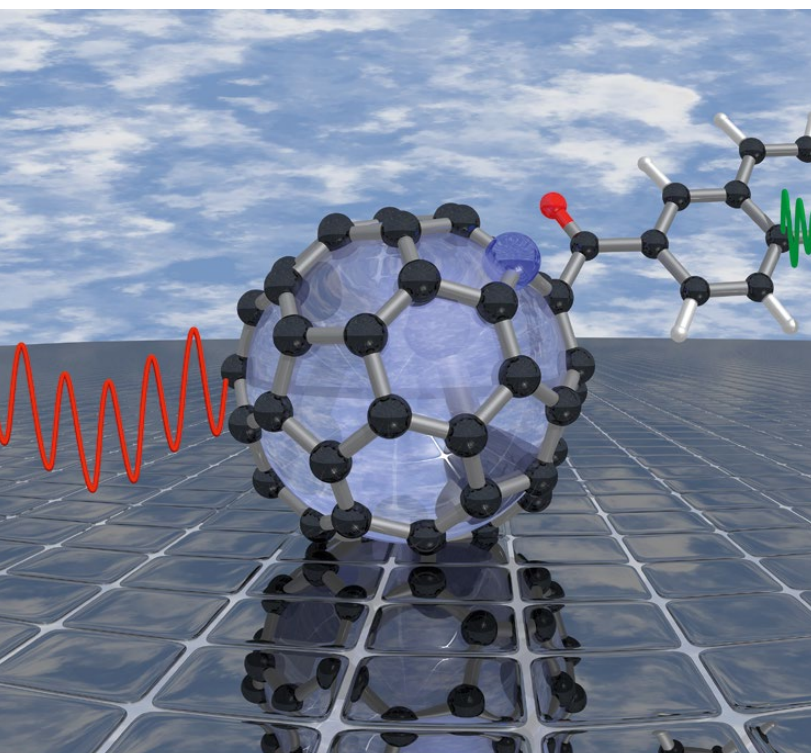
The **Department of Chemistry and Pharmacy (DCP)** is made up of two separate, namely Chemistry, on one hand, and Pharmacy and Food Chemistry, on the other hand. Both are cooperating closely with other Faculties within the FAU, especially with the Faculties of Engineering and Medicine as well as with other departments within the Faculty of Sciences. The cooperations range from joint research projects and interdisciplinary research centers to extensive exchange of students at the undergraduate and graduate levels.

The **DCP** comprises 8 chairs in Chemistry for Inorganic, Organic, Physical, and Theoretical Chemistry and 3 chairs in Pharmacy and Food Chemistry for Medicinal Chemistry, Pharmaceuticals, and Food Chemistry. A total of 28 professors hold appointments in the various areas. Additional support is provided by 32 permanent and 117 non-permanent scientific staff members. External research funds that total up to an average of more than 8 Mio Euro per year enable the means to finance more than 114 additional scientists.

Overall, the compelling research in the **DCP** has received top rankings not only at the national but also at the international level. Most remarkable, the recent, independent study coordinated by the German Science Council rates Chemistry in Erlangen as “world class”. It has been stated that particular strengths of Chemistry in Erlangen—with ratings “five out of five”—are the performance in research quality, impact, and research. In the latest ranking of the German Science Foundation (“Deutsche Forschungsgemeinschaft”, DFG) on third party funding across all German Chemistry departments, the **DCP** came in second place. The aforementioned is rounded off by the “Shanghai Academic Ranking of World Universities 2014” and the “QS World University Rankings 2014”, which list Chemistry at the FAU in the TOP 75 and Pharmacy at the FAU in the TOP 100, respectively.

Currents developments, as outlined in the following sections, are reflections of the national and international standing of the Department:

Since 2005 the **DCP** is a central part of the Cluster of Excellence—“Engineering of Advanced Materials (EAM)”, which is funded by the Federal Government via the DFG (www.eam.fau.de). Among the 25 lead Principal Investigators (PI), 6 come from Chemistry. The PIs from the **DCP** contribute to the cluster research areas “Multiscale Modelling and Simulations”, “Engineering of Nanoelectronic Materials”, and “Engineering of Catalytic Materials”. In 2012, funding for the Cluster of Excellence EAM was renewed for an additional five-year period. Furthermore, 8 additional project leaders from the **DCP** are associated with the Cluster of Excellence, which includes substantial funding for personal and instrumentation.



In 2012, the DFG approved funding for the Collaborative Research Center SFB 953 “Synthetic Carbon Allotropes” and the Research Training Group GRK 1910 “Medicinal Chemistry of Selective GPCR Ligands”. SFB 953 with about 10 Mio Euro for 4 years supports a total of 20 groups with 9 coming from the **DCP**. The GRK 1910, which is a collaborative effort together with the University of Regensburg, finances 7 groups belonging to the **DCP** with 5 Mio Euro for 4.5 years.

In 2012, the State of Bavaria initiated an interdisciplinary consortium “Solar Technologies Go Hybrid—SolTech” by chemists and physicists at five different Bavarian Universities, which is currently coordinated by the **DCP**. In Erlangen, 14 out of the 15 funded groups come from the **DCP** and are supported with 5 Mio Euro for a period of 5 years.

Finally, in 2013, the Research Unit “Functional Molecular Structures on Complex Oxide Surfaces” (funCOS) was established by the DFG in Erlangen. It supports 14 groups with 8 of them from the **DCP** with 3 Mio Euro for an initial period of 3 years.

The Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) supports the **DCP** since 2011 through their “Emerging Field Initiative” in the form of 4 different projects. 2 of them are coordinated by PIs from Chemistry and 1 from Pharmacy/Food Chemistry. Here, a total of 2.4 Mio Euro support a total of 9 groups.

RESEARCH FOCI

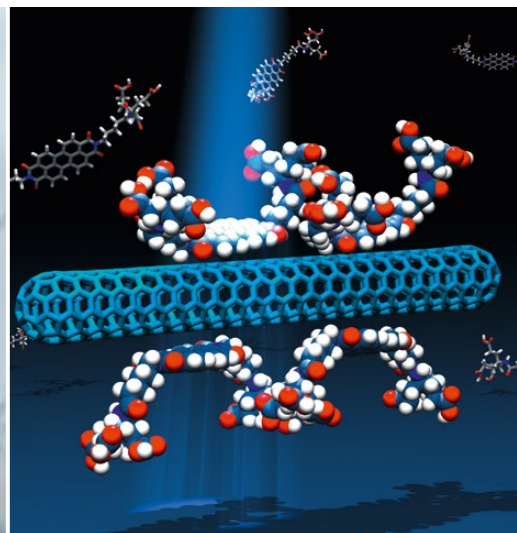
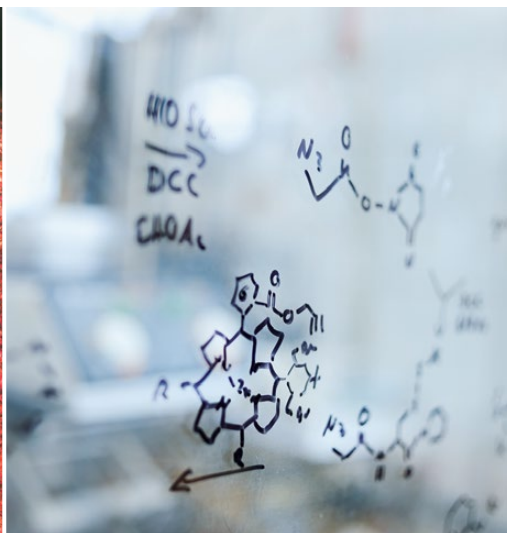
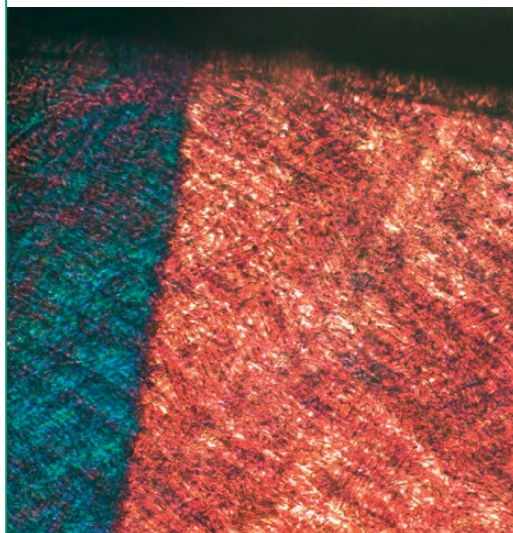
The research activities of the **DCP** cover a wide spectrum in the areas of Chemistry, Materials Science, Biology, and Pharmaceutical Science. The two major research foci of the **DCP**, **Molecular Materials** and **Bioactive Molecules**, constitute the basis for the FAU

research foci “New Materials and Processes” and “Molecular Life Science and Medicine”.

The synthesis and characterization of molecular materials with special emphasis on electronic, photophysical, and catalytic properties constitutes one of the two major research foci of the **DCP**, **Molecular Materials**. To this end, different forms of carbon allotropes and redox-active metal complexes represent some of the most intensively studied classes of molecules. Bioactive molecules, in general, and the design, synthesis, and examination of novel neurotropic agents for their activity towards signaling proteins—G-protein-coupled receptors—in particular, represent the second major research focus, **Bioactive Molecules**, of the Department. The research activities integrate chemical synthesis, biological and pharmacological testing, structure-activity relationships, the technology of drug delivery and investigations of molecular mechanisms of action.

The research foci create the molecular bridge between the Faculty of Engineering, on one side, and the Faculty of Medicine, on the other. The strongly interwoven and multiple interaction nature of these research activities are the inception to a large number of interdisciplinary collaborative research projects within the university (Collaborative Research Centers (SFB), Research Training Units (GRK)) and with other nationally and internationally leading institutions (DFG Priority Programs, EU, BMBF, NIH (US), Volkswagenstiftung, DAAD, Humboldt-Foundation, Bayerische Forschungsförderung, etc.) in which the **DCP** participates in addition to the above presented collaborative research projects lead by the **DCP**.

Moreover, the research foci of the **DCP** are vital for the FAU research focus “Energy, Environment, and Climate”. Microscopic under-



standing of processes relevant for energy, environment, and climate again means understanding at the molecular level. The research activities of the **DCP** furthermore contribute and are related to the FAU research foci “Electronics, Information, and Communication”, “Health Technology”, and “Optics and optical technologies”. In other words, the **DCP** is active in 6 of the 8 FAU research foci.

RESEARCH ENVIRONMENT AND INFRASTRUCTURE

The research activities of the **DCP** are embedded in a number of Centers at the FAU. For example, the *Interdisciplinary Center for Molecular Materials* promotes fundamental and interdisciplinary research at the frontier areas between Chemistry, Physics, and Materials Science, the *Interdisciplinary Center for Interface Controlled Processes* aims at strengthening interdisciplinary research considering interfaces of materials, the *Computer Chemistry Center* amalgamates competences of the Department with respect to simulation and computational science. The *Emil Fischer Center* comprises research groups from the Pharmaceutical Sciences, Food Chemistry and Molecular Medicine and, as such, crosslinks scientific work on bioactive molecules, target proteins and bioanalytics. These centers are coordinated or, in case of the *Computer Chemistry Center*, formed by members of the **DCP**. In addition, the **DCP** is a vital member in the *Erlangen Catalysis Resource Center*, the *Zentralinstitut für Scientific Computing*, and the *Interdisciplinary Center for Neuroscience*. All of the aforementioned foster interdisciplinary research activities across disciplines and are instrumental in joint funding efforts. Moreover, the **DCP** runs the elite *Graduate School Molecular Science*, which is based on the interdisciplinary curriculum Molecular Science as a collaborative effort of Chemistry and Pharmacy. A second graduate program run by the DCP through the *Emil Fischer Center* is the *Emil Fischer Graduate Programme of Pharmaceutical Sciences & Molecular Medicine*. Last but not least, the Helmholtz-Institut Erlangen-Nürnberg as well as the Energie Campus Nürnberg, which both are research platforms for the development and presentation of a closed renewable energy chain, contribute to the stimulating and productive research environment.

TEACHING PROFILE

The Bachelor and Master programs Chemistry and Molecular Science are highly modularized, research-oriented (B.Sc.) and research-focused (M.Sc.) curricula. Both the Pharmacy and Food Chemistry degree programs have been expanded in the last 5 years and continue to attract large numbers of undergraduates with top school grades. University wide, Food Chemistry, for example, has the third highest local Numerus Clausus.

In the Master programs, which are completely taught in English, a tight interplay between contemporary research and teaching leads to a high-class, modern education based on the scientific activities of the Department. Therefore, the aforementioned scientific foci are well reflected in the modules of the M.Sc. curricula. Additionally, the wide spread nature of the offered subjects put the students in a position to select courses according to their personal interest. The teaching philosophy aims at the development of students into well-rounded scientists who can take on leadership roles in industry, academia, etc.

In addition to the scientific education the personnel progress of the students is supported by offered language course and the opportunity to study parts of all study programs abroad. The quality of all study programs is ensured by a tight evaluation and supervision process.

INTERNATIONALIZATION OF RESEARCH AND TEACHING

Internationality is a key character of the **DCP**. 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 of undergraduate and graduate studies. The latter is complemented by international doctoral and post-doctoral students—funded through DAAD, Alexander von Humboldt Foundation, and EU programs. Cooperation with, for example, Osaka University in Japan and the University of Wollongong in Australia are initiated by excellence in research and teaching and are often build up by committed members of the **DCP**. They include frequent exchanges of students and researchers. Since 2004, the **DCP** has appointed 5 professors from the USA, UK, Canada, and the Netherlands and 7 out of the 11 chairs have an international background.

DEPARTMENT OF CHEMISTRY AND PHARMACY

INORGANIC CHEMISTRY

Inorganic and Organometallic Chemistry

Prof. Dr. S. Harder
Prof. Dr. N. Burzlaff

Inorganic and General Chemistry

Prof. Dr. K. Meyer

Prof. Dr. J. Bachmann
Prof. Dr. R. Dorta

Bioinorganic Chemistry

Prof. Dr. I. Ivanović-Burmazović

ORGANIC CHEMISTRY

Organic Chemistry I

Prof. Dr. R. R. Tykwinski
Prof. Dr. J. Schatz
Prof. Dr. S. Tsogoeva

Organic Chemistry II

Prof. Dr. A. Hirsch
Prof. Dr. A. Mokhir
Prof. Dr. W. Bauer
Prof. Dr. N. Jux

PHYSICAL / THEORETICAL CHEMISTRY

Physical Chemistry I

Prof. Dr. D. M. Guldi
Prof. Dr. C. Kryschi
Prof. Dr. T. Drewello

Physical Chemistry II

Prof. Dr. H.-P. Steinrück

Prof. Dr. R. Fink
Prof. Dr. J. Libuda

Theoretical Chemistry

Prof. Dr. A. Görling
Prof. Dr. D. Zahn

PHARMACY AND FOOD CHEMISTRY

Medicinal Chemistry

Prof. Dr. P. Gmeiner
Prof. Dr. J. Eichler
Prof. Dr. M. Heinrich

Food Chemistry

Prof. Dr. M. Pischetsrieder
Prof. Dr. A. Büttner

Pharmaceutics

Prof. Dr. G. Lee

Molecular and Clinical Pharmacy

Prof. Dr. K. Friedland

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)
- Centre for Scientific Computing (ZISC)

DEGREE PROGRAMS

CHEMISTRY

(B.Sc. / M.Sc.)

MOLECULAR SCIENCE NANO SCIENCE / LIFE SCIENCE

(B.Sc. / M.Sc.)

CHEMISTRY TEACHING DEGREE

(State Examination)

PHARMACY

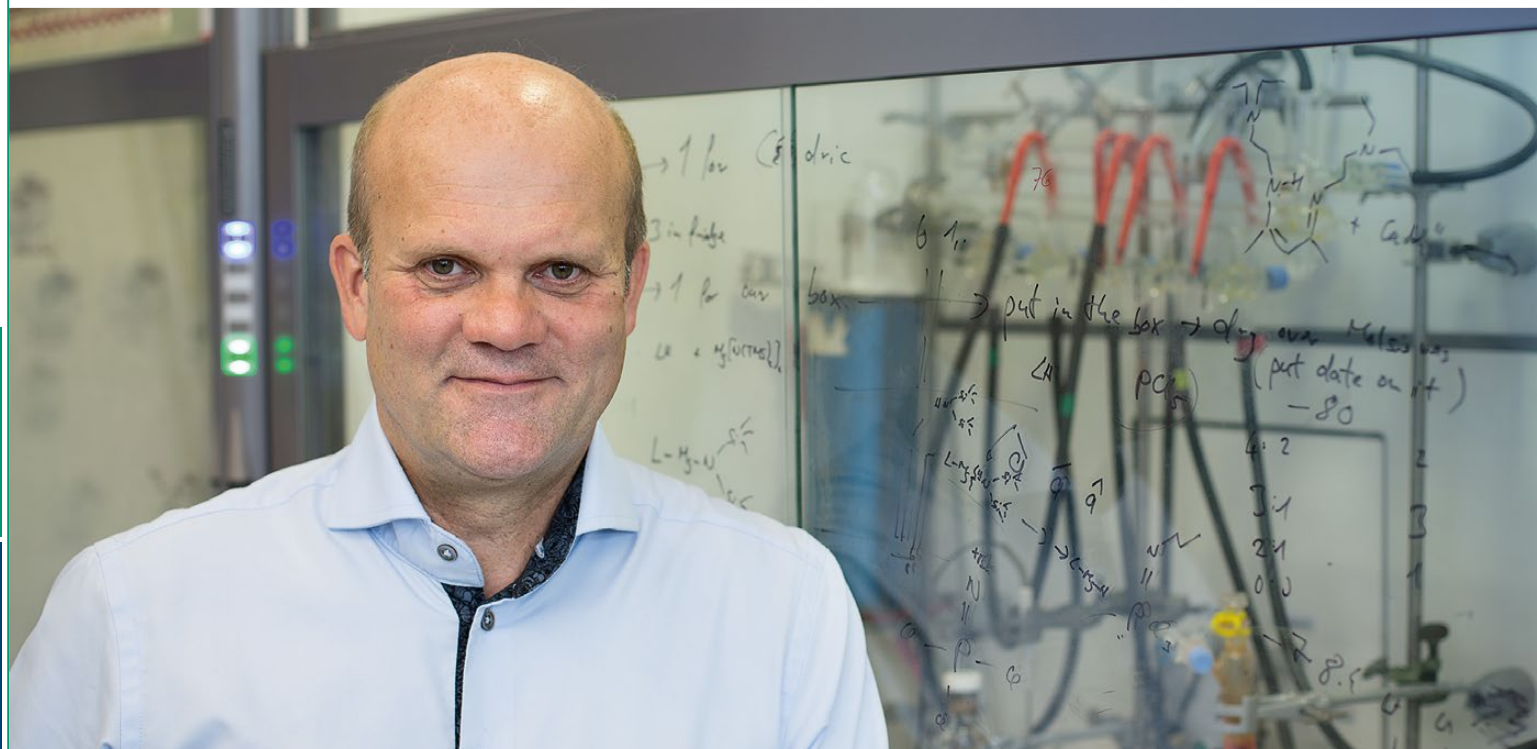
(State Examination)

FOOD CHEMISTRY

(State Examination)

GRADUATE SCHOOLS

- Emil Fischer Graduate Programme
- Graduate School Advanced Materials and Processes
- Graduate School Molecular Science



CHAIR OF INORGANIC AND ORGANOMETALLIC CHEMISTRY

PROF. DR. SJOERD HARDER

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CURRICULUM VITAE

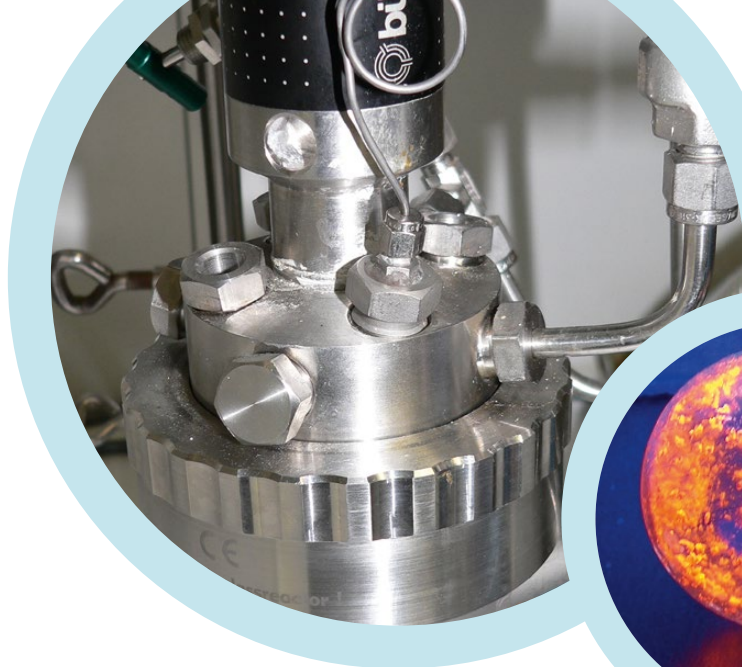
- Since 2012** University Full Professor, Chair of Inorganic and Organometallic Chemistry at the University of Erlangen-Nürnberg, Germany
- 2009 – 2012** Chair of Molecular Inorganic Chemistry at the University of Groningen, Netherlands
- 2004 – 2009** Professor of Inorganic Chemistry at the University Duisburg-Essen, Germany
- 1998 – 2003** Lecturer at the University of Konstanz, Germany, and the University of Cape Town, South Africa
- 1994 – 1998** Habilitation in Inorganic and Organometallic Chemistry at the University of Konstanz, Germany
- 1993 – 1994** Post-doc (Hans-Herbert Brintzinger) at the University of Konstanz, Germany
- 1992** Post-doc (Andrew Streitwieser) at the University of California at Berkeley, USA
- 1991** Post-doc (Paul R. von Schleyer) at the University of Erlangen-Nürnberg, Germany
- 1990** PhD in Organic Chemistry at the University of Utrecht, Netherlands

OBJECTIVES

- Further development of a fundamental understanding of organometallic compounds and reactions
- Application of organometallic chemistry in various fields like catalysis, polymerization chemistry, enantioselective conversions, luminescence, surface science and subjects related to a sustainable energy economy
- Mastering and teaching the skills of working with highly air-sensitive compounds under an inert atmosphere using Schlenk techniques

SCIENTIFIC BACKGROUND

Our group works at the frontiers of the organometallic chemistry of the early main group metals with a special focus on the heavier group 2 metals (Ca, Sr, Ba). This corner in the periodic table has been forgotten for a long time but its chemistry is now starting to develop rapidly. The work with these highly reactive, and consequently also very air-sensitive, organometallic compounds is not only challenging but also requires techniques that allow handling of these complexes under an inert atmosphere. Although we partially work in gloveboxes, we master and develop the original Schlenk techniques at a high level and believe that this is the key to doing chemistry with highly



reactive compounds. The high reactivity of our complexes is exploited in catalysis. Our general motto “Cheap Metals for Noble Tasks” has led to pioneering breakthroughs in the field of calcium-based catalysis. These offer a cheap alternative to transition metal catalysts and are also attractive for reasons of biocompatibility. Our interests, however, are much broader and also venture into areas like lanthanide chemistry and early (Ti, Zr) as well as late (Au, Cu, Zn) d-block metals or in the field of highly Lewis-acidic late main group metal chemistry (Al).

RESEARCH HIGHLIGHTS

We are among the pioneers using early main group metals in catalysis and developed for example methods for the strictly controlled catalytic hydrosilylation of alkenes, a highly atom-efficient key transformation for the production of silicon compounds. The catalyst in this unique reaction is a calcium hydride species that we could also isolate and structurally characterize. Surprisingly, we could use this catalyst also in the hydrogenation of alkenes with H_2 and this method represents a first demonstration of transition metal-free alkene hydrogenation catalysis. Other highlights of our research are the isolation of first calcium carbene complexes of the form $Ca=CR_2$ and our work with “superbulky” ligands among which Cp^{BIG} , a large penta-aryl cyclopentadiene. The latter ligand is the key to a set of interesting lanthanide sandwich complexes with an unusual strong luminescence. Our expertise in group 2 metal hydride chemistry evolved to the synthesis of larger magnesium hydride clusters that represent model systems for hydrogen storage materials like bulk MgH_2 . Especially rewarding are the investigations on metal amidoborane complexes for hydrogen storage.

PERSPECTIVES

We will continue to explore the organometallic chemistry of heavier group 2 metals but also strongly focus on Mg and the closely related Zn chemistry. We believe that the application of these highly

reactive complexes in a large variety of emerging fields could be especially rewarding. We currently start to explore their redox chemistry and use in Frustrated Lewis Pair chemistry but also actively pursue the use and development of nonheterocyclic carbene ligands (NHC's). Investigations of their reactivity towards small molecules will contribute to new catalytic protocols. The high abundance and low prices of these simple metals is the part of the key to a sustainable society based on renewable materials. Apart from that, our future focus will further concentrate on energy-related research themes and polymerization catalysis.

SELECTED PUBLICATIONS

- S. Harder, J. Spielmann, J. Intemann, H. Bandmann, *Angew. Chem. Int. Ed. Engl.* **2011**, 50, 4156–4160
- C. Ruspici, J. R. Moss, M. Schürmann, S. Harder, *Angew. Chem. Int. Ed. Engl.* **2008**, 47, 2121–2126
- J. Spielmann, G. Jansen, H. Bandmann, S. Harder, *Angew. Chem. Int. Ed. Engl.* **2008**, 47, 6290–6295
- J. Spielmann, F. Buch, S. Harder, *Angew. Chem. Int. Ed. Engl.* **2008**, 47, 9434–9438
- F. Buch, J. Brettar, S. Harder, *Angew. Chem. Int. Ed. Engl.* **2006**, 45, 2741–2745
- S. Harder, J. Brettar, *Angew. Chem. Int. Ed. Engl.* **2006**, 45, 3474–3478
- L. Orzechowski, G. Jansen, S. Harder, *J. Am. Chem. Soc.* **2006**, 128, 14676–14684

SELECTED REVIEWS

- S. Harder, Molecular early main group metal hydrides: synthetic challenge, structures and applications, *Chem. Comm.* **2012**, 48, 11165–11177
- S. Harder, From limestone to catalysis: Application of calcium compounds as homogeneous catalysts, *Chem. Rev.* **2010**, 110, 3852–3876

SELECTED AWARDS

- 1994 European Community—Marie Curie Fellowship
- 1993 European Community—Human Capital & Mobility Fellowship
- 1992 NATO Fellowship
- 1991 Alexander von Humboldt Fellowship
- 1990 H. J. Backer Prize of the Royal Dutch Society of Chemistry (Organic Chemistry)



PROFESSOR OF INORGANIC CHEMISTRY

PROF. DR. NICOLAI BURZLAFF

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CURRICULUM VITAE

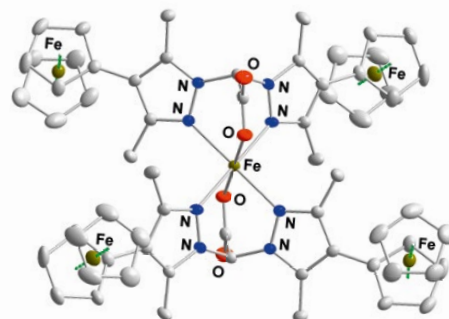
- Since 2004** University Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
- 1999 – 2004** Habilitation at the University of Konstanz, Germany
- 1997 – 1999** Postdoctoral Fellow at the Dyson Perrins Laboratory, Oxford, Great Britain
- 1997** PhD from the University of 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 of the enzymes. Coordination of substrates or substrate analogues and inhibitors to the models are also 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. Several ligands have been grafted on Merrifield resins or on silica. Moreover copolymers of several scorpionate ligands with MMA/EGDMA have been synthesized. Ongoing work focuses on the generation of *imprinted polymers* by template complexes to generate artificial enzymes. Furthermore, various 1D and 2D coordination polymers as well as metal organic frameworks (MOFs) are accessible with the heteroscorpionates or 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.

Recently, we focus especially on carbon-rich allenylidene complexes as a new concept to modify semi-conducting organic materials.

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.

Finally, in cooperation with the university hospital, we study small molecules that control the erythropoietin (EPO) formation by stabilization of the hypoxia inducible transcription factor HIF.

PERSPECTIVES

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, carbon rich molecules such as pentacenes will be modified by organometallic cumulenyldiene complex fragments to vary the electronic properties of the semi-conducting materials.

Finally, in cooperation with the university hospital, we will search for new leads that control the erythropoietin (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. Fluorescing inhibitors will be developed as a tool to monitor the uptake and kinetics of this promising new class of drugs.

SELECTED PUBLICATIONS

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- S. Tampier, S. M. Bleifuß, M. M. Abd-Elzaher, J. Sutter, F. W. Heinemann, N. Burzlaff, *Organometallic* **2013**, 32, 5935 – 5945
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- T. Godau, A. L. Müller, S. M. Bleifuss, T. Roth, S. Hoffmann, F. W. Heinemann, N. Burzlaff, *Dalton Trans.* **2011**, 40, 6547 – 6554

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- N. Burzlaff, Model Complexes for Zinc-Containing Enzymes, in: H.-B. Kraatz, N. Metzler-Nolte, *Concepts and Models in Bioinorganic Chemistry* **2006**, 397 – 431



CHAIR OF INORGANIC AND GENERAL CHEMISTRY

PROF. DR. KARSTEN MEYER

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CURRICULUM VITAE

- 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), Cambridge, USA
- 1995 – 1998** PhD, Max Planck Institute (MPI) for Radiation Chemistry (now MPI for Chemical Energy Conversion), Mülheim / Ruhr, Germany
- 1989 – 1995** Study of Chemistry at the Ruhr-University of Bochum (RUB), Germany; Diploma in Chemistry

OBJECTIVES

General objectives of our research are the syntheses of new chelating ligands and their reactive 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 H_2 , H_2O , N_2 , CH_4 , CO , CO_2 , NO_x , SO_x , O_2 , O_3 , P_4 , As_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.

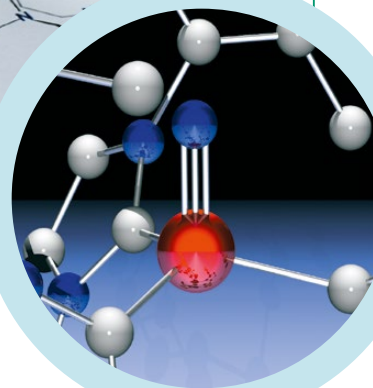
cals and fuels. This is particularly true for the greenhouse gases CO_2 and CH_4 . Functionalization of CH_4 and CO_2 , however, is difficult due to their thermodynamic stabilities. One approach to circumvent this limitation is to coordinate the inert C1 molecules to a redox-active metal ion, which can 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 transformation of small molecules; thus, opening opportunities for activation and functionalization of chemical feedstock.

SCIENTIFIC BACKGROUND

Small molecules such as alkanes, carbon dioxide, and water are attractive natural resources for the synthesis of fine chemi-

RESEARCH HIGHLIGHTS

The Meyer research program is focused on the activation of small molecules of biological and industrial interest using redox-active

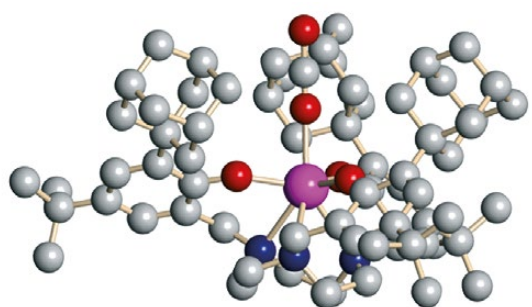


uranium and transition metal complexes in molecularly engineered ligand environments. Highlights of this work include the activation, cleavage, and multiple-bond metathesis of carbon dioxide at uranium complexes and the synthesis of reactive peroxo-, imido-, and nitrido-complexes for the functionalization 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(II) to Fe(V) and U(III) and U(VI), enabling a complete and systematic analysis of the structure-reactivity relationships. A recent highlight is the identification of a new, previously unknown U(III) oxidation state, opening new avenues to uranium reactivity. The analysis of complex series with structural continuity through the oxidation states presents a distinct benefit for the understanding of fundamental uranium and transition metal 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 and have become trademark areas of research.

PERSPECTIVES

Ultimate long-term objectives of the fundamental synthetic research in the Meyer lab are the development of efficient catalysts for the metal complex assisted conversion of abundant natural substrate resources and the discovery of renewable energy sources.

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



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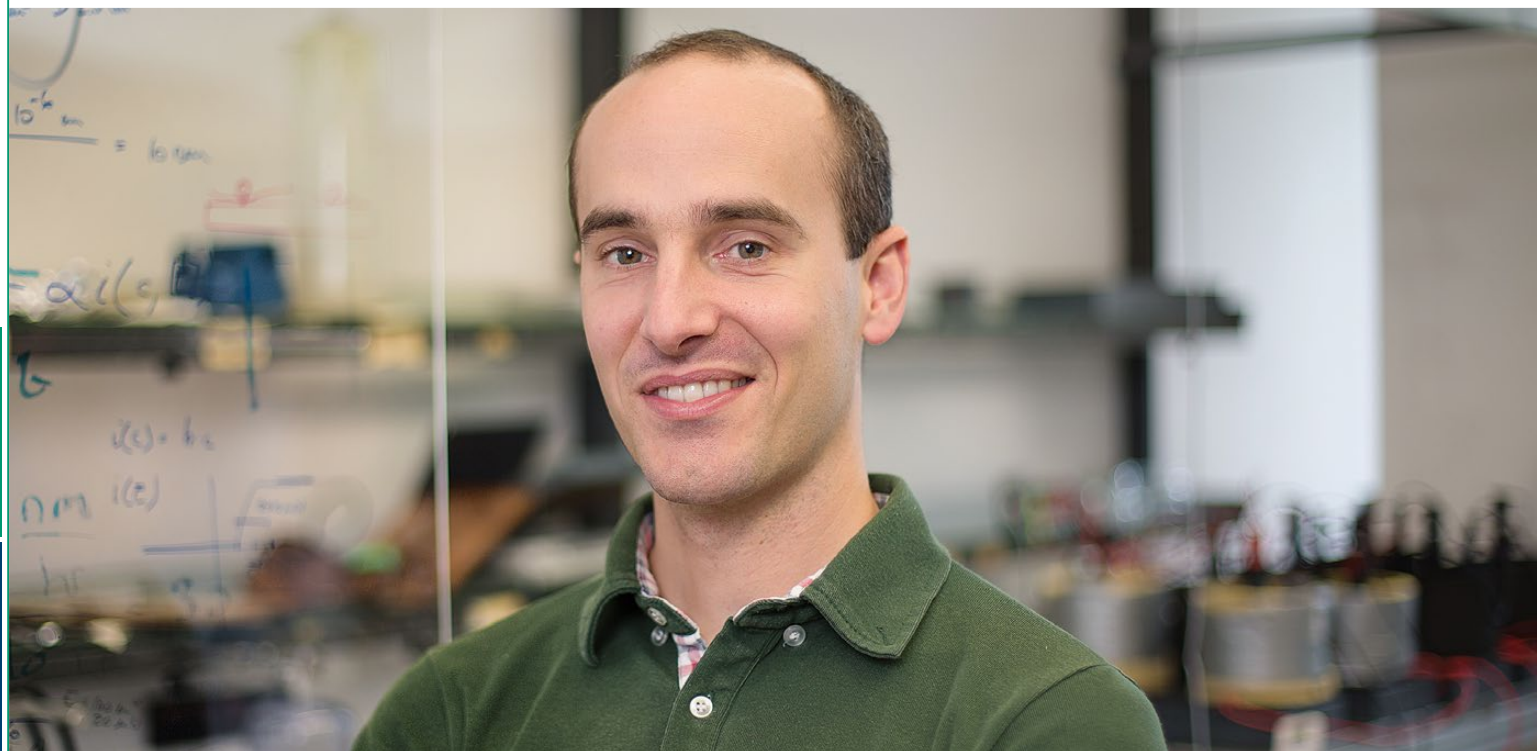
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- S. C. Bart and K. Meyer, Highlights in Uranium Coordination Chemistry, *Structure & Bonding* **2008**, 127, 119–176
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- C. Hauser, K. Meyer, Uranchemie zwischen Phobie und Begeisterung, *Nachr. Chem.* **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

- 2012 Visiting Professorship Award, Université Paul Sabatier, Toulouse, France
- 2012 Visiting Professorship Award, University of Manchester, UK (2009–2012)
- 2011 Fellow of the Royal Society of Chemistry
- 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



PROFESSOR OF INORGANIC CHEMISTRY

PROF. JULIEN BACHMANN PHD

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CURRICULUM VITAE

Since 2012	Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg
2009 – 2012	Junior Professor of Chemical Physics (Physics and Chemistry Departments) at the University of Hamburg, Germany
2007 – 2009	Scientist at the Institute of Applied Physics of the University of Hamburg
2006 – 2007	Postdoctoral Fellow at the Max Planck Institute of Microstructure Physics in Halle, Germany
2006	PhD in Inorganic Chemistry from the Massachusetts Institute of Technology, USA
2001	Chemistry Diploma from the University of Lausanne, Switzerland

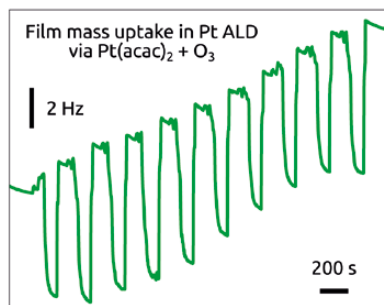
OBJECTIVES

The overarching theme of our research is the systematic investigation of structure-property relationships in nanostructured inorganic materials. To achieve this goal, we develop innovative preparative methods designed for engineering ordered arrays of elongated structures, the geometry of which is accurately tunable, and the surface chemistry of which can be defined at will. We then quantify how the performance indicators of the material depend on the geometric parameters of the structures. We pay particular attention to the interplay of transport and interface phenomena in various types of energy conversion devices, such as the electrodes of fuel cells, electrolyzers, and batteries, as well as solar cells. We also aim at controlling data storage in adequately shaped magnetic elements.

SCIENTIFIC BACKGROUND

Research in nanostructured materials has long been justified by the size- and shape-dependent variation of properties expected, and observed, in confined systems. Their applications in modern solar cells, various types of electrodes, and magnetic data storage media mostly rely on their large specific surface area. Colloidal synthesis has been most instrumental towards fundamental advances and in applied devices, but is limited to disordered, suspended particles. In contrast to this, in our group we start from bulk solid pieces of macroscopic size, then we treat them in order to generate large amounts of parallel structures ordered on a surface or in a matrix. We pay particular attention to the generality of our preparative methods, and the accurate tunability of the geometry.

Julien Bachmann's dual background in molecular coordination and redox chemistry, on the one hand, and in the chemical and phys-



ical preparative and characterization methods of solids and interfaces, on the other hand, is perfectly suited to addressing the challenges of this highly interdisciplinary field of research.

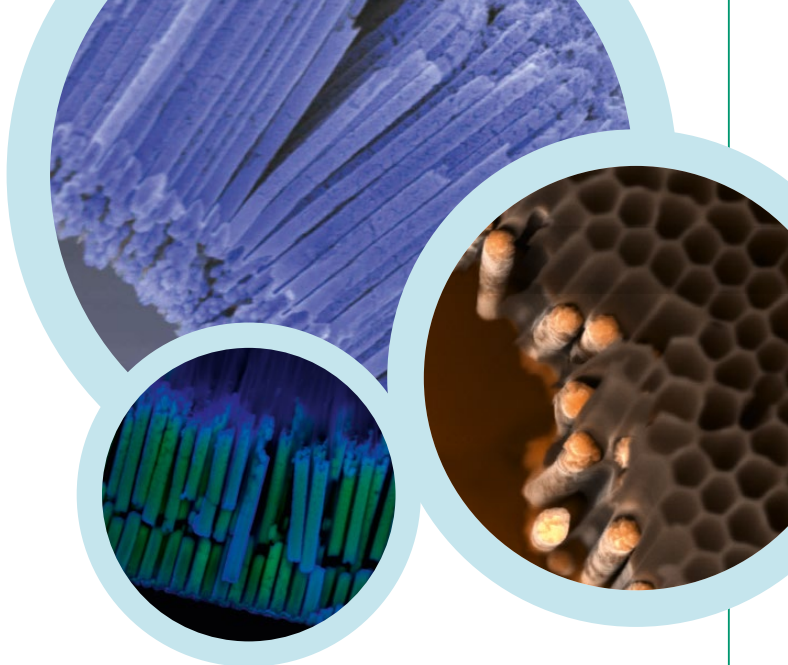
RESEARCH HIGHLIGHTS

We use electrochemical methods (‘anodization’) to generate hexagonally arranged arrays of parallel, cylindrical pores, the length of which can be set to any value between 0.5 μm and 100 μm and the diameter between 10 nm and 300 nm. We introduce diameter modulations, if needed, at arbitrarily defined points along the pores’ length. Subsequently, we use galvanic techniques to either fill the pores completely with solid metallic wires, or to grow hollow metal tubes along the pore walls. These metallic structures may consist of one pure metal, of alloys, or even of alternating segments with different composition. An alternative is provided by atomic layer deposition (ALD), a thin film deposition technique that exploits well-defined surface chemistry to enable the conformal coating of our deep pores with thin layers of oxides and sulfides. One or several consecutive ALD layers can be applied, the thicknesses of which we set between 1 nm and 20 nm typically. Our samples and reactions are characterized by electron microscopy, spectroscopic ellipsometry, piezoelectric microbalance, various steady-state and dynamic electrical, electrochemical, and photoelectrochemical methods, impedance spectroscopy, and magnetometry.

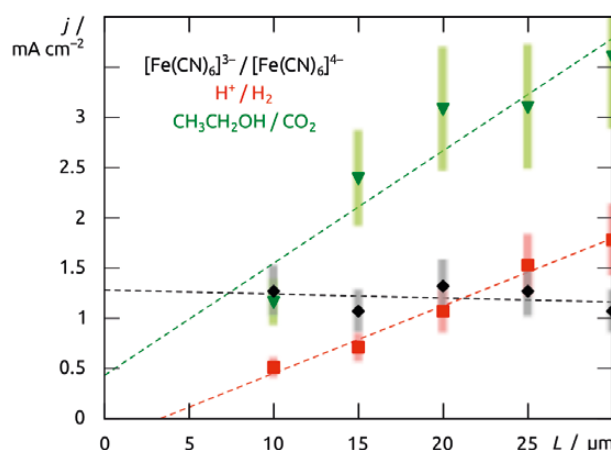
In the magnetic realm, segmented structures enable us to define a large number of ‘bits’ along the length of each object. The shape and length of each segment, as well as the distances between the segments, define the magnetization orientation, the switching field, and the interactions between bits. In ‘extremely thin absorber’ (ETA) solar cells, we find an optimal thickness for the intrinsic light-absorbing layer which balances the requirements of sufficient light absorption and efficient charge carrier collection. For many electrochemical fuel cell reactions at noble metal surfaces, we increase the current density by elongating the electrode’s pores while minimizing the catalyst loading via very thin coatings. We also experiment with iron oxide as a cost-efficient surface for the oxygen evolution reaction, whereby we compensate for the material’s poor intrinsic catalytic activity by increasing its surface area.

PERSPECTIVES

The generality of our methods will enable us to combine materials in a modular manner to create electrochemically and photoelectrochemically optimized systems, in which several functional materials (such as electron conductor, light absorber, and water oxidation catalyst) are combined in a coaxial geometry on the sub-micrometer



scale. In parallel, we will also pay renewed attention to the molecular aspect of multielectron reactivity at solid surfaces, in order to better understand the interfacial catalysis aspects of our work. The physical-chemical insight gained from our geometrically controlled model systems will finally be exploited towards the construction of energy conversion devices based on abundant elements and cost-efficient materials.

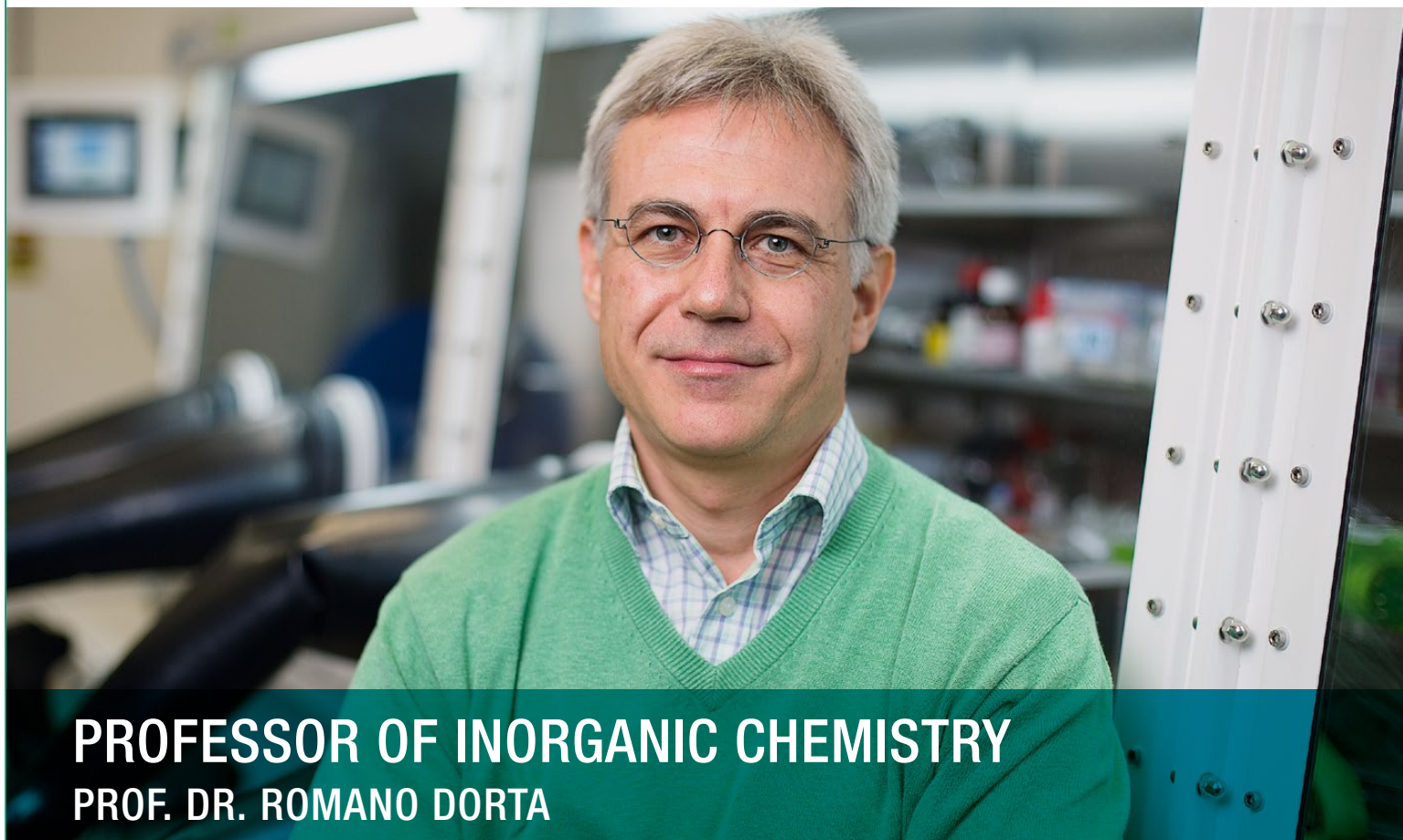


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- V. Roscher, M. Lickleder, J. Schumacher, G. Reyes Rios, B. Hoffmann, S. Christiansen, J. Bachmann, *Dalton Trans.* **2014**, 43, 4345–4350
- T. Grünzel, Y. J. Lee, K. Kueppel, J. Bachmann, *Beilstein J. Nanotechnol.* **2013**, 4, 655–664
- H. Wedemeyer, J. Michels, R. Chmielowski, S. Bourdais, M. Sugiura, G. Dennler, J. Bachmann, *Energy Environ. Sci.* **2013**, 6, 67–71
- J. Gemmer, Y. Hinrichsen, A. Abel, J. Bachmann, *J. Catal.* **2012**, 290, 220–224

SELECTED AWARDS

- 2013 Starting Grant, Cluster of Excellence ‘Engineering of Advanced Materials’, Erlangen
- 2009–2012 Six teaching prizes, University of Hamburg Physics Department (four times first prize, twice second prize)
- 2006 Humboldt Research Fellowship, Alexander von Humboldt Foundation
- 2002 Award for Excellence in Teaching by a Graduate Student, MIT Chemistry Department
- 2001 Presidential Fellowship, MIT



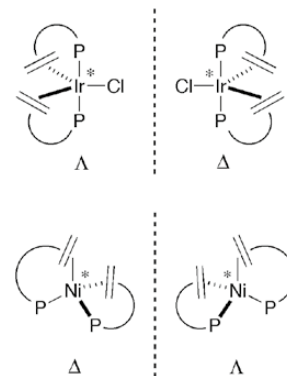
PROFESSOR OF INORGANIC CHEMISTRY

PROF. DR. ROMANO DORTA

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CURRICULUM VITAE

- Since 2013** Professor of Inorganic Chemistry at the University of Erlangen-Nürnberg, Germany
2002 – 2013 Full Professor of Inorganic Chemistry at the Universidad Simón Bolívar, Caracas, Venezuela
2000 – 2002 Research fellow at the Instituto Venezolano de Investigaciones Científicas, Venezuela
1998 – 2000 Postdoctoral fellow at the Weizmann Institute of Science, Rehovot, Israel
1993 – 1998 PhD, ETH Zürich, Switzerland
1988 – 1993 Studies of chemistry at the Université de Lausanne, Switzerland, and the Università degli Studi di Parma, Italy



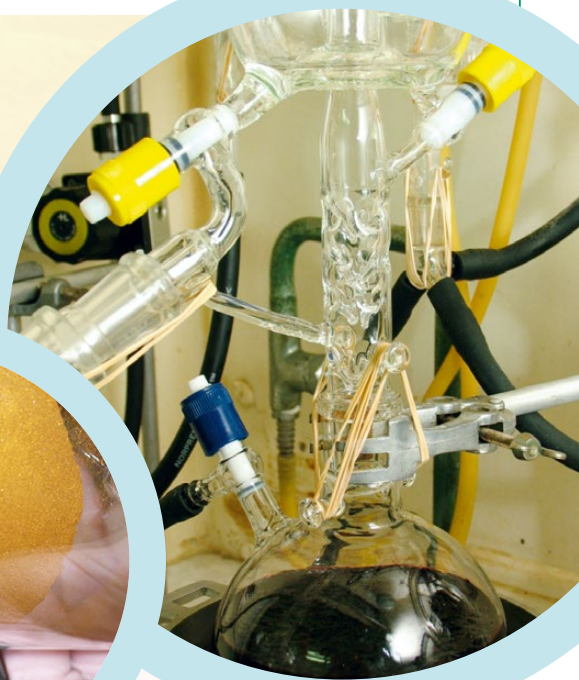
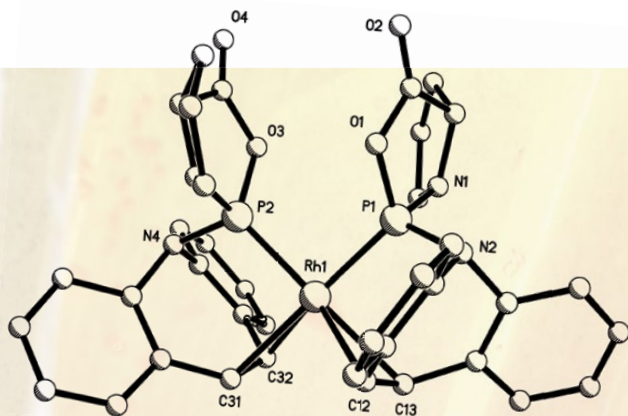
OBJECTIVES

Our research efforts are directed towards the design of novel chiral organometallic transition metal complexes, which serve as catalysts for the asymmetric synthesis of optically active organic molecules. The development of alternative synthetic tools, such as functional ionic liquids is also part of our objectives.

SCIENTIFIC BACKGROUND

Chiral molecules are ubiquitous in nature and biochemical processes. The enantiomers of a biologically active chiral molecule may elicit very distinct responses in living organisms. Many active pharmaceutical ingredients are chiral molecules, which nowadays are mostly commercialized in their non-racemic forms, due also to regulatory constraints. However, the synthesis of enantiomerically pure molecules

is costly, and indeed the added value of such products is very high. Annual single-enantiomer drug sales worldwide are estimated to be worth well over 200 billion Euros. Therefore, the development of new enantioselective synthetic methodologies has high priority. Amongst them, asymmetric catalysis represents a most elegant approach, a fact that was highlighted by the 2001 chemistry Nobel Prize. The idea behind asymmetric catalysis is that the spatial information residing on a chiral catalyst complex be transmitted as efficiently as possible onto the substrate molecules. Ideally, every chiral catalyst molecule would be able to generate thousands or even millions of product molecules of a defined chirality, thereby acting as a chiral multiplier. This technology can be superior to the classic separation of racemates or other stoichiometric enantioselective methods.



RESEARCH HIGHLIGHTS

The design of new chiral ligand systems is the first and most challenging step toward the synthesis of reactive, optically pure metal complexes that are to be used as catalysts for asymmetric organic transformations. Some time ago, we came up with a chiral P-alkene ligand architecture that proved to be synthetically flexible enough to create a small ligand library, which allowed us to synthesize a series of reactive chiral metal complexes. Noteworthy are the optically pure complexes possessing stereogenic metal centers in stereochemically stable tetrahedral and trigonal bipyramidal coordination geometries. Their precise molecular structures and absolute configurations were authenticated by X-ray crystallography. In fact, complexes with stereogenic metal centers represent worthwhile synthetic targets because they appear to play a key role in some of the most successful asymmetric catalytic processes known. Furthermore, our P-alkene ligands exhibit hemilabile behavior thanks to a weakly coordinating alkene function. Hemilability is operational in various catalytic reactions but structural proof thereof is scarce. Such ligand systems protect reactive metal centres from premature decomposition without affecting their inherent reactivity. This is evidenced by our hemilabile Ni(0)-P-alkene complexes that are perfectly air stable in the solid state, but once in solution readily activate small molecules, thus maintaining the high reactivity typical of electron rich Ni(0) species but doing away with their characteristic air-sensitivity. As molecular catalysts we only employ well-defined organometallic species and avoid in-situ formed catalyst mixtures. Examples are our chiral cationic mononuclear Rh-P-alkene complexes that catalyze the formation of certain C–C bonds with almost perfect enantioselection (> 99% *ee*). The focus on structural organometallic chemistry is also aimed at elucidating and modeling industrially relevant catalytic systems, in order to get a better understanding of the interplay between ligands,

metal centers, substrate, and product molecules. Finally, functional ionic liquids represent promising new synthetic tools for stoichiometric and catalytic transformations. For example, transition metal salts that are liquid at room temperature may be used as biphasic, self-supported catalysts for oxygen atom transfer reactions.

PERSPECTIVES

We are currently developing novel chiral P- and S-based ligand systems, synthesizing highly reactive chiral complexes of the less noble and less expensive transition metals, and exploring their rich organometallic chemistry, ranging from activations of small molecules and specific bonds, to new catalytic reactivities. Catalysis development in our group is centered on the atom-economical, enantioselective formation of C–H, C–C, C–N, and C–O bonds. On the other hand, highly reactive functional ionic liquids are also being investigated as new synthetic tools.

SELECTED PUBLICATIONS

- J. Pastrán, G. Agrifoglio, T. González, A. Briceño, R. Dorta, *Tetrahedron: Asymmetry* **2014**, 25, 1280–1285
- A. Linden, L. Llovera, J. Herrera, R. Dorta, G. Agrifoglio, R. Dorta, *Organometallics* **2012**, 31, 6162–6171
- E. Drinkel, A. Briceño, R. Dorta, R. Dorta, *Organometallics* **2010**, 29, 2503–2514
- R. Mariz, A. Briceño, R. Dorta, R. Dorta, *Organometallics* **2008**, 27, 6605–6612
- G. Noguera, J. Mostany, G. Agrifoglio, R. Dorta, *Adv. Synth. Catal.* **2005**, 347, 231–234

SELECTED REVIEWS

- R. Dorta, Iridium-Catalyzed Hydroamination, in: *Iridium Complexes in Organic Synthesis*, L. Oro, C. Claver Editors, Wiley-VCH, Weinheim, **2008**



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 involved in redox signaling and design efficient enzyme mimetics, metal based human pharmaceuticals and chemical catalysts. The approach is to rationally design bio/catalytically-active metal complexes with desirable physiological/catalytic

effects based on understanding of their kinetic, thermodynamic, redox and mechanistic behavior, paving the way for improvements in human health and the energy conversion.

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, weak 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 me-

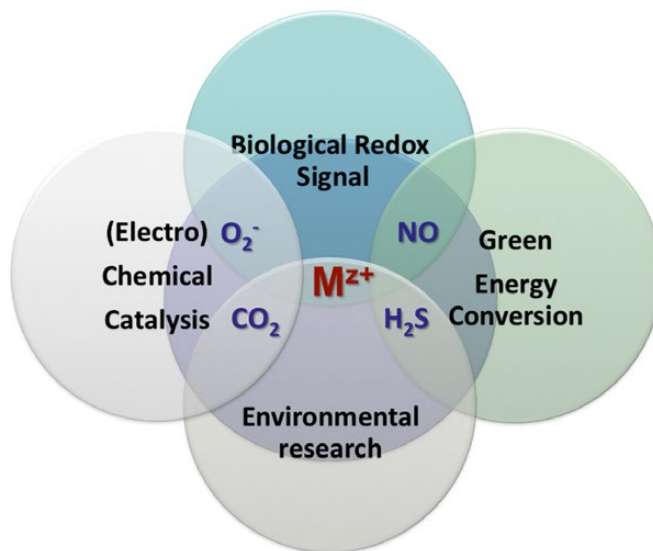
mechanisms in order to predict a potential application of metal based structures and tune their desirable activity. We apply a wide range of instrumentation methods in our research: time-resolved UV/vis low-temperature (down to -90 °C) and high-pressure stopped-flow measurements, high-pressure fluorescence 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

- New insights into the superoxide dismutation (SOD) mechanisms
- Water exchange on Mn(III)
- HNO generation by seven-coordinate SOD mimetics
- 100 years old question, why nitrite acts as an antidote for hydrogen sulfide, is now solved: heme-catalyzed reaction between NO_2^- and H_2S generates HNO in mitochondria
- Interaction between H_2S and $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}]$ as a new pharmacological source of HNO
- HSNO as a new signalling (shuttle) molecule
- Direct interaction between H_2S and NO
- Homogeneous and heterogeneous catalytic removal of H_2S
- Mechanism of fast CO_2 fixation by Ni-OH species
- Confined space reverses the high-pressure behavior of an iron-center, relevant for operation of heme-proteins in deep-sea organisms and a reverse spin-crossover effect

PERSPECTIVES

Our long-term goals is to develop an emerging field of Medicinal Redox Inorganic Chemistry at a global level and to increase the impact of (bio)inorganic chemistry research on health care. 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 work on the effects of H_2S 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. We will also apply our knowledge on tuning the redox reactions by pressure for clarifying and increasing the efficiency of proton coupled electron transfer involved in the energy conversion processes.

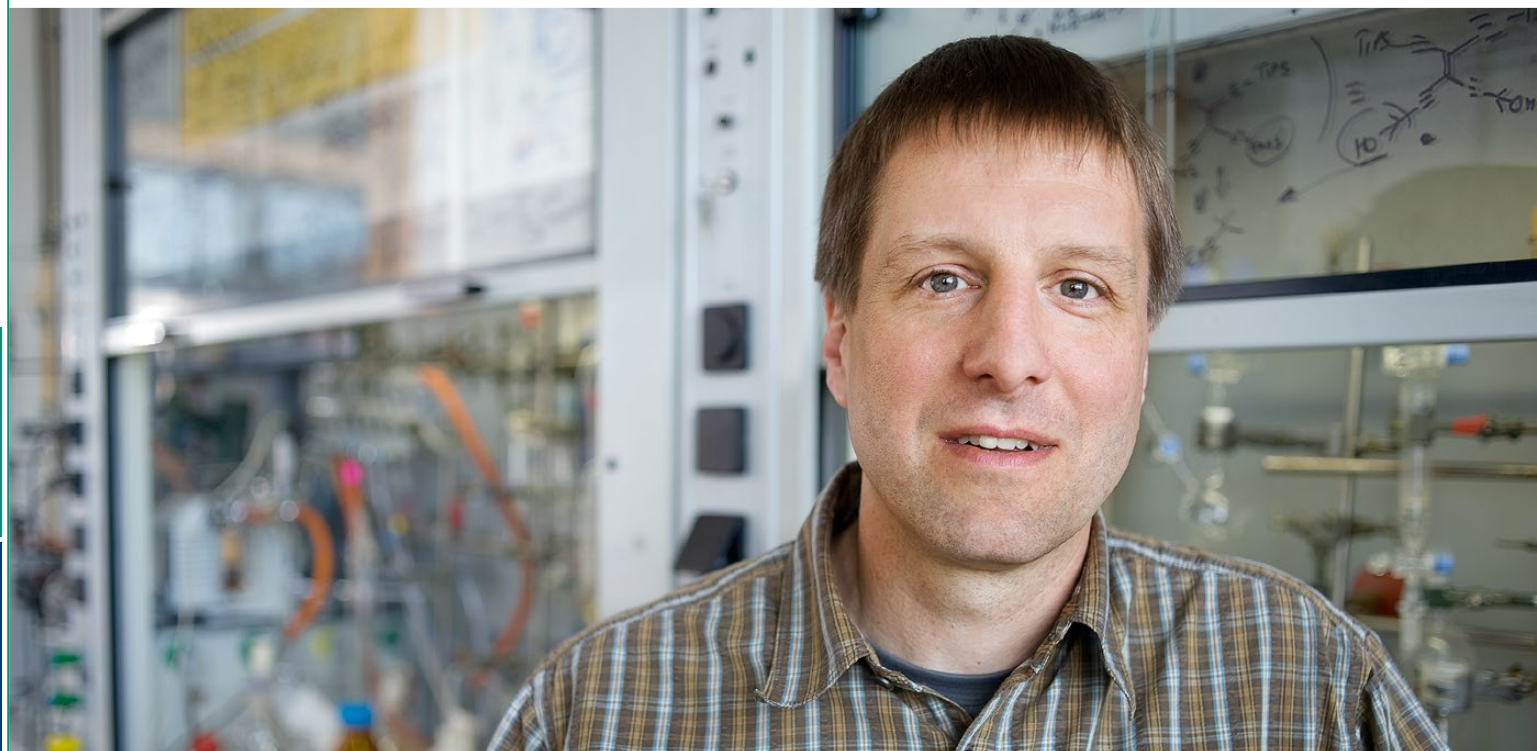


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- O. Troeppner, R. Lippert, T. E. Shubina, A. Zahl, N. Jux, I. Ivanović-Burmazović, *Angew. Chem. Int. Ed.* **2014**, DOI: 10.1002/anie.201406954
- J. Lj. Miljković, I. Kenkel, I. Ivanović-Burmazović, M. R. Filipovic, *Angew. Chem., Int. Ed.* **2013**, 52, 12061–12064
- M. R. Filipovic, M. Eberhardt, V. Prokopovic, A. Mijuskovic, Z. Orescanin-Dusic, P. Reeh, I. Ivanović-Burmazović, *J. Med. Chem.* **2013**, 56, 1499–1508
- I. Ivanović-Burmazović, M. Filipović, *PCT Int. Appl.* **2012**, WO 2012175630 A1 20121227
- M. R. Filipović, J. Miljković, T. Nauser, M. Royzen, K. Klos, T. E. Shubina, W. H. Koppenol, S. J. Lippard, I. Ivanovic-Burmazović, *J. Am. Chem. Soc.* **2012**, 134, 12016–12027
- D. Lieb, A. Zahl, T. E. Shubina, I. Ivanovic-Burmazovic, *J. Am. Chem. Soc.* **2010**, 132, 7282–7284
- M. R. Filipović, K. Duerr, M. Mojović, V. Simeunović, R. Zimmermann, V. Niketić, I. Ivanović-Burmazović, *Angew. Chem. Int. Ed.* **2008**, 47, 8735–8739

SELECTED REVIEWS

- I. Ivanović-Burmazović, M. R. Filipović, *Adv. Inorg. Chem.* **2012**, 64, 53–95



CHAIR OF ORGANIC CHEMISTRY I

PROF. RIK TYKWINSKI PHD

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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 – 1994	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 gen-

eration 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.

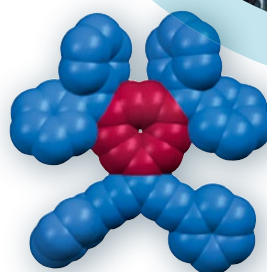
HIGHLIGHTS

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, with up to 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 have provided synthetic routes to many new pentacene derivatives, some of which show unprecedented semiconducting 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 and cumulenes can serve as an ideal, 1-D molecular wires as a result of their linear, conjugated structures. Current synthetic methods are not likely suitable for polyynes and cumulenes longer than those currently known, and innovative routes toward encapsulation of the conjugated skeleton are a challenging goal, as are methods toward incorporating end-groups to allow polyynes and cumulenes 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 π -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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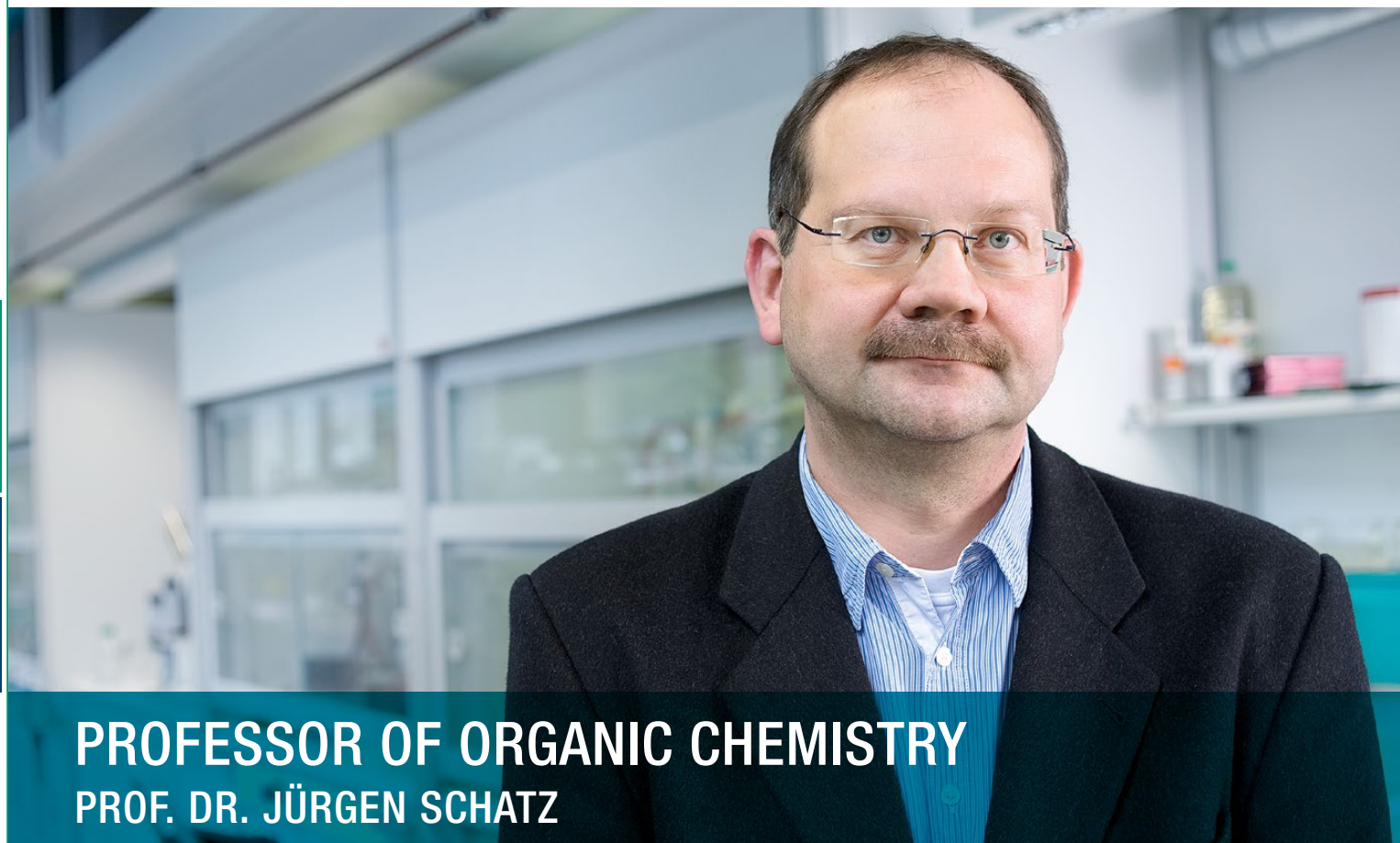
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- K. Campbell, C. A. Johnson II, R. McDonald, M. J. Ferguson, M. M. Haley, R. R. Tykwinski, *Angew. Chem. Int. Ed.* **2004**, 43, 5967–5971

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- J. A. Januszewski, R. R. Tykwinski, *Chem. Soc. Rev.* **2014**, 43, 3184–3203
- 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

- 2013 Inductee, University of Minnesota-Duluth Academy of Science and Engineering
- 2004 Faculty of Science Research Prize, University of Alberta
- 2001 PetroCanada Young Innovator Award



PROFESSOR OF ORGANIC CHEMISTRY

PROF. DR. JÜRGEN SCHATZ

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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 alternative 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.

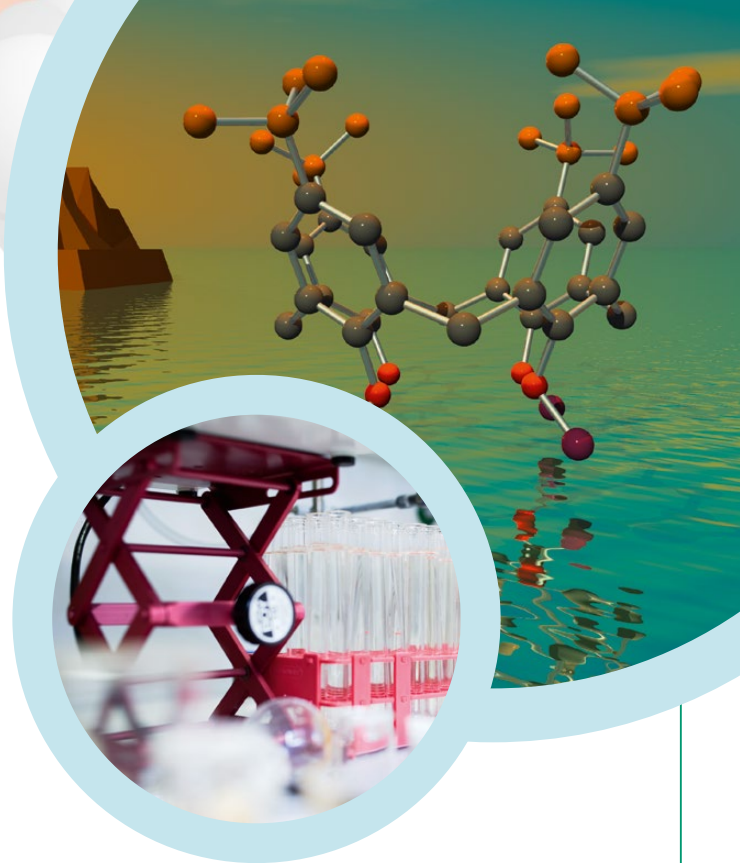
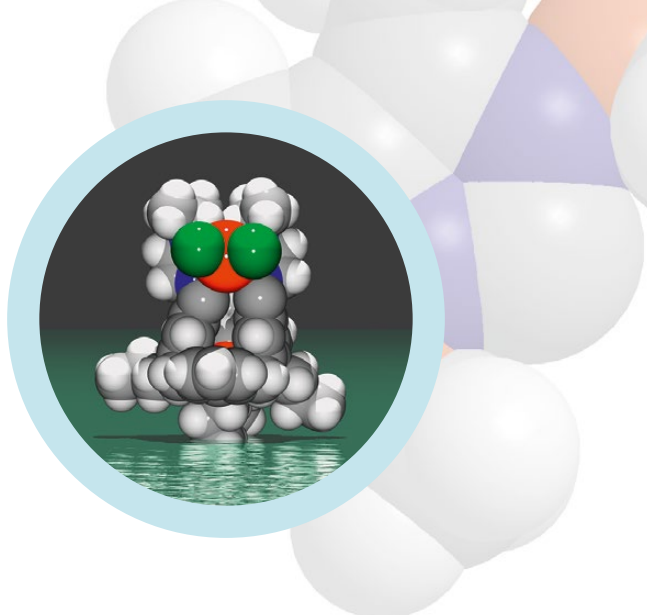
Here, our general interest in organic chemistry, which uses pure water as a solvent, can help to develop methodologies which allow organic transformations in aqueous media. We focus on the use of water-soluble macrocycles, e.g., calixarenes, cyclodextrins, cyclo-

phanes, 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 years we developed methods to perform standard organometallic reactions in pure water. For example, 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-azacrown-ether-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—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 an 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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- J. Schatz, D. Schühle, Supramolecular Metal Complexes for Imaging and Radiotherapy, *Supramolecular Systems in Biomedical Fields* **2013**, 10, 300–330
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- 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

- 2008–2013 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

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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

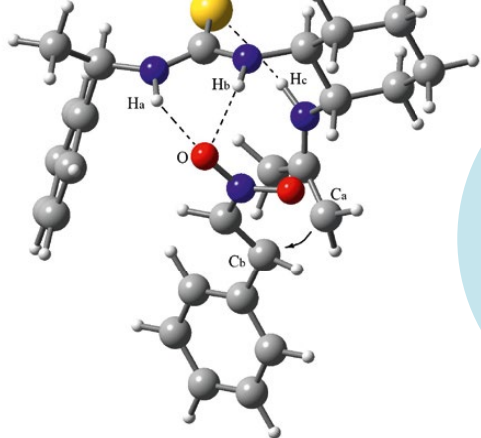
OBJECTIVES

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 pharmaceuticals or material science for compounds with high enantiopurity, e.g., for single enantiomer chiral drugs and their precursors. Stereochemistry therefore aims at intro-

ducing 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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- 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
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- S. B. Tsogoeva, When chiral product and catalyst are the same: discovery of asymmetric organoautocatalysis, *Chem. Commun.* **2010**, 46, 7662–7669
- 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
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- 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

- 2012 Otto-Röhm Research Award
- 2008 Tetrahedron: Asymmetry “Most Cited Paper 2005–2008 Award”
- 2007 Thieme Journal-Preis



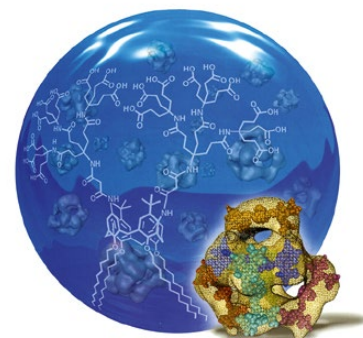
CHAIR OF ORGANIC CHEMISTRY II

PROF. DR. ANDREAS HIRSCH

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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 in Organic Chemistry at the University of Tübingen, Germany



OBJECTIVES AND SCIENTIFIC 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 bio-medical properties. Andreas Hirsch's work in synthetic organic chemistry includes synthesis of oligoynes, development of new covalent, ionic and H-bonded dendrimers, porphyrines, calixarenes, perylenes and redox-active ionic liquids.

RESEARCH HIGHLIGHTS

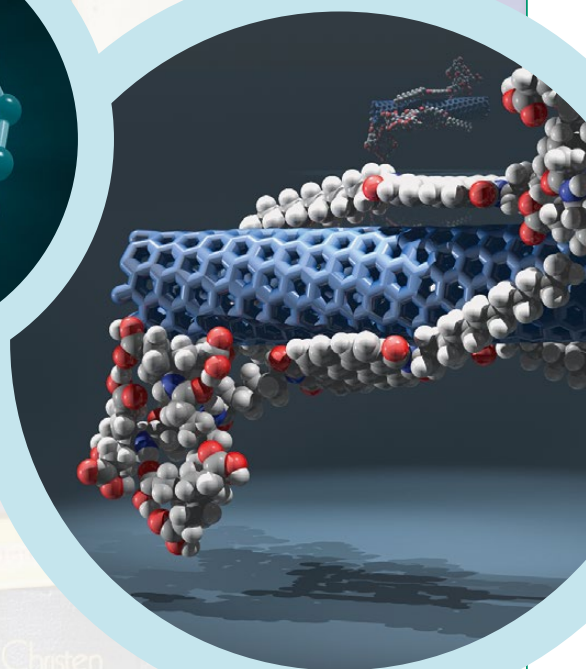
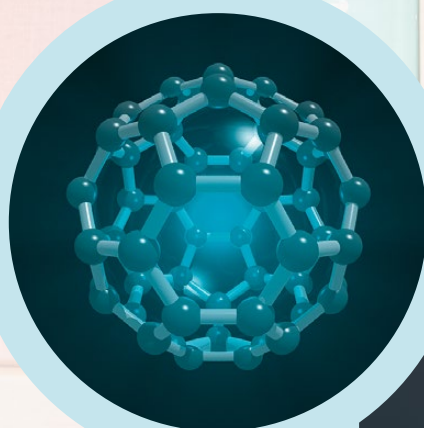
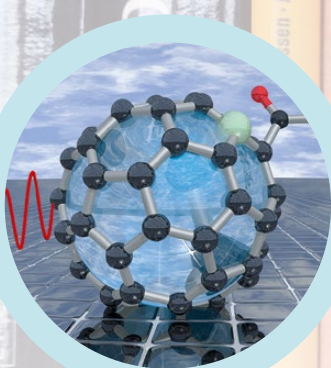
The research of the Hirsch group is characterized by its uncompromising commitment to *interdisciplinarity*. Among the most important achievements are: control over the regiochemistry of multiple addition reactions, the shape dependent difference of endohedral and exohedral functionalization, the $2(n+1)^2$ -rule for the description of spherical aromaticity of fullerenes, which is named as 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. Numer-



ous 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 carbene $sp-C_{\infty}$.

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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- R. Neubauer, F. W. Heinemann, F. Hampel, Y. Rubin, A. Hirsch, *Angew. Chem. Int. Ed.* **2012**, 51, 11722 – 11726
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- S. Eigler, A. Hirsch, Chemistry with Graphene and Graphene Oxide – Challenges for Synthetic Chemists, *Angew. Chem. Int. Ed.* **2014**, 52, 7720 – 7738
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- M. Bühl, A. Hirsch, Spherical Aromaticity of Fullerenes, *Chem. Rev.* **2001**, 101, 1153 – 1183

SELECTED AWARDS

- 2009 ERC Advanced Grant
- 2006 Elhuyar-Goldschmidt-Prize



PROFESSOR OF ORGANIC CHEMISTRY

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CURRICULUM VITAE

Since 2013 Professor of Organic Chemistry at the University of Erlangen-Nürnberg, Germany
2011 – 2012 Associate Professor for Bioinorganic Chemistry, Ruprecht-Karls-Universität Heidelberg, Germany
2010 Habilitation at the Ruprecht-Karls-Universität Heidelberg, Germany
1997 PhD, Kiev Shevchenko University, Ukraine

OBJECTIVES

To control biochemical processes and to monitor concentration and localization of biomolecules (nucleic acids and proteins) in live cells by using reagents based on chemical catalysts.

SCIENTIFIC BACKGROUND

The group is involved in synthesis of organic and coordination compounds as well as bioconjugates of oligonucleotides with chemical fragments including fluorescent dyes, reactive substrates and catalytic moieties. The activity of these substances is tested in vitro using NMR, UV-visible, fluorescence spectroscopy, chromatography (HPLC, TLC and others) and mass spectrometry (ESI, MALDI-TOF) as well as in cell cultures.

RESEARCH HIGHLIGHTS

We develop nucleic acid controlled photocatalysts based on natural and semi-synthetic tetrapyrroles and their analogues. We use these catalysts to design catalytic and autocatalytic reactions, which are applied for the amplified detection of nucleic acids in living cells. The ultimate goal of this project is to develop a robust assay for detection of a single copy of a particular nucleic acid per cell (*Figure 1*). The same photocatalysts are used to design “caged” reagents (e.g., oligonucleotides, siRNAs), whose biological activity (antisense, RNAi or immunostimulatory activity) is controlled by non-toxic red light (*Figure 2*).

Finally, we work on discovery of ferrocene-based prodrugs. In the cancer cell—specific microenvironment these compounds are converted in the quick autocatalytic reaction into highly toxic species, which kill cancer cells selectively. In the microenvironment of normal cells these metallodrugs are stable and not toxic (*Figure 3*).

Figure 1

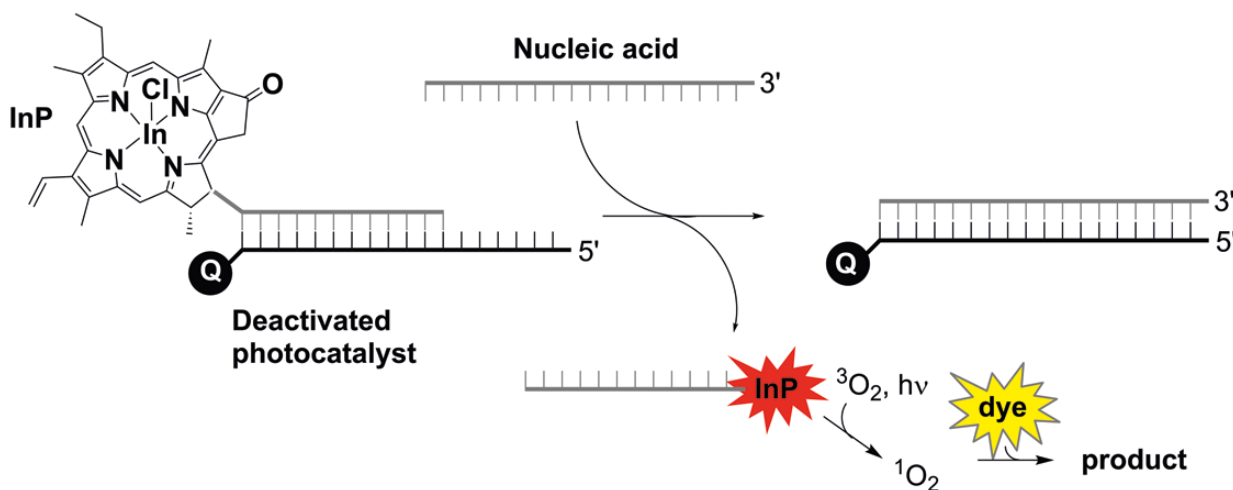


Figure 2

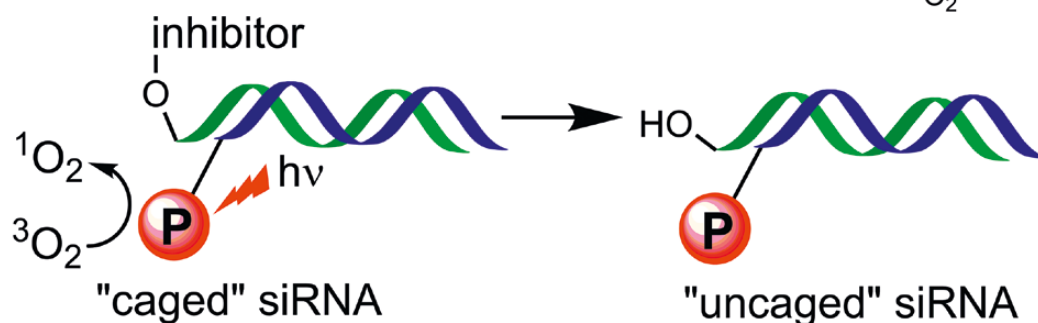
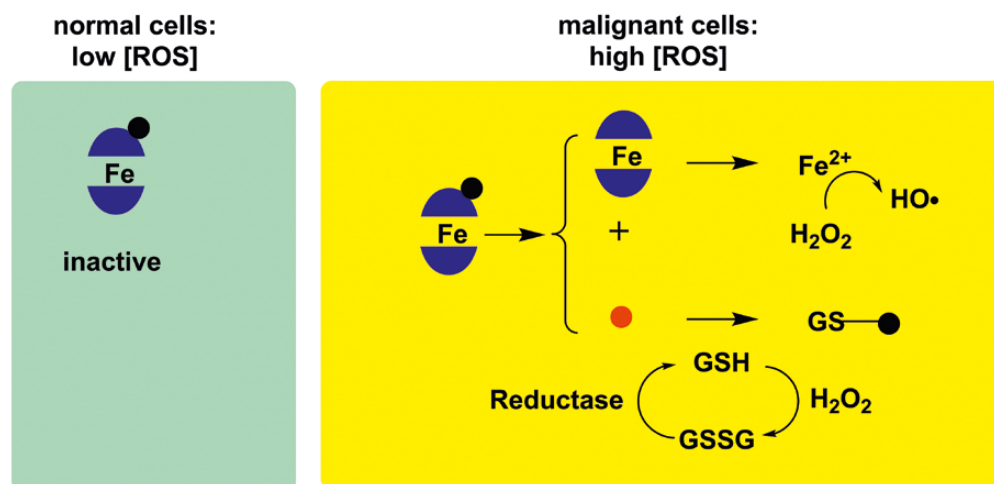


Figure 3



**suppression of the antioxidant system
and generation of highly reactive ROS**

PERSPECTIVES

Our long term goals include development of (a) side effect-free anticancer drugs and (b) membrane-permeable reagents for robust and highly sensitive detection of biomolecules in live cells and for regulation of their biological activity.

SELECTED PUBLICATIONS

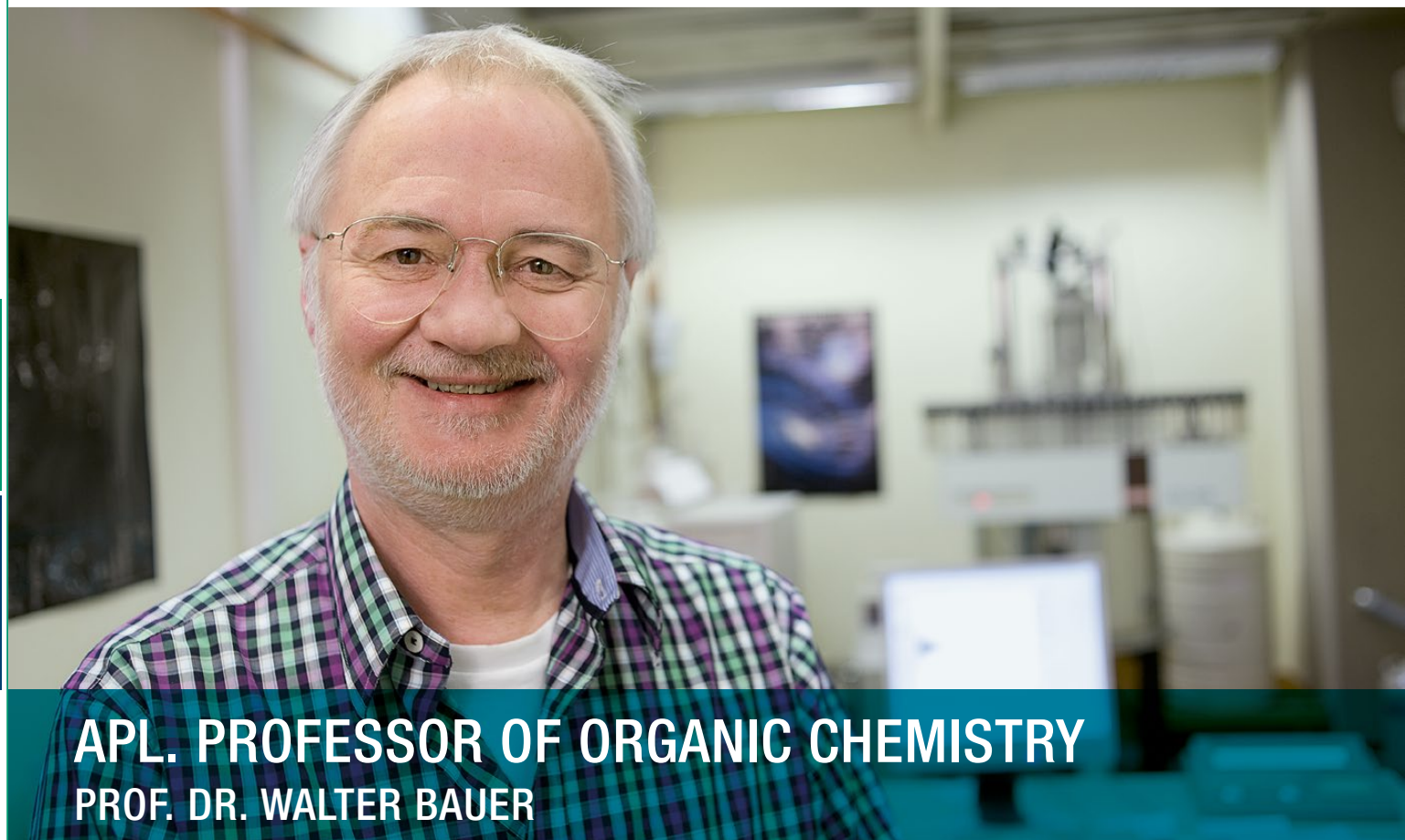
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- A. Rotaru, A. Mokhir, *Angew. Chem.* **2007**, 119, 6293–6296
- J. Kovács, T. Rödlér, A. Mokhir, *Angew. Chem.* **2006**, 118, 7979–7981

SELECTED REVIEWS

- A. Mokhir, Chemical reactions controlled by nucleic acids, in: *DNA in Supramolecular Chemistry and Nanotechnology*, John Wiley & Sons, Ltd, Eds. E. Stulz and G. H. Clever, **2014**
- R. Krämer, A. Mokhir, A. Metal Complex Derivatives of Peptide Nucleic Acids, in: *Interplay between Metal Ions and Nucleic Acids*, Vol. 10 of series *Metal Ions in Life Sciences*, A. Sigel, H. Sigel, R. K. O. Sigel, Eds.; Springer Science + Business Media B.V., Dordrecht, **2012**

SELECTED AWARDS

- 2005 selected in the Emmy Noether – Programme of the Deutsche Forschungsgemeinschaft (DFG)
- 2011 selected in the Perspectives Programme "PLUS 3" for independent young group leaders and endowed professorships of Boehringer Ingelheim 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 2003** Apl. 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
- 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, indispensable 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., ^1H , ^1H -NOESY) and heteronuclear (e.g., ^1H , ^{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

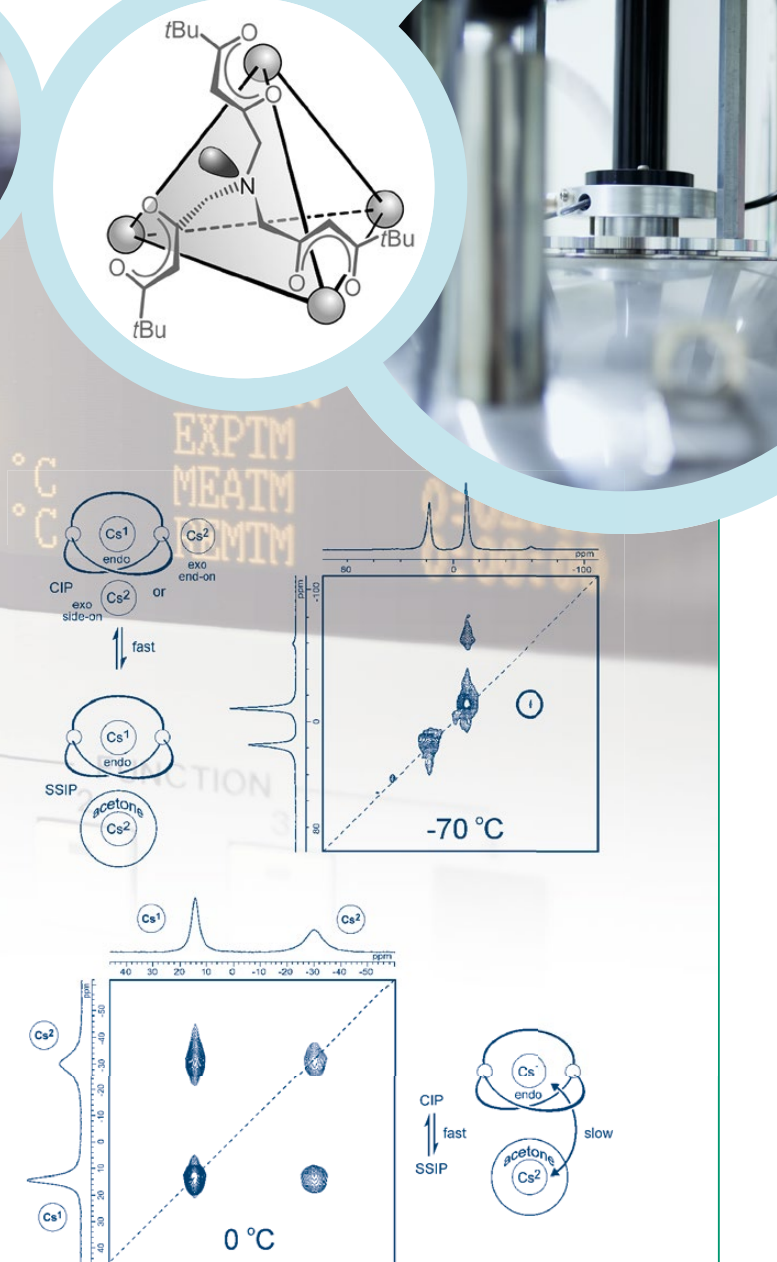
NOE methods based on pulsed field gradients and on gradient echoes (“excitation sculpting”) have become popular in recent years (DPFGSE-NOE). However, the well-known problem of “NOE zero-crossing” for $\omega\tau_c = 1.12$ still persists for DPGSE-NOE. We have described the application of the rotating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

We have applied DPGSE-ROE to a variety of organolithiums, calixarene inclusion compounds and other “normal” organic molecules. Though DPGSE-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, DPGSE-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

One of the current research projects 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 , ^1H -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. Fig. 1 summarizes the findings obtained by ^{133}Cs , ^{133}Cs -EXSY for the depicted molecule.



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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
- R. W. Saalfrank, C. Deutscher, H. Maid, A. M. Ako, S. Sperner, T. Nakajima, W. Bauer, F. Hampel, B. A. Heß, N. J. R. van Eikema Hommes, R. Puchta, F. W. Heinemann, *Chemistry Eur. J.* **2004**, 10, 1899–1905
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- H. Maid, F. W. Heinemann, A. Scheurer, N. Mooren, R. W. Saalfrank and W. Bauer, *Helv. Chim. Acta* **2012**, 95, 2429–2445
- 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



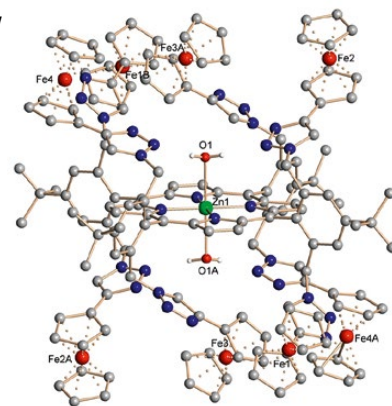
APL. PROFESSOR OF ORGANIC CHEMISTRY

PROF. DR. NORBERT JUX

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CURRICULUM VITAE

Since 2013	apl. Professor, Organic Chemistry at the University of Erlangen-Nürnberg, Germany
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



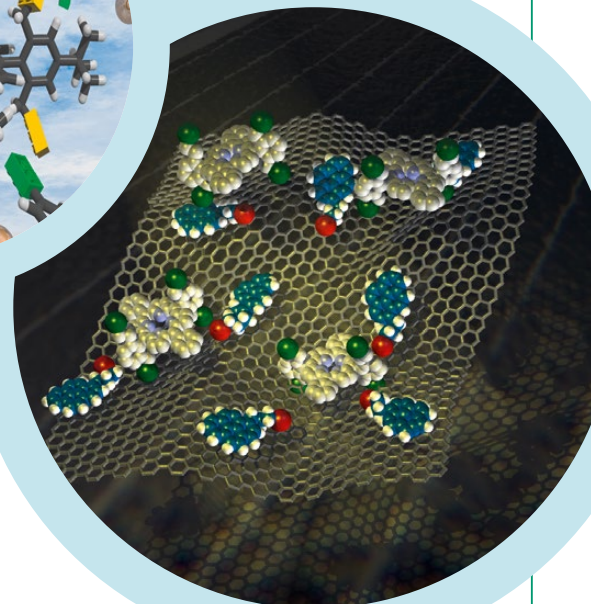
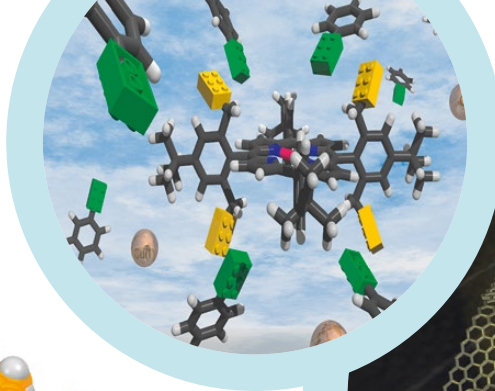
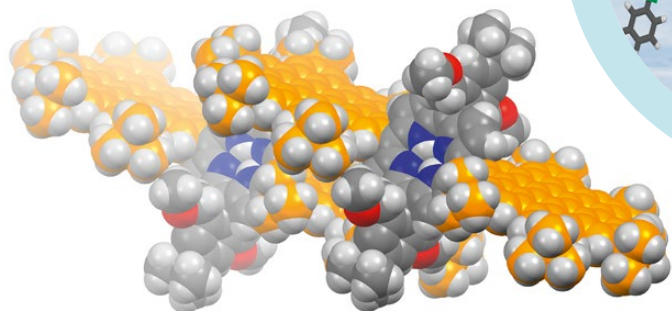
OBJECTIVES

To synthesize and characterize novel porphyrins and porphyrinoids, develop synthetic tools for their efficient functionalization; to explore their potential as a) components for solar energy conversion devices, b) as model systems for heme enzymes to gain insight into mechanisms of dioxygen activation and processing, c) as photosensitizers in elaborate modular carrier systems for photodynamic therapy of tumors and photodynamic inactivation of bacteria, fungi, molds, etc., d) as central parts of porphyrin-containing carbon-rich molecules and superstructures.

SCIENTIFIC BACKGROUND

Porphyrins are ubiquitous dyes in nature which govern the most important transformations in living organism—making them aptly named “pigments of life”.

Their inherent photophysical, photochemical, and redox properties are likely responsible for their extensive appearance in Nature. In photosynthesis, porphyrins act as light harvesters in stunningly complex arrays, as electron donors in the reaction center and as electron transporting cofactors. In the respiratory chain, these cofactors play indispensable roles as dioxygen carriers, repositories



and activators, the latter essentially delivering the “energy of life” in cytochrome c oxidase. It is not surprising that huge efforts are made to better understand these vital processes, because this may lead to improved artificial solar energy conversion in terms of light—energy—gathering and water splitting. As heme enzymes catalyze very important oxidations in nature, they are also in the focus of intense pharmaceutical research. Even without looking at Nature, porphyrins are fascinating molecules by themselves. They are able to form complexes with all metal ions, some half and even non-metals, often with several oxidation states available and strongly varying coordination geometries. Porphyrins act as sensitizer for singlet oxygen, thus are able to generate highly reactive species from dioxygen in the presence of light. This process, although detrimental in Nature, is used in the photodynamic therapy of tumors (PDT) as well as the photodynamic inactivation of germs. The highly polarizable π -electron system of porphyrins, their ability to either take-up or give-up two electrons in often reversible manner offers a high potential in molecular electronics.

RESEARCH HIGHLIGHTS

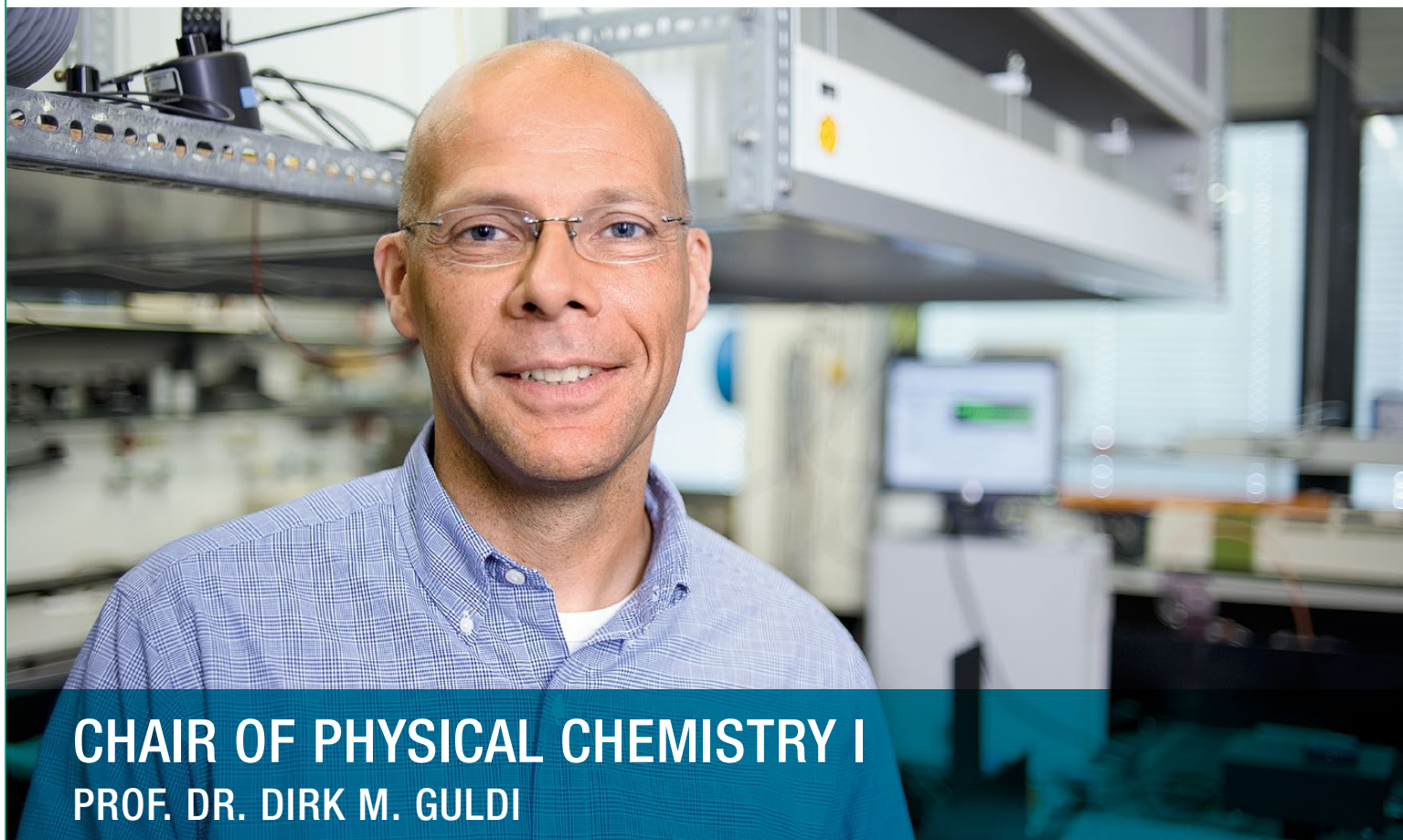
Our research is aimed at the synthesis and functionalization of porphyrins. Having the amazing properties of natural systems in mind, we prepare model compounds for, for example, enzymes, light harvesters, and reaction centers with organic chemical transformations—but we also look further into porphyrin chemistry. Recent highlights of our research are a) crown-ether appended metalloporphyrins which give deep insights into the mechanism of dioxygen activation, even under rather extreme high-pressure conditions as found for deep-sea organisms; b) antibody-conjugated modular carrier systems for the transport of photosensitizers for PDT; c) highly charged cationic and anionic metalloporphyrinoids in layer-by-layer-constructed photovoltaic devices; d) organization, metallation, and switching experiments of porphyrins on surfaces; and e) carbon-rich porphyrin conjugates containing hexa-peri-hexabenzocorone (HBC) moieties. Our work is on the one side based on powerful organic synthetic methods and, on the other hand, highly interdisciplinary. We strongly collaborate with various groups in Erlangen within several initiatives, such as the Collaborative Research Center 953 “Synthetic carbon allotropes”, or the Bavarian project “Solar Technologies go Hybrid”.

PERSPECTIVES

We are currently deeply involved in the preparation of porphyrins with high carbon content. Such compounds can be obtained by various approaches, such as introduction of acetylenic or polyaromatic hydrocarbon (i.e., HBC) substituents. Microwave-assisted transformations such as Diels-Alder reactions or Pd-catalyzed couplings are turning out to be more and more important. We have now established a flash-vacuum pyrolysis line where we investigate thermal reactions such as dehydrochlorinations or dehydrogenations of appropriately substituted porphyrins. We are convinced that carbon-rich porphyrins with their extended π -systems are ideal materials for molecular electronics and photovoltaics. We have shown that supramolecular interactions such as π - π -stacking govern their structures in the crystal. Such effects may play a vital role in successful applications in the aforementioned fields.

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- O. Troppner, R. Lippert, T. Shubina, A. Zahl, N. Jux, I. Ivanović-Burmazović, *Angew. Chem. Int. Ed.* **2014**, 53, 11452–11457
- W. Brenner, J. Malig, R. D. Costa, D. M. Guldi, N. Jux, *Adv. Mater.* **2013**, 25, 2314–2318
- J. M. Englert, J. Malig, V. Zamolo, A. Hirsch, N. Jux, *Chem. Commun.* **2013**, 49, 4827–4829
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- J.-F. Gnichwitz, R. Marczak, F. Werner, N. Lang, N. Jux, D. M. Guldi, W. Peukert, A. Hirsch, Andreas, *J. Am. Chem. Soc.* **2010**, 132, 17910–17920
- K. Dürr, B. P. Macpherson, R. Warratz, F. Hampel, F. Tuczek, M. Helmreich, N. Jux, I. Ivanović-Burmazović, *J. Am. Chem. Soc.* **2007**, 129, 4217–4228
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- 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



CHAIR OF PHYSICAL CHEMISTRY I

PROF. DR. DIRK M. GULDI

dirk.guldi@fau.de • www.chemie.fau.de/guldi

CURRICULUM VITAE

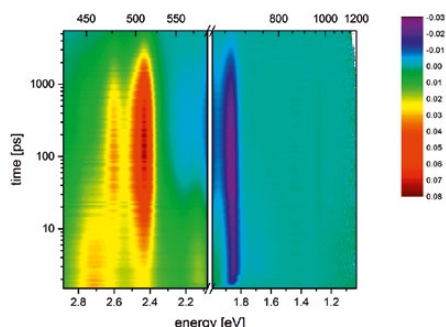
- Since 2014** Member of Australian Research Council Centre of Excellence for Electromaterials Science, University of Wollongong, Australia
- Since 2013** Vice Dean for Research, Faculty of Sciences, University of Erlangen-Nürnberg, Germany
- Since 2004** University Full Professor, Chair of Physical 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 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



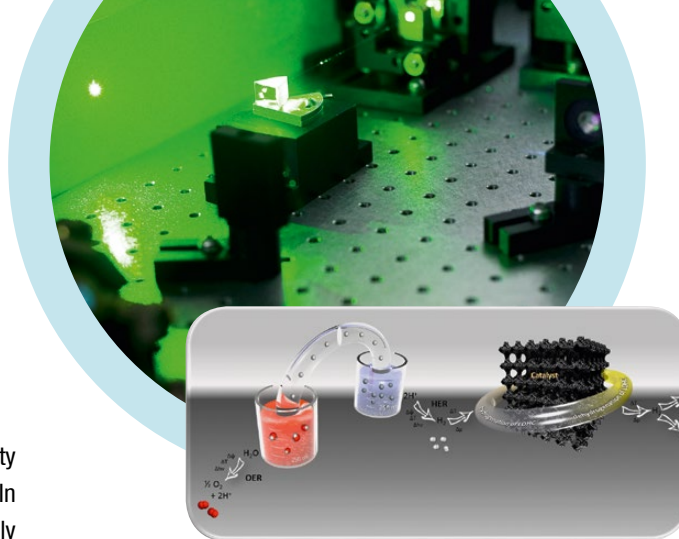
Dirk M. Guldi back to Germany, despite major efforts by the University of Notre Dame (2004) and the University of Bowling Green (2005). In the Scientist Ranking in Chemistry, Dirk M. Guldi is among the Highly Cited Researchers 2014/Thomson Reuter based on a track record that includes around 400 publications, an H-index of 80.

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/*Nature Chemistry* 2014) 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/*Nature Chemistry* 2014). 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 μ s. 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 photo-



induced 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.

SELECTED PUBLICATIONS

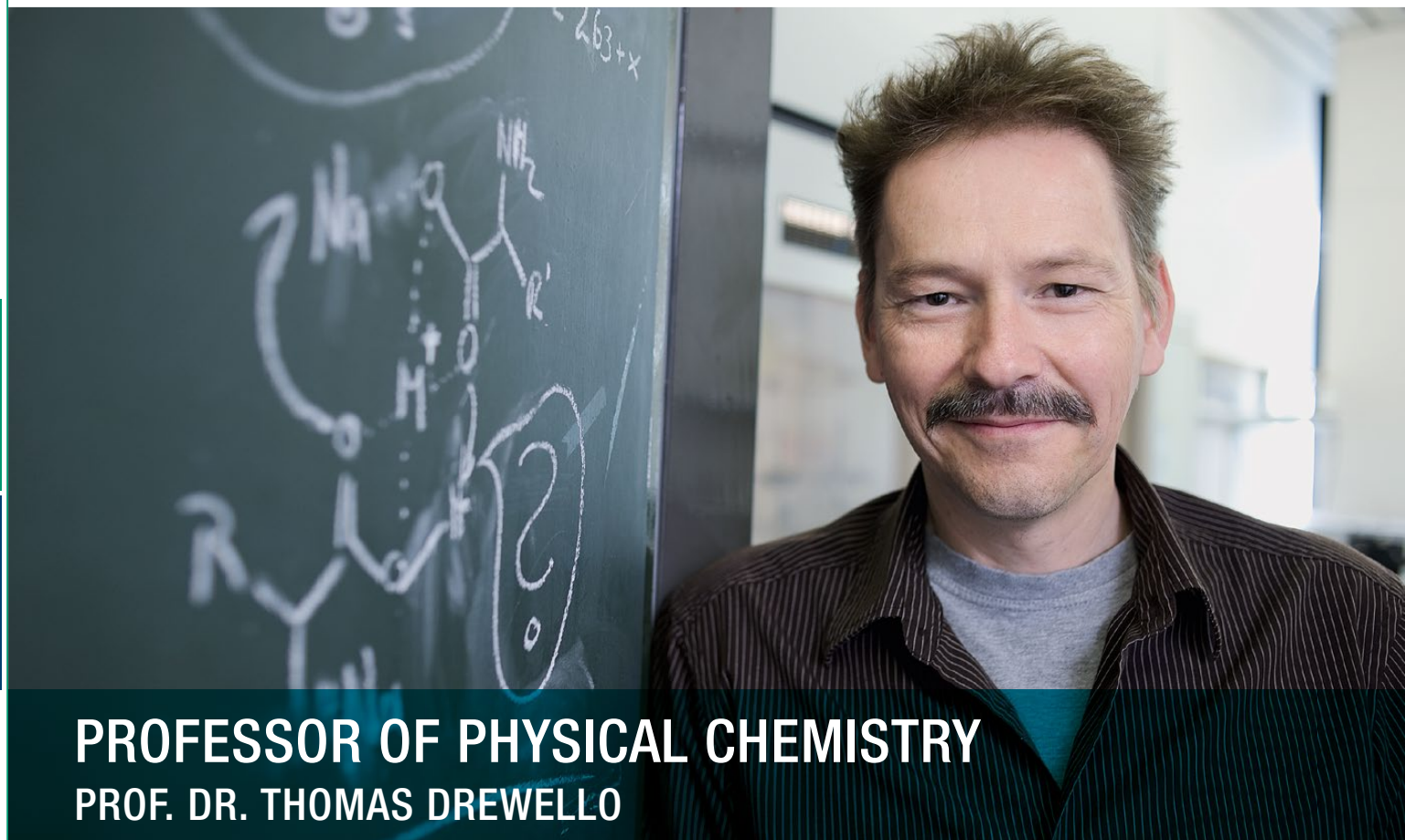
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- J. L. Lopez, C. Atienza, F. G. Brunetti, C. Romero-Nieto, D. M. Guldi, N. Martin, *Nature Communications* 2014, 5, 3763
- B. Grimm, J. Schornbaum, H. Jasch, O. Trukhina, F. Wessendorf, A. Hirsch, T. Torres, D. M. Guldi, *Proc. Natl. Aca. Sci.* 2012, 109, 15565–15571
- C. Ehli, C. Oelsner, D. M. Guldi, A. Mateo-Alonso, M. Prato, C. Schmidt, C. Backes, F. Hauke, A. Hirsch, *Nature Chemistry* 2009, 1, 243–249

SELECTED REVIEWS

- J. Malig, N. Jux, D.M. Guldi, Toward Multifunctional Wet Chemically Functionalized Graphene—Integration of Oligomeric, Molecular, and Particulate Building Blocks that Reveal Photoactivity and Redox Activity, *Acc. Chem. Res.* 2013, 46, 53–64
- 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, 110, 6768–6818

SELECTED AWARDS

- 2014 Fellow of the Electrochemical Society (Electrochemical Society)
- 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

thomas.drewello@fau.de • www.chemie.fau.de/drewello

CURRICULUM VITAE

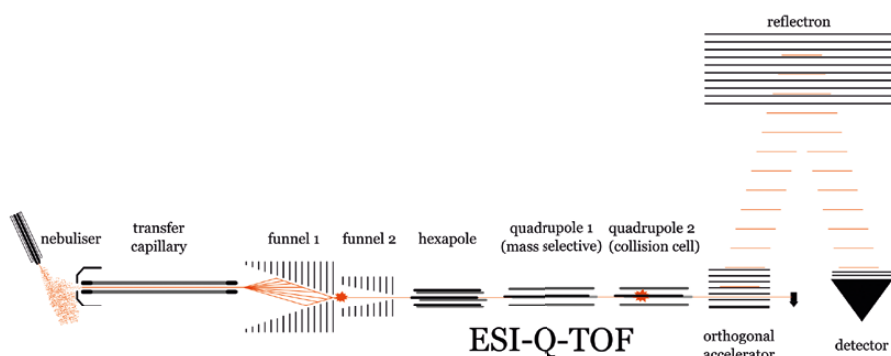
- Since 2008** University Professor of Physical Chemistry at the University of Erlangen-Nürnberg, Germany
1995 – 2007 Associate Professor at the University of Warwick, Great Britain
1990 – 1995 Researcher, Hahn-Meitner-Institute, Berlin, Germany
1989 – 1990 Postdoctoral Fellow, University of Amsterdam,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

OBJECTIVES

Research in this group is concerned with the development of mass spectrometry-based methods for the improved characterization 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.

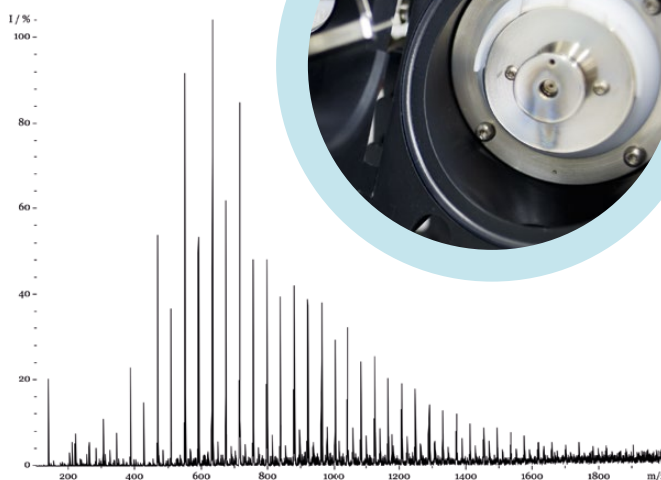
Jointly with several groups (Derrick, Warwick/Auckland; Woodruff, Warwick; Mackenzie; Warwick/Oxford; Beyer, Munich/Innsbruck) we were involved in the creation of a laser ablation/expansion source for the efficient production of metal clusters in conjunction with FT-ICR MS which allowed the investigation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

PERSPECTIVES

The further development of soft ionization methods for the sensitive and informative analysis of new materials continues to be a challenging task. 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, end group-protected polyynes, ionic liquids and polyoxometalates.

We will focus on the investigation of different carbon allotropes, elucidating their properties and reactivity by laser- and spray-based methods, with emphasis on affinities and interconversion.



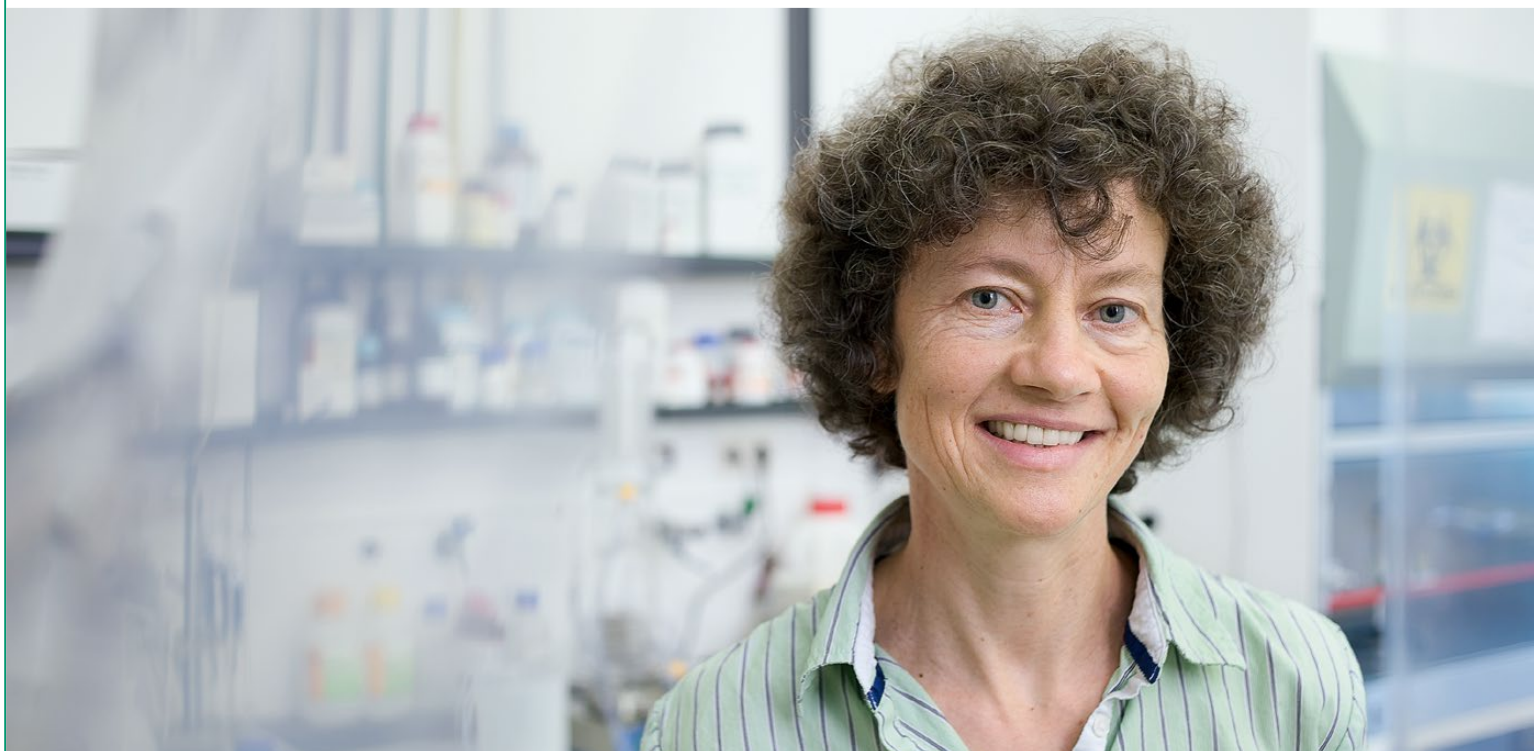
Finally, extending our cluster research, future investigations will focus on the formation, characterization and reactivity of different types of clusters.

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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

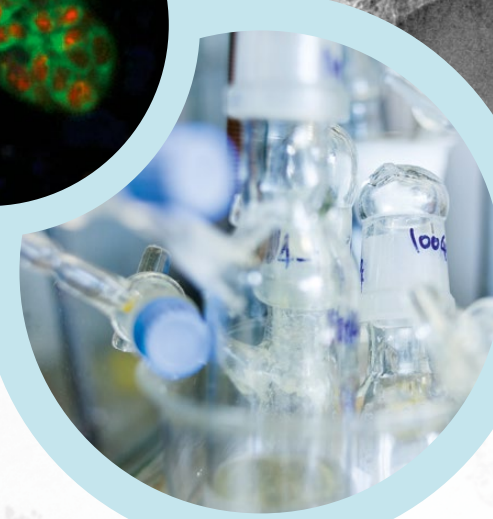
OBJECTIVES

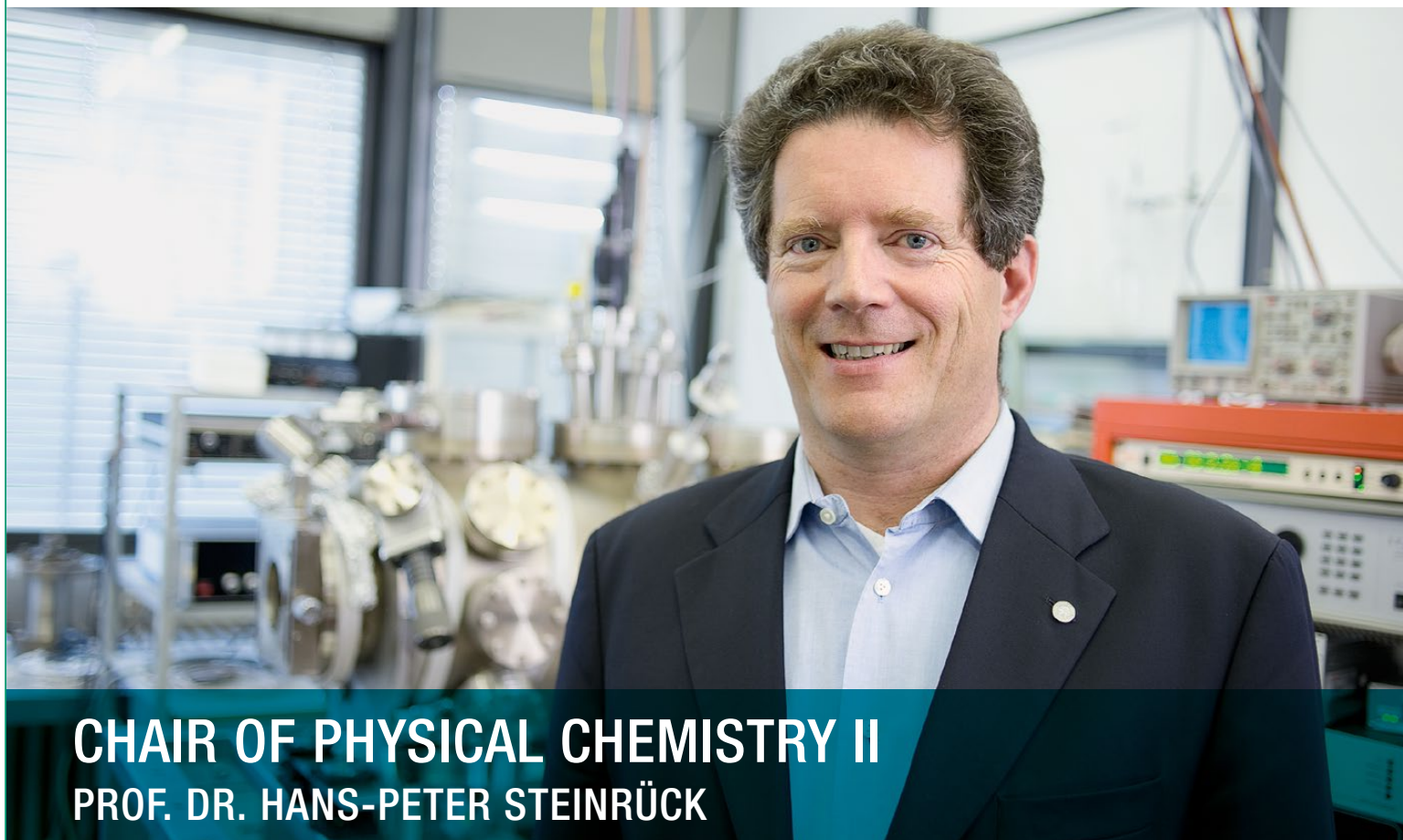
Current and future research activities focus on advanced non-linear spectroscopic methods and are directed to engineering of functionalized luminescent silicon quantum dots for optoelectronic applications, surface-stabilized metal noble-metal clusters for catalysis and superparamagnetic iron oxide nanoparticles as transfection reagent for gene therapies and X-ray enhancer for radiation cancer therapy.

SCIENTIFIC BACKGROUND

Carola Krysch 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, she is Professor of Physical Chemistry at the University of Erlangen-Nürnberg.





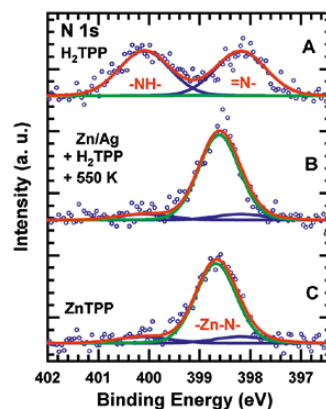
CHAIR OF PHYSICAL CHEMISTRY II

PROF. DR. HANS-PETER STEINRÜCK

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CURRICULUM VITAE

- 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

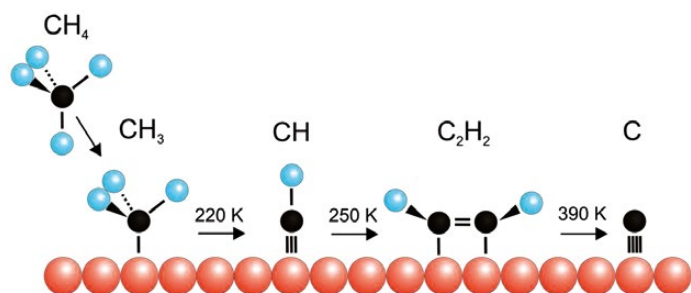


OBJECTIVES

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,



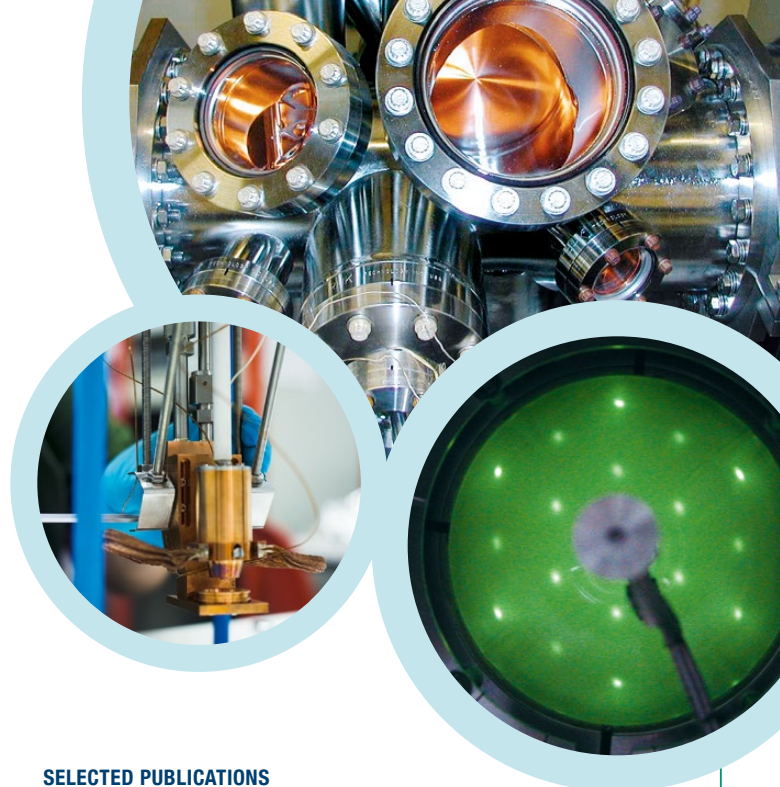
at an atomic level. For these investigations a large variety of experimental methods is applied, including synchrotron radiation-based photoelectron spectroscopy, scanning electron and scanning tunneling microscopy, and molecular beam methods.

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. The “*Chemical modification of graphene*” addresses different routes to functionalize graphene supported on metal substrates. 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 ultraclean metal and oxide nanostructures of an arbitrary shape. 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

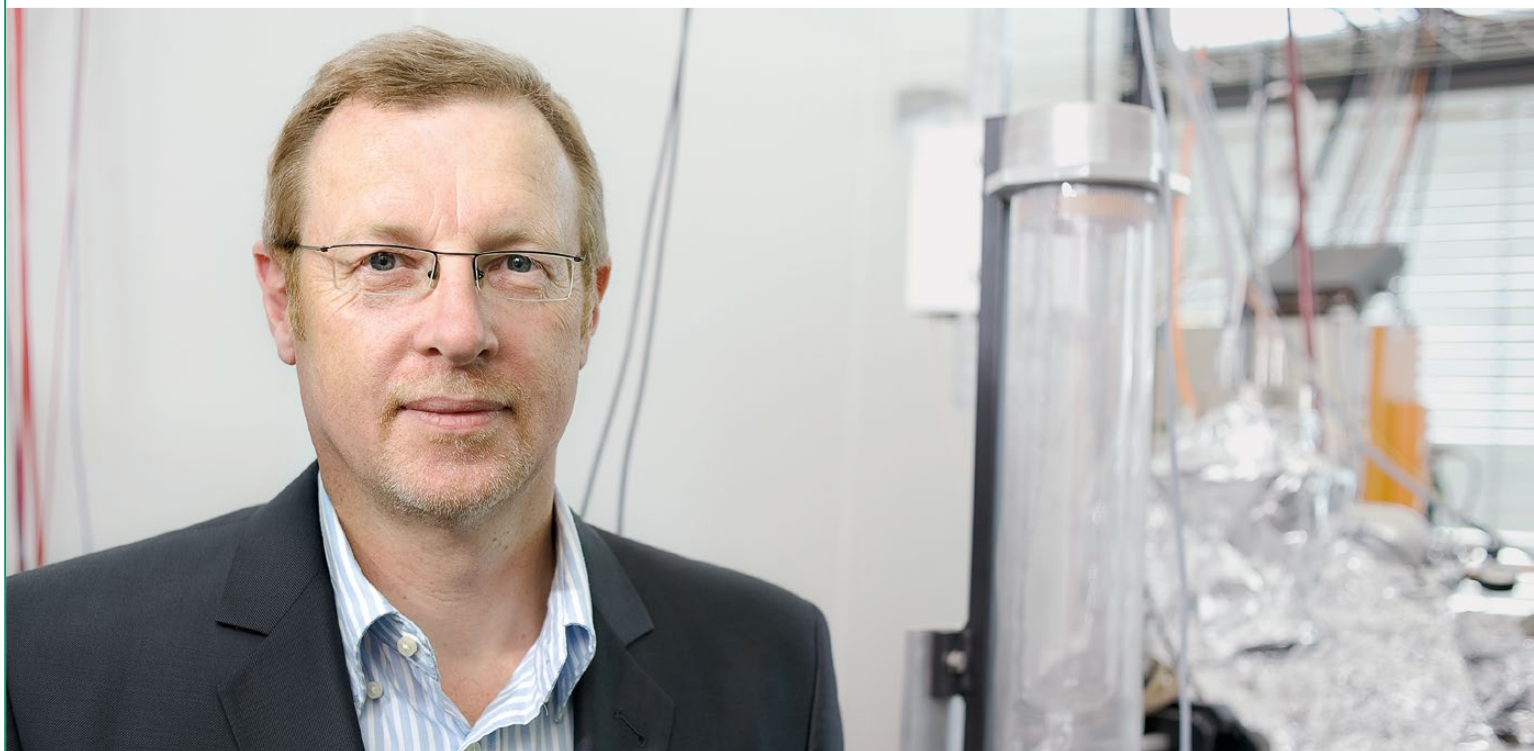
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- C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, Liquid Organic Hydrogen Carriers: Surface Science Studies of Carbazole Derivatives, *Chem. Rec.* (in press), DOI 10.1002/tcr.201402014
- H. Marbach, H.-P. Steinrück, Studying the dynamic behaviour of porphyrins as prototype functional molecules by scanning tunnelling microscopy close to room temperature, *Chem. Commun.* **2014**, 50, 9034–9048
- C. Papp, H.-P. Steinrück, In-situ high-resolution X-ray photoelectron spectroscopy – Fundamental insights in surface reactions, *Surface Science Reports* **2013**, 68, 446–487
- H.-P. Steinrück, Recent developments in the study of ionic liquid interfaces using X-ray photoelectron spectroscopy and potential future directions, *Phys. Chem. Chem. Phys.* **2012**, 14, 5010–5029
- H.-P. Steinrück, Angle-resolved photoemission studies of adsorbed hydrocarbons, *Journal of Physics: Condens. Matter* **1996**, 8, 6465–6509

SELECTED AWARDS

- 2013 Fellow of the American Physical Society
- 2012 Member of Academia Europaea—The Academy of Europe
- Since 2009 Guest Professor, University of Science and Technology of China (USTC), Hefei, China



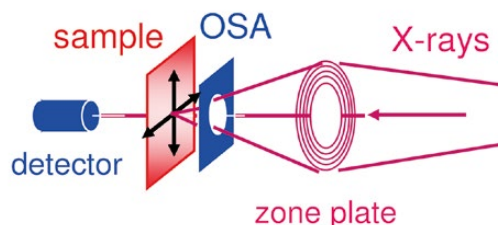
PROFESSOR OF PHYSICAL CHEMISTRY

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, organic nanocrystals, organic devices, and hybrid materials.

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.

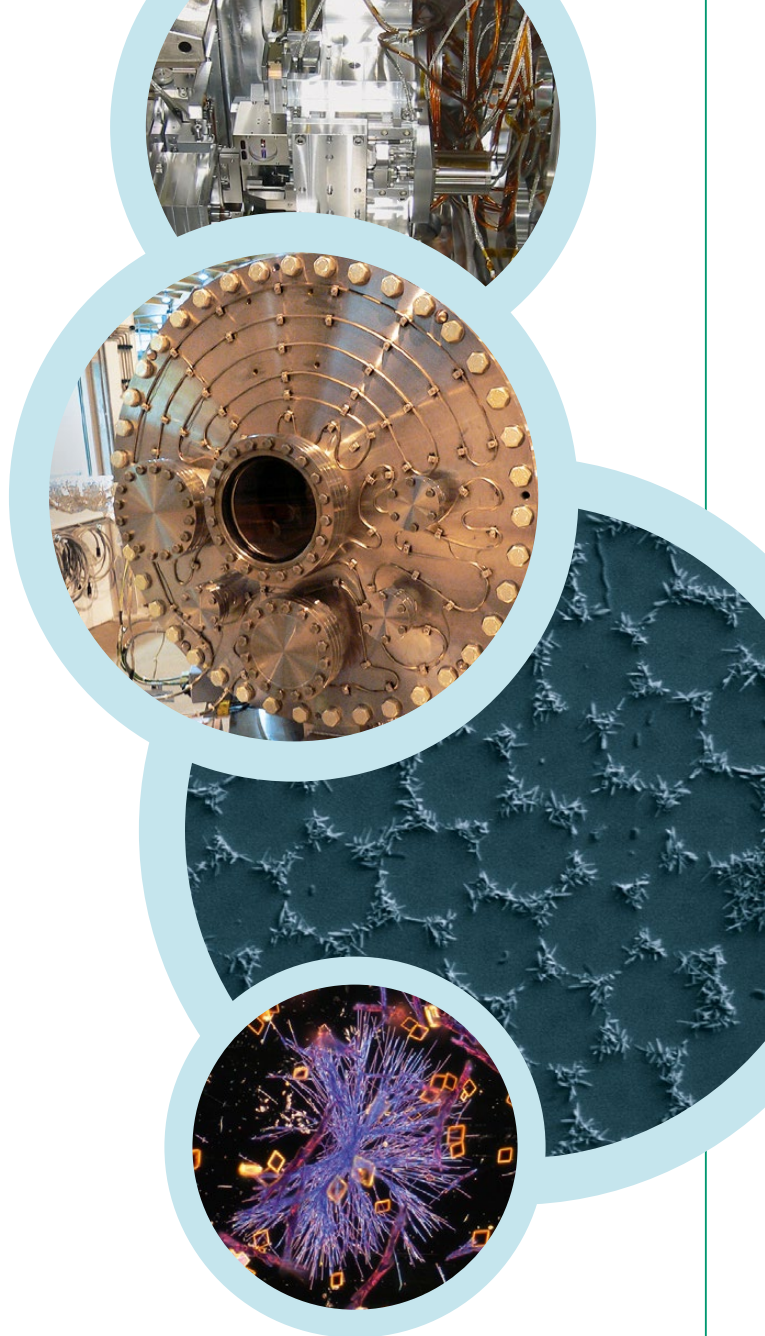
RESEARCH HIGHLIGHTS

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 polyvinyl 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 or transport in molecular wires. Using the local NEXAFS probe we were able to monitor the electronic structure within the active area while the OFET or device 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. Confocal imaging using short wavelengths will overcome the diffraction-limit in 3D microscopy. Present studies evaluate the realization of a zone-plate based confocal microscope in the soft x-ray regime. These developments will be supported by experiments that implement higher-order diffraction to improve the lateral resolution in STXM into the regime below 10 nm. 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. Here, in-situ studies shall give insight into the growth kinetics and molecular self-organization on the mesoscale using LEEM and PEEM as direct imaging techniques.

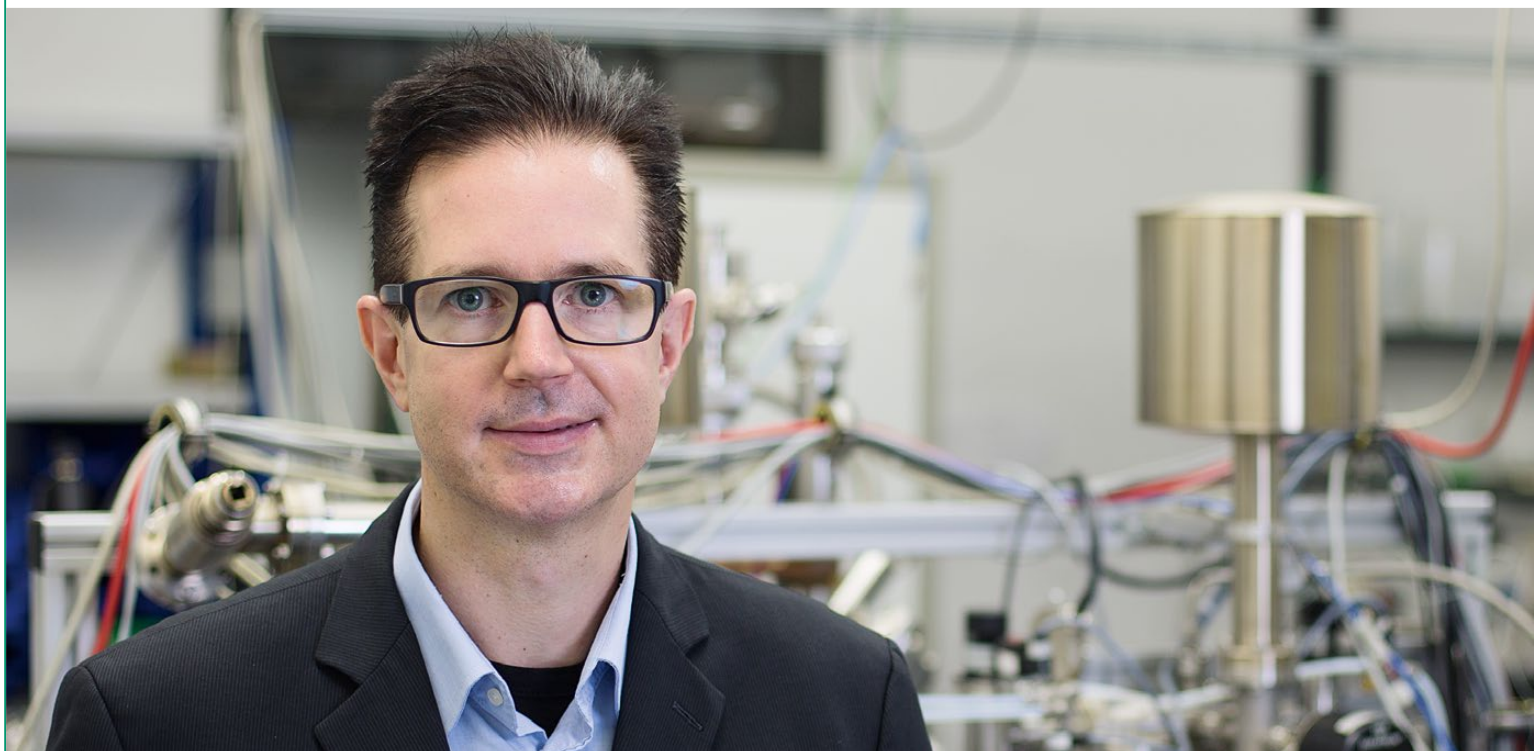


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- N. Schmidt, T. Clark, S. G. Urquhart, R. H. Fink, *J. Chem. Phys.* **2011**, 135(14), 144301
- A. Schöll, L. Kilian, Y. Zou, J. Ziroff, S. Hame, F. Reinert, E. Umbach, R. H. Fink, *Science* **2010**, 329, 303–305
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- 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. Tyliczszak, PoLux: 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, Department of Chemical Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft (MPG), Berlin, Germany
2003 Habilitation, Humboldt University of Berlin, Germany
1998 – 1999 Postdoctoral Fellow, Department of Chemistry, Princeton University, USA
1996 PhD, Ruhr-University Bochum, Germany

OBJECTIVES

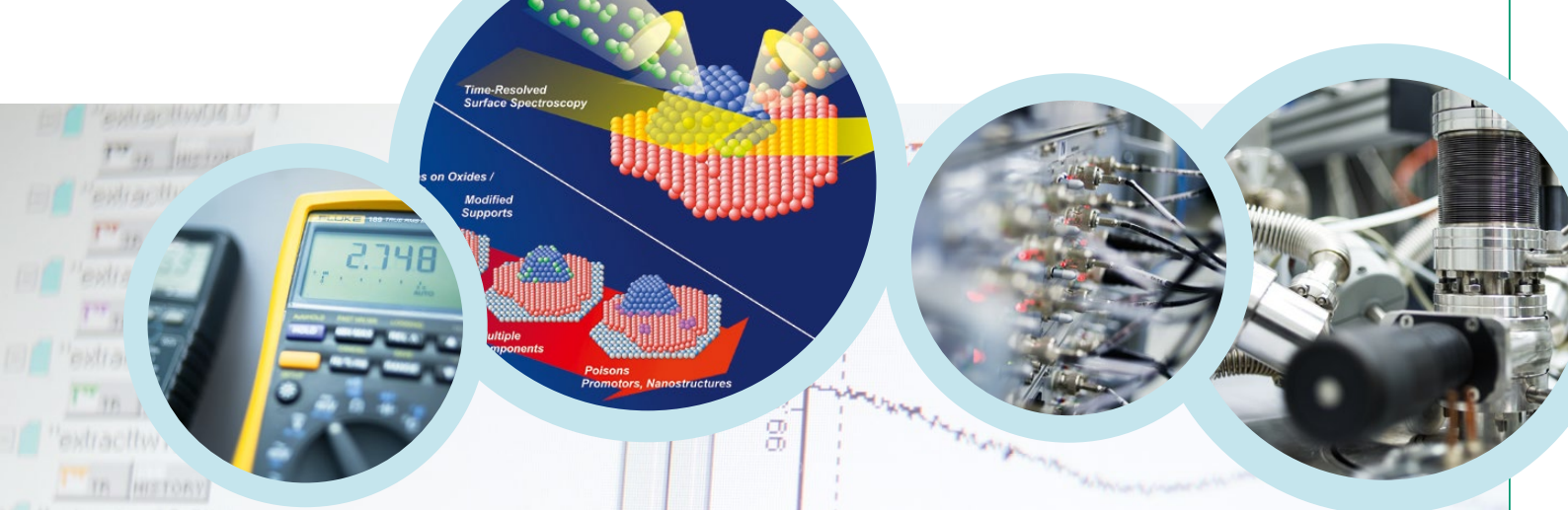
Chemical reactions and physical processes at complex surfaces play a pivotal role in many areas of today's technology. Towards a better understanding of the underlying physical and chemical phenomena at the microscopic level, we develop and investigate complex nanostructured model surfaces. Mechanisms, 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 and under electrochemical 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 inter-

face 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 complexity of materials 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 current project in energy-related catalysis we investigate, for instance, novel fuel-cell catalysts with lower demand for critical materials such as noble metals. Together with partners from academia and industry we develop model systems to explore the fundamental surface chemistry of such materials using a surface science approach and transfer this knowledge to realistic materials and environments, i.e., ambient pressure and electrochemically controlled conditions. 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. In the DFG Research Unit “fun-COS”, an interdisciplinary team from chemistry, physics and engineering, we study the fundamental properties of organic thin films on oxide surfaces, systems that are used in molecular electronics, solar cells, or catalysis. Within the Excellence Cluster Engineering of Advanced Materials, our projects aim at energy-related materials, such as hydrogen storage, for example in so-called Liquid Organic Hydrogen Carriers, and at novel concepts in catalysis, such as ionic-liquid-based model catalysis and material synthesis. For instance, we develop new ionic liquid model catalysts following a surface science approach. Such model systems provide insights into the interfacial chemistry of ionic liquid films at an unprecedented level of detail.

PERSPECTIVES

The group is involved in several new activities, most of them emerging at the interface between fundamental sciences and engineering. A special focus is on the development of spectroscopic methods that directly link fundamental surface science and model catalysis to studies under realistic conditions and on real materials.

To this aim a new facility for time-resolved in-situ and operando spectroscopy has been set up within the Excellence Cluster Engineering of Advanced Materials. So-called operando methods combine measurements of catalytic activity with spectroscopic investigations performed at the same time. Currently, new spectroscopy facilities are developed to study atomically well-defined liquid-solid interfaces under electrochemically controlled conditions. In a unique fashion, these methods allow us to link scientific results obtained under ideal surface-science conditions to model studies on complex surfaces and, finally, to real-life catalysts. Such spectroscopic links close the often-cited gap between model studies and applied research and provide mechanistic insights that help to develop new catalytic systems at a knowledge-driven basis.

SELECTED PUBLICATIONS

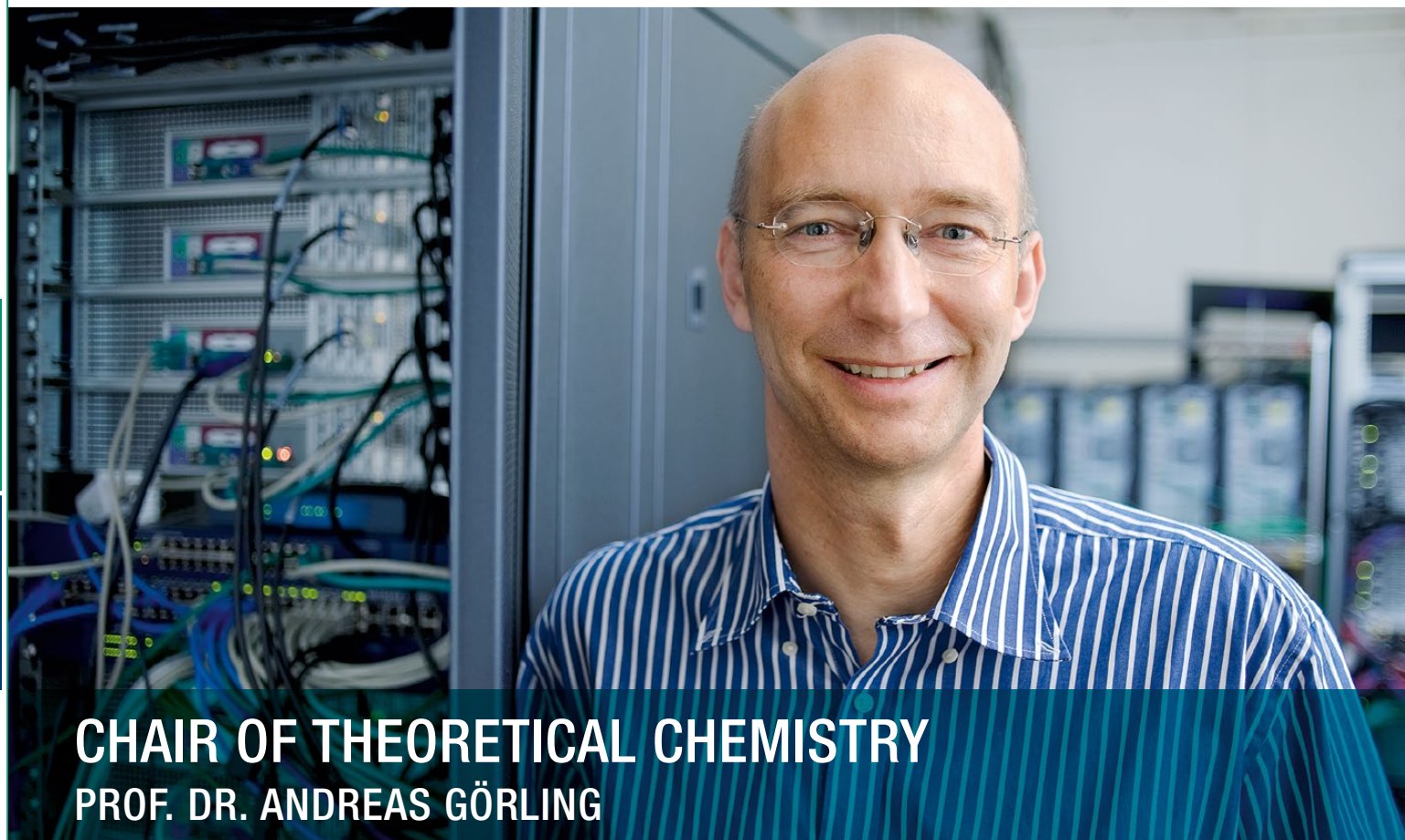
- M. Amende, Ch. Gleichweit, K. Werner, S. Schernich, W. Zhao, M. P. A. Lorenz, O. Höfert, C. Papp, M. Koch, P. Wasserscheid, M. Laurin, H.-P. Steinrück, J. Libuda, *ACS Catal.* **2014**, 4, 657–665
- A. Bruix, Y. Lykhach, I. Matolínová, A. Neitzel, T. Skála, N. Tsud, M. Vorokhta, V. Stetsovych, K. Ševčíková, J. Mysliveček, K. C. Prince, S. Bruyère, V. Potin, F. Illas, V. Matolín, J. Libuda, K. M. Neyman, *Angew. Chem. Int. Ed.* **2014**, 53, 10531–10535
- M. Kusche, F. Enzenberger, S. Bajus, H. Niedermeyer, A. Bösmann, A. Kaftan, M. Laurin, J. Libuda, P. Wasserscheid, *Angew. Chem. Int. Ed.* **2013**, 52, 5028–5032
- G. N. Vayssilov, Y. Lykhach, A. Migani, T. Staudt, G. P. Petrova, N. Tsud, T. Skála, A. Bruix, F. Illas, K. C. Prince, V. Matolín, K. M. Neyman, J. Libuda, *Nat. Mater.* **2011**, 10, 310–315
- T. Schalow, B. Brandt, D. E. Starr, M. Laurin, Sh. K. Shaikhutdinov, S. Schauermaier, J. Libuda, H.-J. Freund, *Angew. Chem. Int. Ed.* **2006**, 45, 3693–3697
- V. Johánek, M. Laurin, A. W. Grant, B. Kasemo, C. R. Henry, J. Libuda, H.-J. Freund, *Science* **2004**, 304, 1639–1644

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- C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, Liquid Organic Hydrogen Carriers: Surface Science Studies of Carbazole Derivatives, *Chem. Rec.* **2014**, DOI 10.1002/tcr.201402014
- H.-P. Steinrück, J. Libuda, P. Wasserscheid, T. Cremer, C. Kolbeck, M. Laurin, F. Maier, M. Sobota, P. S. Schulz, M. Stark, Surface Science and Model Catalysis with Ionic Liquid-modified Materials, *Adv. Mater.* **2011**, 23, 2571–2587
- J. Libuda, H.-J. Freund, Molecular Beam Experiments on Model Catalysts, *Surf. Sci. Rep.* **2005**, 57, 157–298

SELECTED AWARDS

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



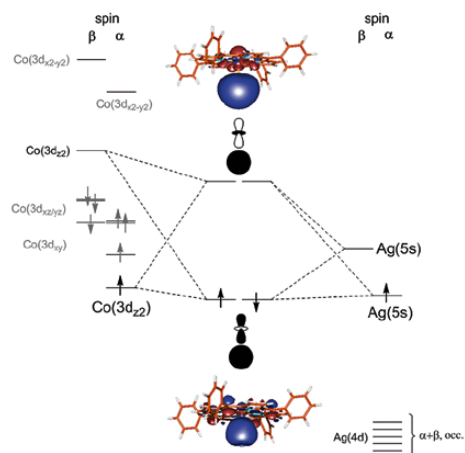
CHAIR OF THEORETICAL CHEMISTRY

PROF. DR. ANDREAS GÖRLING

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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. Röscher), Germany
- 1986** Diploma in Chemistry, Technische Universität München, Germany



OBJECTIVES

The research group of Andreas Görling develops and applies 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 experimen-

tal 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 joint projects by

theoreticians and experimentalists have become the rule. Today, theory not only helps interpreting and understanding experimental findings but makes predictions suggesting promising experiments or synthetic targets. 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 activities of the group of Andreas Görling have to be seen in this context.

About half of the group focuses on the development of formal theory and new methods, including the implementation of the latter, both in homegrown computer codes and commercially available quantum chemistry packages. The other 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

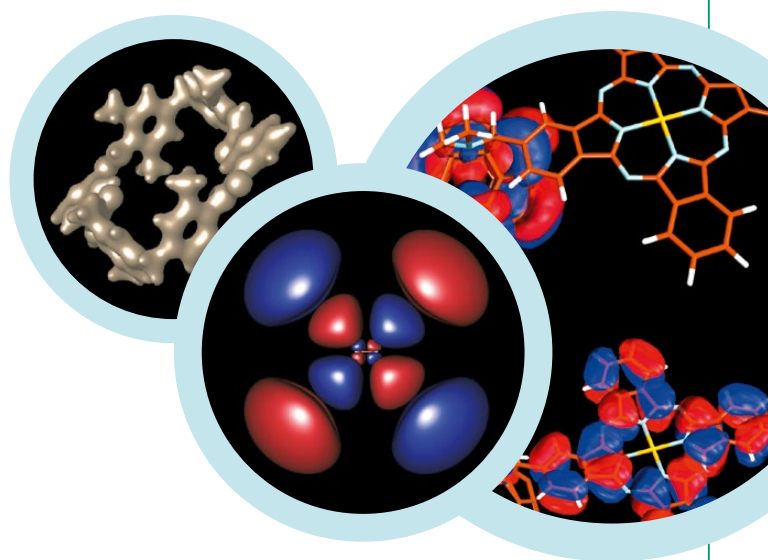
In recent years novel density-functional methods employing orbital-dependent functionals were developed, in particular, methods treating the electron correlation on the basis of the adiabatic-connection fluctuation-dissipation theorem. These methods do not suffer from the shortcomings of conventional density-functional methods and therefore, in contrast to the latter, can describe Van-der-Waals interactions and electronic structures characterized by static correlation which typically occur during the breaking and forming of bonds. The accuracy of the new density-functional methods is comparable to that of high-level, wave-function-based quantum chemistry methods while the required computational effort is distinctively lower. This opens up new exciting new perspectives for quantum chemistry, most importantly, the treatment of molecules or assemblies of molecules containing more than hundred atoms with unprecedented accuracy enabling predictions of their properties and reactivities with, so far, unmatched reliability.

Recent examples of applications of methods from theory in joint projects with experimental groups here in Erlangen comprise work on synthetic carbon allotropes in the framework of the collaborative research centre 953 which is located in Erlangen and is funded by the German Research Foundation. Together with the group of Hans-Peter Steinrück of Physical Chemistry doping and chemical functionalization of graphene adsorbed on metal surfaces is investigated, collaborations with Rik Tykwinski and his group from Organic Chemistry aim at the synthesis of polynes and cumulenes as well as graphynes, and with the group of Andreas Hirsch from Organic Chemistry new approaches to separate different carbon nanotubes are explored. Within the research unit 1878 funded by the German Research Foundation functional molecules on complex oxide surfaces are investigated with various groups from chemistry and physics. In collaborations with the group of Peter Wasserscheid from Chemical Reaction Engineering new catalytic concepts are developed which reduce the need for costly precious metals. The role of dispersion interactions

on efficiency and chemo-, regio-, and stereoselectivity of organocatalysts is investigated with the group of Svetlana Tsogoeva from Organic Chemistry. Together with the group of Heiko Weber of Applied Physics vibrational signatures in single molecule current-voltage experiment are interpreted and assigned.

PERSPECTIVES

In the future the interplay between method development and applications shall become even closer. The new methods developed in recent years will be further developed and optimized and will be made available to the quantum chemistry community in widely used computer packages. In this way, the arsenal of available methods for investigating questions in chemistry and materials science is going to be enlarged. In the future, furthermore, work on materials for energy conversion and storage shall develop into a new research focus of the group.



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- A. Heßelmann, A. Görling, *Phys. Rev. Lett.* **2011**, 106, 093001
- S. M. Kozlov, F. Viñes, A. Görling, *Adv. Mater.* **2011**, 23, 2638–2643
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- A. Heßelmann, A. Görling, Random-phase approximation correlation methods for molecules and solids, *Mol. Phys.* **2011**, 109, 2473–2500
- 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

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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.

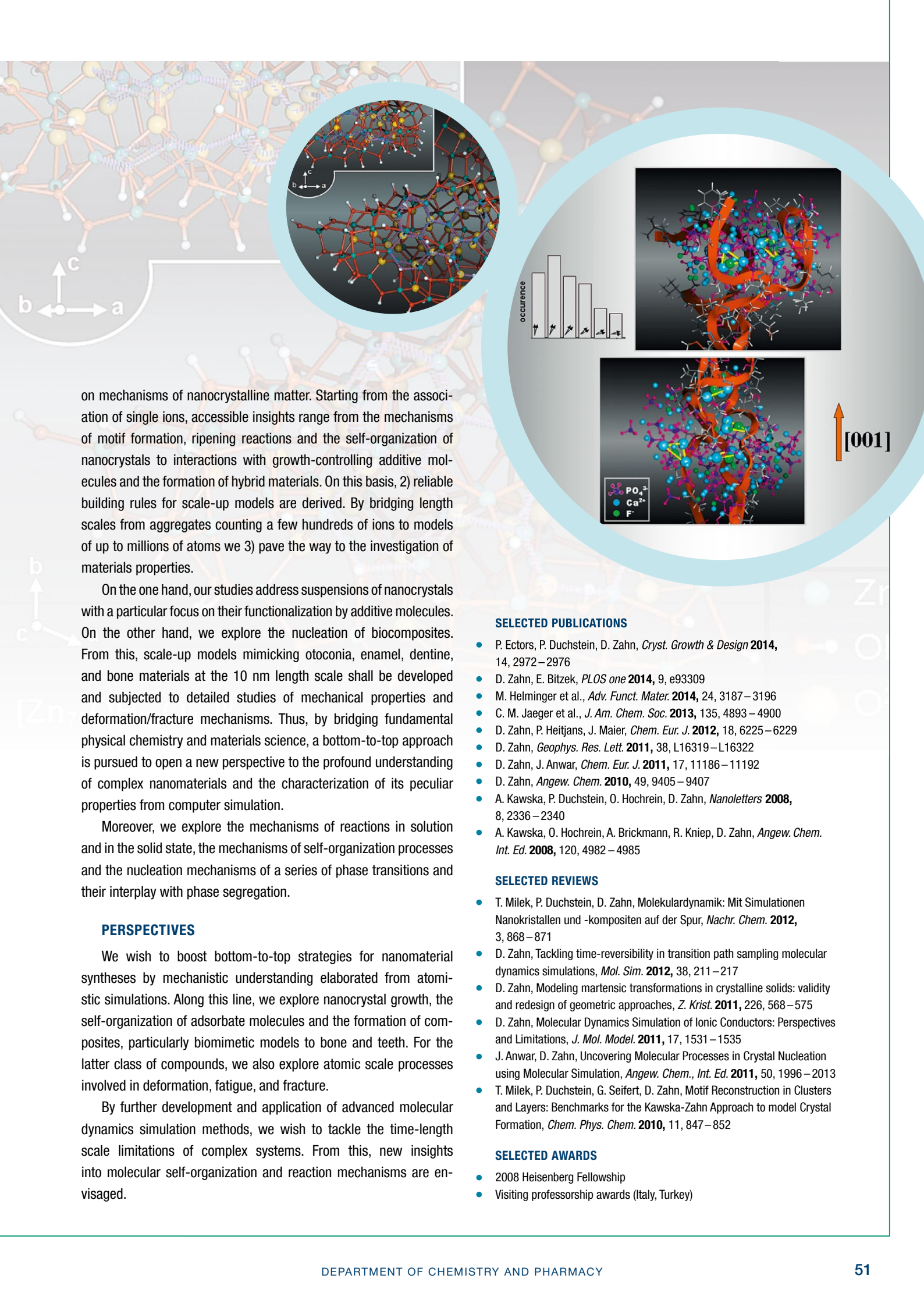
SCIENTIFIC BACKGROUND

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 1) to explore the nucleati-



on 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, 2) 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 3) pave the way to the investigation of materials properties.

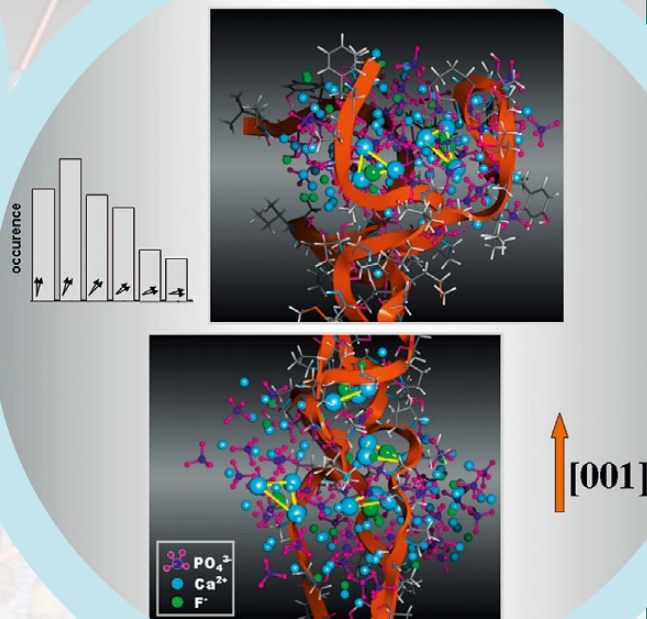
On the one hand, our studies address suspensions of nanocrystals with a particular focus on their functionalization by additive molecules. On the other hand, we explore the nucleation of biocomposites. From this, scale-up models mimicking otoconia, enamel, dentine, and bone materials at the 10 nm length 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.



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- D. Zahn, E. Bitzek, *PLOS one* **2014**, 9, e93309
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- D. Zahn, P. Heitjans, J. Maier, *Chem. Eur. J.* **2012**, 18, 6225–6229
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- T. Milek, P. Duchstein, D. Zahn, Molekulardynamik: Mit Simulationen Nanokristallen und -kompositen auf der Spur, *Nachr. Chem.* **2012**, 3, 868–871
- D. Zahn, Tackling time-reversibility in transition path sampling molecular dynamics simulations, *Mol. Sim.* **2012**, 38, 211–217
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- D. Zahn, Molecular Dynamics Simulation of Ionic Conductors: Perspectives and Limitations, *J. Mol. Model.* **2011**, 17, 1531–1535
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- T. Milek, P. Duchstein, G. Seifert, D. Zahn, Motif Reconstruction in Clusters and Layers: Benchmarks for the Kawaska-Zahn Approach to model Crystal Formation, *Chem. Phys. Chem.* **2010**, 11, 847–852

SELECTED AWARDS

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



CHAIR OF MEDICINAL CHEMISTRY

PROF. DR. PETER GMEINER

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CURRICULUM VITAE

- Since 1999** University Full Professor, Chair of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany
1994 – 1996 Professor of Medicinal 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 novel molecular probes and drug candidates, Peter Gmeiner's group investigates design, chemical synthesis, and pharmacological properties selective ligands for G protein-coupled receptors. In this context, radioligand binding studies, X-ray crystal structures and functional assays reveal the structural origins of subtype selectivity, intrinsic activity and biased signalling. Within these topics, the Gmeiner laboratory has proven substantial experience in the design, organic synthesis, and biological investigation of bioactive molecules and contributes to highly attractive developments in CNS-active drugs.

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 200 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 and International Advisory Board Member of scientific journals including Bioorganic & Medicinal Chemistry, Bioorganic & Medicinal Chemistry Letters, and ChemMedChem. Peter Gmeiner's research spans the design, organic synthesis and pharmacological investigation of bioactive molecules.

Prof. Peter Gmeiner is the spokesman of the Research Training Group “Medicinal Chemistry of Selective GPCR Ligands” (GRK 1910).

RESEARCH HIGHLIGHTS

G-Protein coupled receptors (GPCRs) are of particular interest as pharmaceutical target proteins in Medicinal Chemistry since a large number of diseases can be treated by selective GPCR agonists or antagonists. Peter Gmeiner's group investigates design, chemical synthesis and pharmacological properties of subtype-selective GPCR ligands. Using an integrative approach, the group develops molecular probes to understand, control and engineer receptor-ligand binding, selectivity and function. 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 (neutral)-antagonist properties at the dopamine D4 receptor. Behavioral pharmacological investigations indicated atypical antipsychotic activities for the azaindole derivative FAUC 213. 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 designed, which had not been investigated in drug discovery, yet. As an example, metallocene and paracyclophane derived bioisosteres showed excellent ligand binding properties.

PERSPECTIVES

Although G-protein coupled receptors (GPCRs) have been studied extensively in the past, our understanding of their function at the molecular level is still incomplete. It has been shown that GPCRs mediate diverse signal-transduction pathways by similar mechanisms by binding a variety of ligands and G-proteins. Their interaction with agonists leads to a low-affinity conformation of the active state that is thought to facilitate G-protein binding. Only in the presence of both agonist and G-protein is the high-affinity receptor state formed, which promotes signal transduction. The β 2-adrenergic receptor (β 2AR), which represents an important target for cardiac and asthma drugs, is an extensively studied model system for the large superfamily of G-protein coupled receptors (GPCRs). To overcome relatively rapid association and dissociation rates of commercial β 2AR agonists, our strategy depends on a combination on a covalent β 2AR agonist incorporating a β 2-adrenergic agonist core and a reactive chemical group that could be targeted to a specific residue on the receptor. Employing the structure of the carazolol-bound β 2AR as a template, a flexible linker was added to bridge these two components. Thus, the covalent attachment would not inhibit binding of the agonist core or conformational flexibility of the transmembrane he-



lices. The covalent β 2AR-agonist complex formed efficiently, and was able to activate a heterotrimeric G protein. A covalent agonist-bound β 2AR-T4L fusion protein could be crystallized and determined for its structure. Applying our newly developed methodology, we could determine active-state crystal structures of the muscarinic M2 receptor and the β 2AR in presence of a covalent adrenaline analog, in collaboration with Prof. Brian Kobilka at the Department of Molecular Physiology/Stanford University. Our current projects aim to exploit the covalent ligand strategy to the discovery of highly innovative GPCR-ligand complexes in multiple activation states. Taking advantage of such structural information, we aim to develop highly specific allosteric ligands, biased agonists and bivalent modulators.

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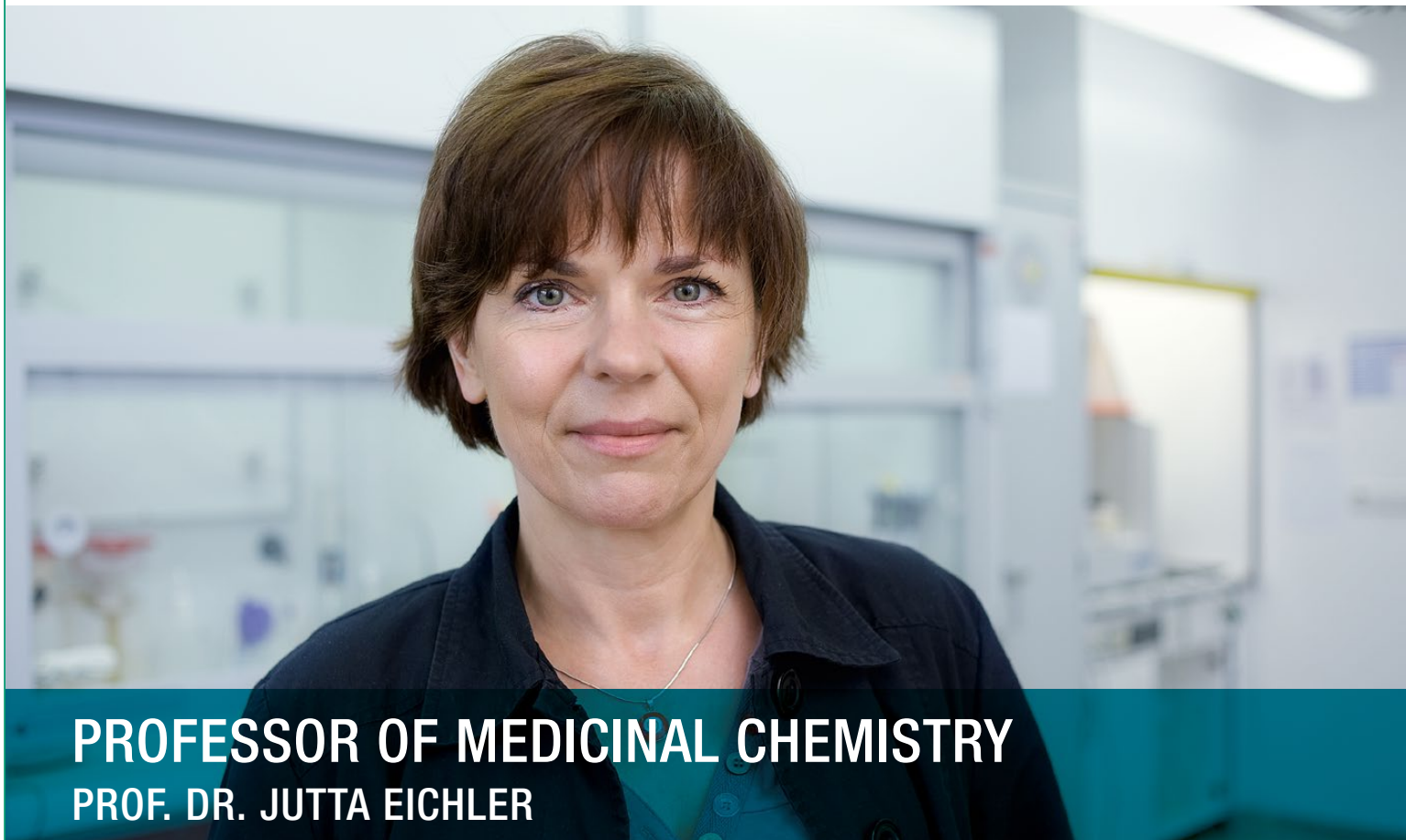
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- Stefan Löber, Harald Hübner, Niska Tschammer, Peter Gmeiner, *Recent advances in the search for D₃- and D₄-selective drugs: probes, models and candidates*, *Trends Pharmacol. Sci.*, **2011**, 32, 148–157
- F. Boeckler, P. Gmeiner, *The Structural 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

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CURRICULUM VITAE

- Since 2008** University Professor of Medicinal Chemistry at the University of Erlangen-Nürnberg, Germany
2004 Habilitation in Bioorganic Chemistry at Technische Universität 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 using synthetic binding site mimics.

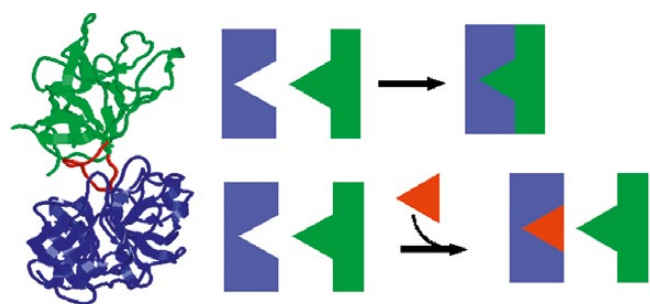
SCIENTIFIC BACKGROUND

Essentially all biological processes are based on specific binding events, which are initiated by molecular recognition between bio-macromolecules. 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 pro-

mising 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

Entry of the AIDS virus HIV-1 into its host cells is mediated by a precise cascade of molecular interactions between viral proteins and cellular receptors. Attachment of the HIV-1 exterior envelope glycoprotein gp120 to the coreceptors CXCR4 and CCR5 is a pivotal element of this entry process. Recently, we have extended the scope of using scaffolded and assembled peptides for the synthetic



mimicry of large, discontinuous protein binding sites, to the extracellular domain of the HIV-1 coreceptor CXCR4, which belongs to the family of GPCRs. The functionality of the CXCR4 mimetic peptide was demonstrated by its affinity to HIV-1 gp120, and, more importantly, by its ability to discriminate between gp120 from X4- and R5-tropic HIV-1 in binding assays involving recombinant proteins, as well as in cellular infection assays. Apart from their potential biomedical applications, such molecules are useful tools for the exploration of HIV-1 tropism at the molecular level. Furthermore, we could show that the interaction of gp120 with CXCR4 can be functionally mimicked by peptides presenting the binding sites of the two proteins for each other, i.e., the V3 loop of gp120 and the three extracellular loops of CXCR4.

PERSPECTIVE

Our ongoing and future research plans include the design and generation of hybrid molecules that target two or more protein-protein-interactions simultaneously, as well as probing the concept of mimicking protein-protein interactions by peptide-peptide interactions in the context of other proteins. Furthermore, we want to address the relationship of functional and structural mimicry, i.e., the question whether protein binding site mimics 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. The goal is to understand the structural features that govern the affinity of these mimicry, which will in turn guide the design of improved molecules.

SELECTED PUBLICATIONS

- A. Berthelmann, J. Lach, M. A. Gräwert, M. Groll, J. Eichler, *Org.Biomol.Chem.* **2014**, 12(16), 2606–2614
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- K. Möbius, R. Dürr, C. Haußner, U. Dietrich, J. Eichler, *Chem.Eur.J.* **2012**, 18, 8292–8295
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- K. Möbius, J. Eichler, HIV-derived peptide mimics, *Drug Discovery Today: Technologies*, **2009**, 6, (1–4), e19–e25
- 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

- Since 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.

We therefore focus on the development of radical reactions which can be conducted under very mild and simple reaction conditions with solvents such as water. To maintain a wide and general applicability, our aim is use only non-toxic metals or metal-free conditions.

SCIENTIFIC BACKGROUND

The applicability of organic radical chemistry is still restricted by the fact that even newly developed reactions 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. Against this background, the synthetic potential of radical reactions appears to be by far not exploited.

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 carbhydroxylation 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

- S. Fehler, S. Maschauer, S. Höfling, A. Bartuschat, N. Tschammer, H. Hübner, P. Gmeiner, O. Prante, M. R. Heinrich, *Chem. Eur. J.* **2014**, 20, 370–375
- C. de Salas, M. R. Heinrich, *Green Chem.* **2014**, 16, 2982–2987
- G. Pratsch, T. Wallaschkowski, M. R. Heinrich, *Chem. Eur. J.* **2012**, 18, 11555–11559
- S. B. Höfling, A. L. Bartuschat, M. R. Heinrich, *Angew. Chem. Int. Ed.* **2010**, 49, 9769–9772
- A. Wetzel, V. Ehrhardt, M. R. Heinrich, *Angew. Chem. Int. Ed.* **2008**, 47, 9130–9133
- A. Wetzel, V. Ehrhardt, M. R. Heinrich, *Angew. Chem. Int. Ed.* **2008**, 47, 9130–9133
- 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 in Food Chemistry, 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 bio-

logical 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

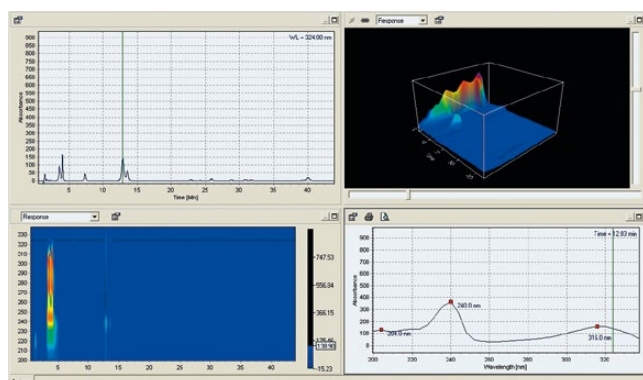


the influence of coffee on the gut health, *activity guided fractionation* led to the identification of hydrogen peroxide as the cytotoxic component of roasted coffee. Using a *synthesized substructure library* as an alternative approach, aminoreductones were identified as major immunomodulating compounds 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 allowed the systematic mapping of non enzymatic posttranslational modifications (nePTMs) in the milk proteome. Furthermore, non-targeted proteome analysis opened an insight into the low molecular weight peptidome of milk leading to the identification of novel bioactive peptides.

Another scientific focus of the work group is the interaction between food components and neurofunction, which is studied in the interdisciplinary Emerging Field Project “Neurotrition”. In cooperation between food chemists and neuroscientists, it was demonstrated for example by magnetic resonance imaging, how snack food modulates brain activity pattern leading to changes in food intake.

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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- T. Hoch, S. Kreitz, S. Gaffling, M. Pischetsrieder, A. Hess, *PLoS ONE* **2013**, 2, 55354
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- A. Wühr, M. Deckert, M. Pischetsrieder, *Mol. Nutr. Food Res.* **2010**, 54, 1021–1030
- J. Hegele, G. Münch, M. Pischetsrieder, *Mol. Nutr. Food Res.* **2009**, 53, 760–769

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- M. Pischetsrieder, R. Bärlein, Proteome research in food science, *Chem. Soc. Rev.* **2009**, 38, 2600–2608
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- T. Kislinger, A. Humený, 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



PROFESSOR OF AROMA RESEARCH

PROF. DR. ANDREA BÜTTNER

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CURRICULUM VITAE

- Since 2012** University Professor of Aroma Research at the University of Erlangen-Nürnberg, Germany
- Since 2007** Head of Department of Sensory Analytics, Fraunhofer Institute for Process Engineering and Packaging IVV, Freising, Germany
- 2007 – 2012** Assistant Professor and Head of a BMBF Junior Research Group at the University of Erlangen-Nürnberg, Germany
- 2006** Habilitation at Technical University of Munich (TUM), Germany
- 2002 – 2006** Internship for Excellent Junior Researchers (HWP II) at the Technical University of Munich (TUM), Germany and of the German Research Community at the German Research Center for Food Chemistry (DFA), Garching, Germany
- 1999 – 2002** Postdoctoral Fellow at DFA, Garching, Germany and the Institute for Food Chemistry, TUM, Germany
- 1999** PhD in Food Chemistry, Technische Universität München (TUM), Germany

OBJECTIVES

The Büttner research group undertakes to investigate topics relating to the analysis and characterisation of aromas and smells, as well as non-odorous volatiles encountered in everyday life. Identification of novel substances and a characterisation of their smell properties based on structure-odour activity considerations are key aspects of this work. Novel smells are created and strategies are developed for the avoidance of unwanted smells based on a combined chemo-analytical and human-sensory decoding of the underlying substances. We elucidate the formation and liberation pathways of odorants and develop techniques for controlling such processes, both in foods as well as non-food materials.

Our odour research encompasses the entire chemo-analytical side of odorant characterisation using experimental tools such as high resolution two-dimensional gas chromatography-mass spectrometry coupled to olfactometry (HR-2D-GC-MS/O), online mass spectrometric gas phase analysis, e.g., in breath aroma monitoring, and stable-isotope dilution assays (SIDA) analysis for quantification of trace odour compounds; furthermore, we endeavour to monitor, characterise, and positively influence the human responses to odour exposure/perception, both on a physiological and/or psychological-behavioural basis.

Consequently, our studies are focussed on investigating the underlying processes in human odorant perception and how these are rated, with an aim to broaden our understanding of behavioural res-

ponses that are associated with acceptance, preference or rejection of smells or smell-associated materials and situations.

SCIENTIFIC BACKGROUND

Odour exposure, for instance in food aromas or material or environmental emissions, is one facet of the diverse sensory factors that may strongly impact humans during their everyday life, albeit often being perceived quite unconsciously, which has led to the sensation of smell to be widely rated as being of comparatively lower relevance than other sensations, e.g., sound or vision.

On the other hand, smells play a crucial role in shaping our lives. From birth we learn to interact with our environment using our sense of smell. Evolutionary processes have engendered a multi-faceted communication that is supported—even dominated—by olfaction.

Today, humans are increasingly exposed to smells that were not encountered by our ancestors. These are ubiquitous in our present-day environment and are met in all aspects of daily life, with sources ranging from manmade materials, industry, cars, household products, etc.; the list is practically endless. Surprisingly, odorous molecules responsible for modern smells are often unknown, as is their influence on perception, physiology and wellbeing. This is especially true for smells that are encountered in everyday living and working situations. In particular, humans are exposed to a whole host of smells, e.g., whilst commuting, during periods at work or school, or when conducting other physical activities, all commonly in indoor environments.

RESEARCH HIGHLIGHTS

A comprehensive treatment of modern smells and their impact on human life currently does not exist. The two research groups of Prof. Büttner at University of Erlangen and Fraunhofer IVV align the senso-chemo-analytical characterisation of everyday smells encountered by mankind with the elucidation of perceptual, hedonic, behavioural and physiological responses of humans to such odours at different stages of life.

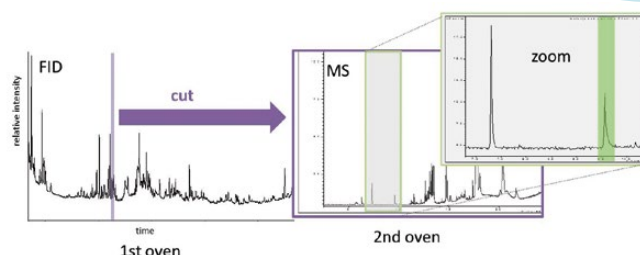
In view of this, our groups investigate physiological and psychological effects of odorants on humans, specifically in relation to foods but also non-food materials such as polymers and plastic materials and other materials that humans encounter in every-day life. Some of our recent studies have dealt with the characterisation of odorants by sensory and chemo-analytical techniques such as HR-GC-MS/O and SIDA. Thereby, we have reported for the first time on specific extremely potent odorants that could be identified as sources of common odour nuisances in daily life. Structure-odour activity relationship studies have targeted diverse substance groups such as alkylated, halogenated and methoxylated phenols, homologous enones and dienones as well as their corresponding alcohols, to name but a few. Characterisation of uptake and metabolism processes within the human body has been achieved in vivo as well as in vitro studies, and is the basis for investigating other physiological effects of odorants in vivo and in vitro such as the activation of brain receptor systems involved in sedative and anxiolytic processes.

Moreover, the immediate as well as the post-oral or post-inhalation human-physiological and behavioural responses to odorants are

monitored, for example, by biofeedback parameters such as electroencephalography (EEG), heart rate, breathing patterns, as well as mimic analysis. Unconscious processing and response of humans to odorant exposure is thereby another important topic of our joint research groups, as is the individual odour rating based on inter-individual differences in olfactory skills and personal experience.

PERSPECTIVES

- Characterisation of odorants relevant to human food, non-food materials and the environment
- Resorption, transfer and metabolism processes of odorants in humans
- Physiological and psychological/behavioural responses of humans from odorant exposure

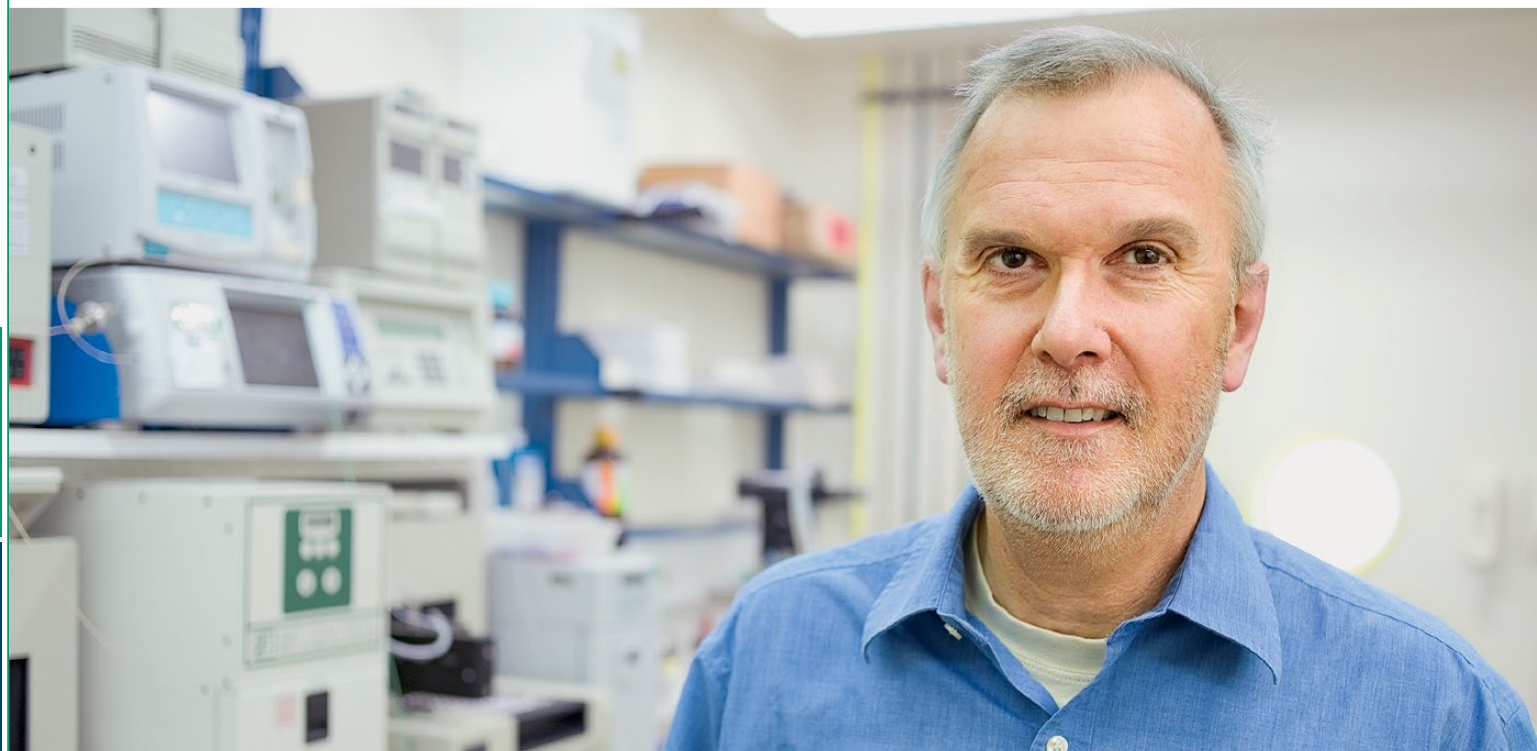


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- M. Wagenstaller, A. Buettner, *Metabolites* **2013**, 3, 637–657
- C. Hartmann, A. Triller, M. Spehr, R. Ditttrich, H. Hatt, A. Buettner, *ChemplusChem* **2013**, 78, 695–702
- F. Kirsch, K. Horst, W. Röhrig, M. Rychlik, A. Buettner, *Metabolomics* **2013**, 9, 483–496
- A. Kessler, C. Villmann, H. Sahin, M. Pischetsrieder, A. Buettner, *Flavour Fragr. J.* **2012**, 27, 297–303
- M. Czerny, R. Brueckner, E. Kirchhoff, R. Schmitt, A. Buettner, *Chem. Senses* **2011**, 36, 539–553
- A. Buettner, A. Beer, C. Hannig, M. Settles, *Chem. Senses* **2001**, 26, 1211–1219

SELECTED AWARDS

- 2013 Nutricia Wissenschaftspreis
- 2012 Danone Innovation Prize
- 2011 Young Investigator Award Food and Agricultural Division, American Chemical Society (ACS)
- 2010 Kurt-Tüffel Award for Young Scientists, Society of Food Chemistry (LChG), German Chemical Society (GDCh)
- 2004 Firmenich Flavor and Fragrance Science Award
- 1999 Weurman Flavour Best Poster-Award



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 Technology 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 pharmaceuticals 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 pharmaceuticals—I worked on the colloidal stability of emulsions supervised by Tharwat Tadros in London. It was in Los Angeles where 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 to include a detailed study of how the barrier property of human skin is related to its morphology at the cellular and molecular levels. After moving to Erlangen I developed a further major research area in the process engineering of proteins for use in drug products. The major thrust is to detail the damaging effects of operational processes on the molecular structure of proteins. The operations are those involved in the processes of spray-drying and freeze-drying and include atomization, droplet drying and particle formation and particle collection. In the past couple of years a further research interest has developed out of contact to Biomedical Engineering in Oxford. This is the design and preparation of nanoparticulate structures that show inertial cavitation in a low-energy ultrasonic field. The use of nanoparticles as drug delivery

$x = 0$	$x = a$	$x = b$	$x = c$
$C_d(x, t)$	$C_m(x, t)$	$C_m(x, t)$	$C_m(x, t)$
D_1	D_2	D_1	D_1
$D_1 \frac{\partial^2 C_d(x, t)}{\partial x^2} - \frac{\partial C_d(x, t)}{\partial t} = 0; t > 0$	$D_2 \frac{\partial^2 C_m(x, t)}{\partial x^2} - \frac{\partial C_m(x, t)}{\partial t} = 0; t > 0$	$D_1 \frac{\partial^2 C_m(x, t)}{\partial x^2} - \frac{\partial C_m(x, t)}{\partial t} = 0; t > 0$	$D_1 \frac{\partial^2 C_m(x, t)}{\partial x^2} - \frac{\partial C_m(x, t)}{\partial t} = 0; t > 0$
$\frac{\partial C_d(a, t)}{\partial x} = 0; t > 0$	$D_1 \frac{\partial C_d(a, t)}{\partial x} = D_2 \frac{\partial C_m(a, t)}{\partial x}; t > 0$	$D_2 \frac{\partial C_m(b, t)}{\partial x} = D_1 \frac{\partial C_m(b, t)}{\partial x}; t > 0$	$\frac{\partial C_m(c, t)}{\partial x} = 0; t > 0$
$C_d(a, t) = K C_m(a, t)$	$C_m(b, t) = K C_m(b, t)$		
$C_d(x, 0) = C_{d1}$	$C_m(x, 0) = 0$ $C_m(x, t) \leq C_{d2}$	$C_m(x, 0) = 0$ $C_m(x, t) \leq C_{d1}$	

systems has become a big issue in pharmaceuticals research; the design of sonosensitive polymeric or inorganic nanoparticles is novel and promising, but highly challenging.

RESEARCH HIGHLIGHTS

I manage three research groups.

1. **Biologic Particles:** microparticles containing biological molecules such as proteins or diagnostic reagents are designed, manufactured and characterized. The production processes are spray-drying, spray freeze-drying and cryopelletization with which we have extensive expertise. For each biomolecule a suitable formulation is developed and processing conditions identified but produce microparticles having the required properties. Of strong interest (also for industry) is the use of spray-drying to produce flowable, storage-stable protein particles as an alternative to freeze-drying of bulk. The particle formation process and the kinetic changes occurring to a protein—unfolding, aggregation, inactivation—are researched using single droplet acoustic levitation. The second current interest is the use of cryopelletization to produce large microparticles ($> 1000 \mu\text{m}$ in diameter) as carriers for diagnostic agents.

2. **Thin Films & Membranes:** this means transdermal drug delivery. The thin films aspect involves research into thin self-adhesive polymeric films whose drug release rate is controlled by the saturation solubility of the drug within the polymer. By reducing saturation solubility in the polymer, the drug release and permeation rate through an adjacent skin membrane can be enhanced. This has great potential applications to allow reduced drug loading of such transdermal films. The preparation of ultrathin polymer films ($< 20 \mu\text{m}$) is a particular challenge and is required to allow measurement of saturation solubility without supersaturation. A major research effort is the design of a fully-synthetic membrane which can simulate the barrier property of human stratum corneum (SC). This membrane must have a high tortuosity of up to 1000 to simulate the effects of the internal morphology of the SC on macroscopic diffusion rate. Our membranes are prepared from ceramic colloidal dispersions that are freeze-dried in such a way that directional freezing occurs to produce and long chimney-like pores. Once cross-linked and filled with lipid this directional pore structure should achieve our goal.

3. **Nanostructures:** polymeric and inorganic highly-rugged nanoparticles have the potential for inertial cavitation when treated with an ultrasonic pressure wave. The challenge is to produce stealth-type nanoparticles of the correct size (around 100 nm) that have the correct surface morphology for gas entrapment. Two morphologies are



being attempted: the 'Grand Canyon' model based on brittle fracture; and the 'hub cap' model based on microcollapse of a highly porous particle. Both are being developed using freeze-drying technologies. This whole research area runs in cooperation with Biomedical Engineering in Oxford.

PERSPECTIVES

The biologic particles group will become more centered on the acoustic levitator to examine the kinetics of drying and particle formation. This has many potential applications, not only in the field of pharmaceuticals but also in other areas as adhesives technology. Thin films and membranes group will concentrate on developing the fully synthetic surrogate for human SC based on high membrane tortuosity. The nanostructures group is still in its infancy, but has potential to become a major research thrust.

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- S. Reismann, W. Bansch, G. Lee, *Pharm. Devel. Technol.* **2014**, 19, 634–640
- S. Wiedemann, S. Fey, P. Grail, G. Lee, *Proc 19th World Meet Pharm Tech Pharm Biopharm, Lisbon* **2014**, 340
- A. Grebner, C. Coussios, G. Lee, *Proc 12th World Meet Pharm Tech Pharm Biopharm, Lisbon* **2014**, 500
- E. Lorenzen, G. Lee, *J. Pharm. Sci.* **2013**, 102, 4268–4273



PROFESSOR OF MOLECULAR AND CLINICAL PHARMACY

PROF. DR. KRISTINA FRIEDLAND

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CURRICULUM VITAE

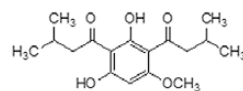
- Since 2011** University Professor of Molecular and Clinical Pharmacy at the University of Erlangen-Nürnberg, Germany
- 2001 – 2005** Postdoctoral Fellow (Goethe-University, Frankfurt, Germany with W.E. Müller and University of Alabama in Birmingham/USA with Lucas Pozzo-Miller)
- 2001 – 2005** PhD thesis, Institute of Pharmacology, Goethe-University Frankfurt Germany
- 2000 – 2001** Placement student at a pharmacy and at Knoll GmbH, Ludwigshafen, Germany
- 1995 – 2000** Studies in Pharmacy at the Free University of Berlin, Germany

OBJECTIVES

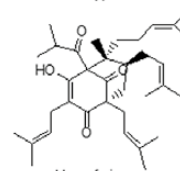
The research group of Prof. Kristina Friedland aims to better understand the pathophysiology of psychiatric diseases, to identify and design new compounds for the treatment of these diseases and to improve the pharmacological treatment of patients in the clinics. This approach closes the gap between bench to bedside. Her research activities follow an interdisciplinary approach with local, national as well as international cooperations with colleagues in pharmacy, food chemistry, biochemistry, medicinal chemistry and medicine, which are documented in collaborative research projects and publications. Special emphasis lays, also, on the education of undergraduate students, on lectures, problem based learning and bed-side-teaching.

SCIENTIFIC BACKGROUND

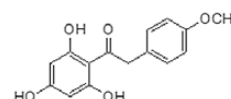
Prof. Kristina Friedland studied Pharmacy at the Free University of Berlin. She received her PhD at the Institute of Pharmacology for natural scientists at the Goethe-University in Frankfurt in 2005, where she worked on the identification of the molecular target of the plant derived antidepressant active compound Hyperforin isolated from St. John's wort extract. During her postdoctoral stay at the Goethe-University and the University of Alabama in the USA, Prof. Friedland got further interested in the neurobiological causes of psychiatric diseases and clinical questions of drug therapy in psychiatric patients such as drug-drug interactions, clinical relevant side effects and causes for patients non-compliance to drug treatment. In 2011, Kristina Friedland was appointed as a Professor of Molecular and Clinical Pharmacy at the University of Erlangen-Nürnberg. In the



Hyp4



Hyperforin



Hyp6



same year, she became a member of the board of the Interdisciplinary Center for Neuroscience at the University of Erlangen-Nürnberg. In 2012, she was elected as the chairperson of the Clinical Pharmacy Section of the German Pharmaceutical Society, she is also a member of the scientific advisory board of the Institute for Prevention (WIPIG), the Bavarian Academy for Clinical Pharmacy and board member of the Lesmüller Stiftung. In Erlangen, she started her research group, which consists on one hand of PhD students dealing with molecular topics in the laboratory but also on the other hand of PhD students and pharmacists, which work with patients in the psychiatric clinic of the University Hospital in Erlangen. Preclinical and clinical research dealing with psychiatric disorders such as depression, schizophrenia or dementia are hampered by several pitfalls. The pathophysiology of these diseases is still not finally understood and the pharmacological treatment is restricted by limited clinical efficacy and drug related problems such as side effects or drug-drug interactions, which hamper patients' compliance. Regarding these problems, we are focusing on ion channels as novel targets for mood disorders and on the role of mitochondrial dysfunction for the pathology of neurodegenerative diseases. In addition, we investigate if intensive pharmaceutical care regarding drug therapy improves patients' compliance.

RESEARCH HIGHLIGHTS AND PERSPECTIVES

Depression is a widespread illness characterized by low mood, pleasure, motivation and reward. The treatment of major depressive disorders is confounded by high rates of treatment resistance and low rates of lasting remission. These clinical realities, paired with the high economic burden of treating depression necessitate a better understanding of the pathophysiology of depression and the development of alternative therapeutic approaches to treating this disease. Current treatment strategies are based primarily on the monoamine hypothesis of depression. Recent work, however, suggests that the neuropathology of depression is stratified across the reduction of synaptic plasticity. Evidence suggests that the canonical transient receptor potential channel 6 (TRPC6) regulates synaptic plasticity, most likely via the influx of calcium and zinc ions. TRPC6 channels are the molecular target of hyperforin, the active antidepressant constituent of St. John's wort extracts, which have been used since Paracelsus to treat mild to moderate depression. Hyperforin is chemically unstable and is only modestly potent in TRPC6 channels. These qualities limit its use as a lead compound for a new class of antidepressants. Therefore, we focus on the identification of novel plant derived TRPC6 activators and on the synthesis and detailed pharmacological and behavioural characterization of new derivatives of hyperforin in the EFL project "Neurotrition" and the European

funded trinational project HYPZITRP. In addition, we try to understand the interplay of TRP channels and other ion channels with proteins such as G-protein coupled receptors, which are highly involved in the pathogenesis of depression and schizophrenia (GRK1910).

In clinical research, we just completed a clinical trial, where we could show that intensive pharmaceutical care comprising detailed patient information about the biological cause of their psychiatric disease as well as their drug treatment results in reduced drug related problems and strongly improves patients' compliance. We will continue this work and focus on improving psychiatric patients' compliance in the community pharmacy setting.

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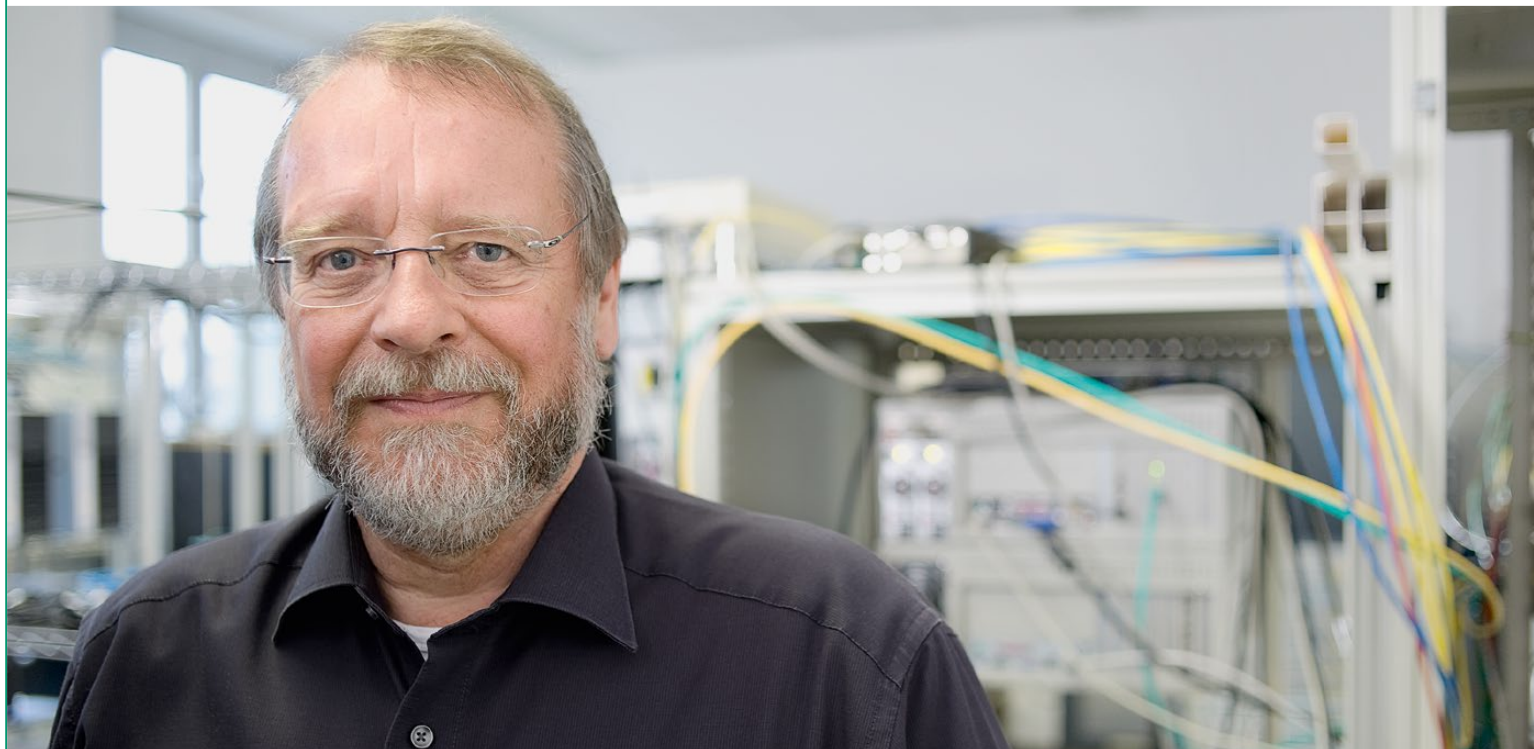
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- K. Leuner, J. Heiser, S. Derksen, M. I. Mladenov, C. J. Fehske, R. Schubert, M. Gollasch, G. Schneider, C. Harteneck, S. S. Chatterjee, W. E. Müller, *Mol. Pharmacol.* **2010**, 77(3), 368–377
- K. Leuner, V. Kazanski, M. Müller, K. Essin, B. Henke, M. Gollasch, C. Harteneck, W. E. Müller, *FASEB J.* **2007**, 21(14), 4101–4111

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- C. Harteneck, K. Leuner, TRP Channels in Neuronal and Glial Signal Transduction, *Neurochemistry, InTech* **2014**, DOI: 10.5772/58232
- K. Friedland-Leuner, C. Stockburger, I. Denzer, G. P. Eckert, W. E. Müller, Mitochondrial dysfunction—cause and consequence of Alzheimer disease, *Prog Mol Biol Transl Sci.* **2014**, 127, 183–210
- K. Leuner, W. E. Müller, A. S. Reichert, From mitochondrial dysfunction to amyloid beta formation: novel insights into the pathogenesis of Alzheimer's disease, *Mol Neurobiol.* **2012**, 46 (1), 186–193
- K. Leuner, S. Hauptmann, R. Abdel-Kader, I. Scherping, U. Keil, J. B. Strosznajder, A. Eckert, W. E. Müller, Mitochondrial dysfunction: the first domino in brain aging and Alzheimer's disease?, *Antioxid. Redox. Signal.* **2007**, 9(10), 1659–1675

SELECTED AWARDS

- 2009 AGNP research prize, psychopharmacology
- 2008 Phoenix Pharmazie research prize, best publication, pharmacology in 2007
- 2007 "Faculty of 1000 Biology", identification of a novel target for the treatment of depression



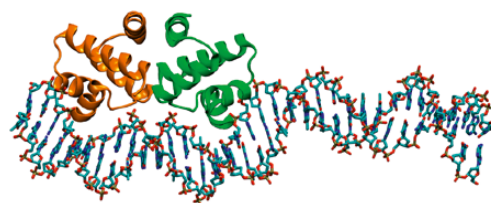
APL. PROFESSOR OF COMPUTATIONAL CHEMISTRY

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 structure, function and properties. A broad spectrum of theoretical techniques from classical force fields to high-level quantum mechanics is used for this purpose. Topics of special interest are peptide hormones and G-protein coupled receptors, simulating molecular electronic devices and the theory of non-covalent interactions. The methods developed are designed to bridge the gap between classical and quantum mechanical modeling techniques on the atomistic and mesoscales and to calculating the electronic properties of extremely large (100,000 atom) systems with semiempirical molecular orbital theory.

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 the-

ory 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. Traditionally, computational chemistry techniques have been used most in the life sciences but modeling new materials and molecular electronic devices is becoming more important. Our work on G-protein coupled receptors and their peptide-hormone ligands, for instance, has revealed new binding sites and modes of action and provided details of the conformations of peptide hormones such as vasopressin in solution. Simulating electronic devices not only allows us to support experimentalists in developing prototypes, but also leads to new understanding of the bonding in electroactive organic aggregates. Simulating self-assembled monolayer field-effect transistors, for instance, led to the discovery of a new type of interstitial electron trap between C₆₀ fullerenes. In order to be able to simulate the electronic properties of devices on the nanometer scale, we have developed a massively parallel semiempirical MO program that is capable of calculating 100,000 or more atoms. Finally, detailed high-level *ab initio* calculations first led to a complete understanding of halogen bonding as a subset of the more general σ -hole bonding and later revealed other directional non-covalent interactions such as anisotropic dispersion.

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, technical and biological questions. Experimentalists are increasingly working with molecules, particles and aggregates that 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. Modeling and simulation has been called the “third pillar of science” along-



side experiment and theory. Modern computer capabilities are now making direct comparisons between nanoscale experiments and simulations possible.

SELECTED PUBLICATIONS

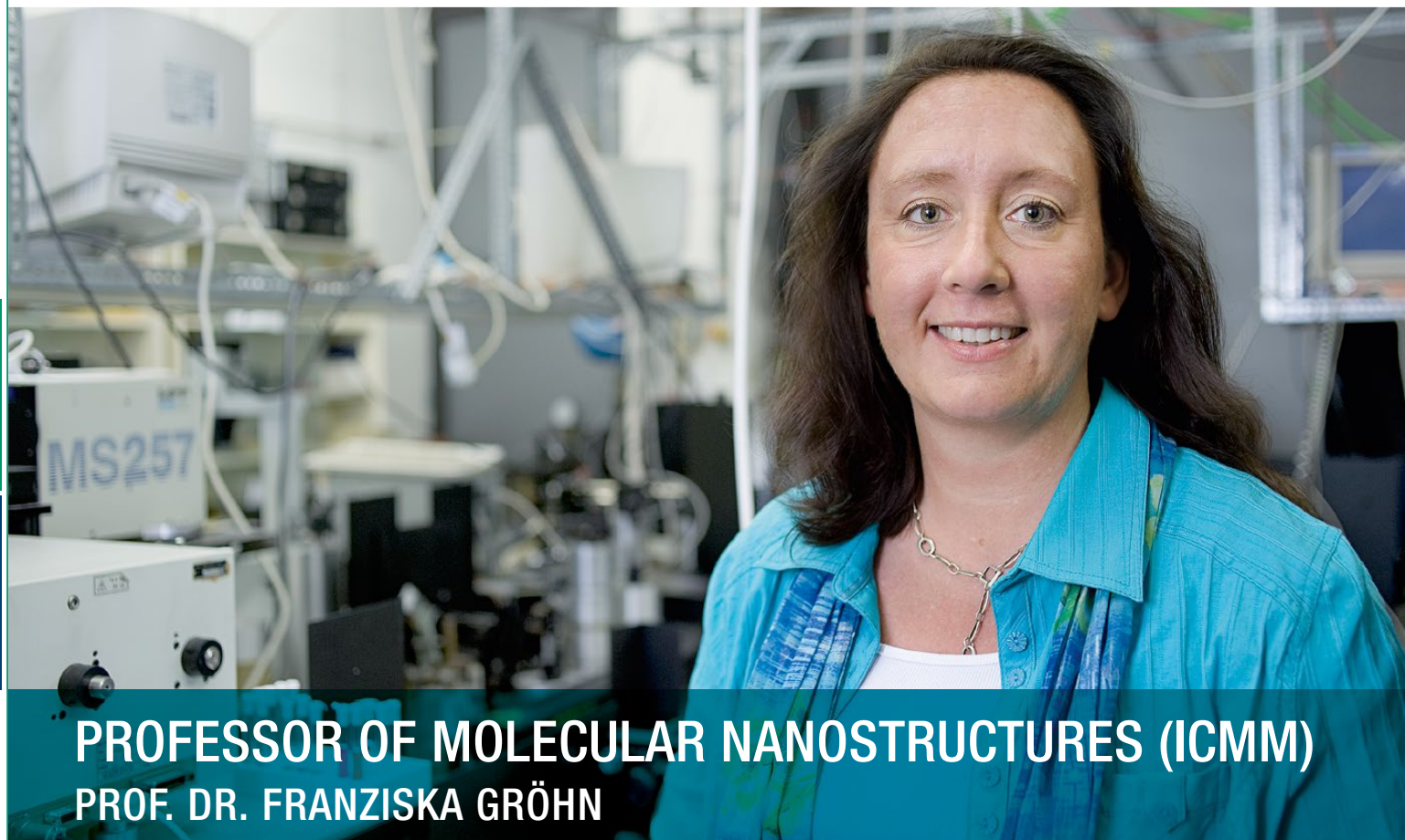
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- T. Clark, M. Halik, M. Hennemann, C. M. Jäger, Simulating “Soft” Electronic Devices, Molecular Engineering and Control (M. G. Hicks and C. Kettner, Eds), **2013**, 137–150
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- T. Clark, Predictive Modeling of Molecular properties: Can We Go Beyond Interpretation?, *Modeling of Molecular properties*, (P. Comba, Ed.), **2011**, 91–106
- T. Clark, J. J. P. Stewart, MNDO-like Semiempirical Molecular Orbital Theory and its Application to Large Systems, *Computational Methods for Large Systems* **2011**, Chapter 8
- P. Politzer, J. S. Murray, T. Clark, Halogen bonding: an electrostatically-driven highly directional noncovalent interaction, *Phys. Chem. Chem. Phys.* **2010**, 12, 7748–7757

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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CURRICULUM VITAE

- 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 and Institute of Physical Chemistry, University of Mainz, Germany
- 1998 – 2000** Postdoctoral fellow at National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA
- 1998** PhD from Max Planck Institute of Colloids and Interfaces 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 important functions in natural systems such as cell membranes or DNA-protein complexes consists of supramolecular nanoscale architectures. Therefore, great potential lies in synthetic nanostructure design through self-assembly. The prospect is a simple way to build complex architectures with tailored properties. Large advantage is the capability for rearrange-

ments, leading to responsive and switchable systems. Exciting potential lies in areas as solar energy conversion, smart materials or 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. This is one of the motivations to investigate the formation of synthetic hybrid structures, for example by polymer templating. The approach can also lead to various inorganic nanoparticles with special optical, electrical or magnetic properties.

With these inspirations in mind, 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 such as scattering and imaging techniques, spectroscopy and thermodynamic investigations, including instrumental developments.

RESEARCH HIGHLIGHTS

Recently we established a new concept for the formation of versatile supramolecular assemblies: electrostatic self-assembly of macroions and oppositely charged organic molecules. A variety of nanoscale architectures such as spheres, rods, networks, rings, and hollow spheres can be built. The approach is based on the interconnection of polyelectrolytes through structural multivalent counterions, combining different types of interactions and effects, e.g., ionic forces, π - π stacking and 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. Such pH responsive carriers are of interest in tumor research.

New self-assembled morphologies involving porphyrins bear potential as light harvesting systems. Ionic porphyrins can interconnect cylindrical polyelectrolyte brushes into finite networks of several hundred nanometer size which show significantly enhanced catalytic activity and a special selectivity in photocatalysis.

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 important natural polymers such as DNA and proteins 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 inorganic nanoparticles in dendrimer templates based on a purely hydrophilic precursor assembly in which for example a certain number of gold ions accumulate inside the ionic dendrimer template. The size of the resulting gold nanoparticle is controlled through the number of gold ions added per macroion. Thus, again electrostatic interaction invol-



ving polyelectrolytes represents an effective route for designing particles on the nanoscale.

PERSPECTIVES

With these concepts of electrostatic self-assembly we have opened routes to versatile nanostructures. In future, in particular the potential to build complex functional assemblies will be exploited. The advantage of this approach lies in its wide applicability without relying on specific binding motifs. Therefore, a variety of functional building blocks can be introduced to build novel composite nanoparticles with targeted properties. Future potential also lies in structures that respond to external triggers, in particular to light. Furthermore, electrostatic self-assembly is combined with the nanotemplating of metal and semiconductor nanoparticles to create functional organic-inorganic hybrid structures that can be used in catalysis, medicine or energy conversion. 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

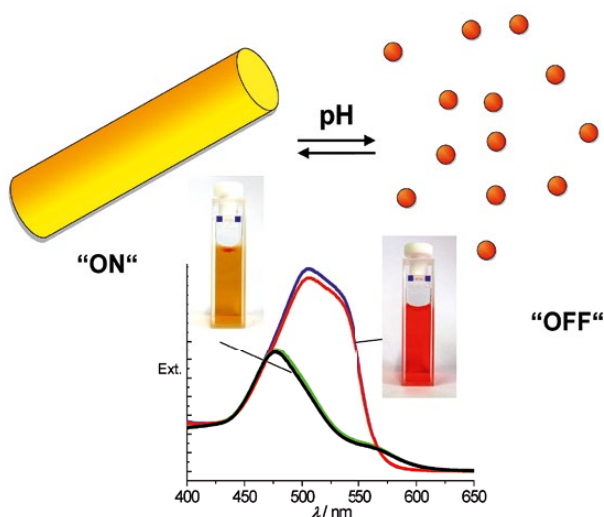
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- S. Frühbeißer, F. Gröhn, *J. Am. Chem. Soc.* **2012**, 134, 14276–14270
- G. Gröger, W. Meyer-Zaika, C. Böttcher, F. Gröhn, C. Ruthard, C. Schmuck, *J. Am. Chem. Soc.* **2011**, 133, 8961–8971
- I. Willerich, F. Gröhn, *J. Am. Chem. Soc.* **2011**, 133, 20341–20356
- I. Willerich, F. Gröhn, *Angew. Chem. Int. Ed.* **2010**, 49, 8104–8108
- 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**, 6, 4296–4302
- 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





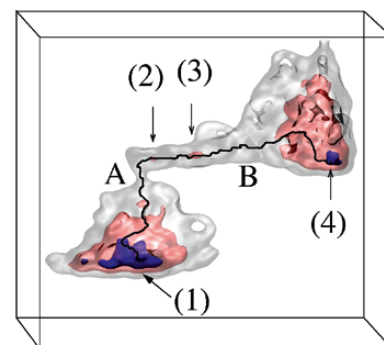
PROFESSOR OF COMPUTATIONAL CHEMISTRY (ICMM)

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 the physical and chemical properties of surfaces are modified by adsorbates. In particular, we focus on identifying relevant surface structures forming under reaction conditions, 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 nano-structures.

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, which both 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 electro-

nic 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 oxide surfaces, for example, in dye-sensitized solar cells or in molecular electronics.

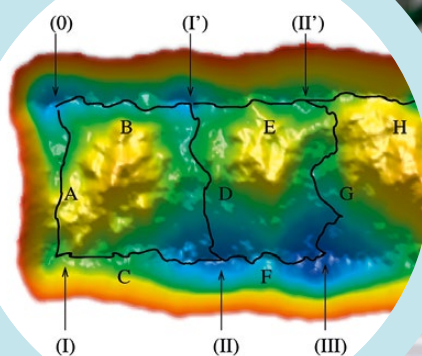
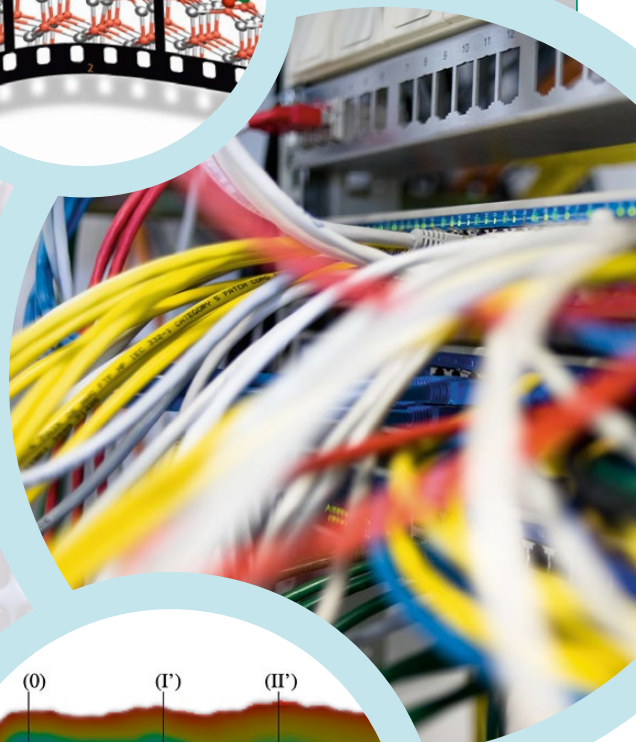
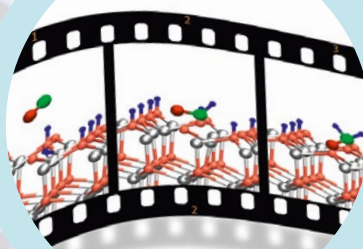
RESEARCH HIGHLIGHTS

A main research focus in the past years has been the study 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 H₂ and CO to methanol.

Further research projects comprise investigations of the structure and dynamical behavior of the first water layer in contact with oxide 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 a few hundred atoms due to the high computational cost. To be able to study larger systems we are currently developing a more approximate, semi-empirical method which is based on a parametrization of the electronic structure problem (density-functional-based tight-binding). This parametrization, however, will be derived without fitting 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.



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- J. Frenzel, J. Kiss, N. N. Nair, B. Meyer, D. Marx, Methanol Synthesis on ZnO from Molecular Dynamics, *Phys. Stat. Sol. B* **2013**, 250, 1174 – 1190



PHARMACEUTICS

PD DR. HENNING GIESELER

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CURRICULUM VITAE

Since 2011	Lecturer (PD), Pharmaceutical Sciences at the University of Erlangen-Nürnberg, Germany
Since 2010	CEO, GILYOS GmbH, Würzburg, Germany
2010	Habilitation in Pharmaceutical Sciences, University of Erlangen-Nürnberg (Prof. G. Lee), Germany
2006 – 2010	Postdoctoral Fellow, Pharmaceutical Sciences, University of Erlangen-Nürnberg (Prof. G. Lee), Germany Founder & Head of the "Freeze Drying Focus Group" (FDG)
2004 – 2006	Postdoctoral Fellow, School of Pharmacy, University of Connecticut (Prof. M. Pikal), Storrs, CT, USA
2001 – 2004	Graduate student, Pharmaceutical Sciences, University of Erlangen-Nürnberg (Prof. Lee), Germany
2000	Licensed Pharmacist, Germany
1995 – 1999	Undergraduate student, School of Pharmacy, University of Würzburg, Germany

RESEARCH HIGHLIGHTS

Our research targets many areas around freeze drying (lyophilisation) of pharmaceutical and biological products. Here, one of our key interests in the last years has been the development and evaluation of innovative Process Analytical Technology (PAT) tools to



gain improved freeze drying process understanding. Based on more refined tools to monitor the drying behaviour of the product, optimized processes with shorter process times are possible (positive process economics) while maintaining or even improving the final product quality attributes. In this regard, Quality by Design (QbD) has grown more attention to regulatory authorities to erase trial-and-error approaches during formulation and process development in industry. The group has already presented a profound QbD concept for process design of freeze dried products, combining both analytical, formulation and process related aspects.

Besides PAT in freeze drying, the groups major achievements could be derived in the field of physicochemical characterization of materials by Freeze Dry Microscopy (FDM) and Modulated DSC (MDSC), freeze drying from atypical container systems (syringes, tubes, capillary systems, PCR plates, etc), formulation development of partially crystalline systems, formulation and process development for oral disintegrating tablets (ODT), and scale-up principles. Since 2006, the Freeze Drying Focus Group has also established an annual freeze drying seminar, entitled "ERLANGEN Seminar" which is well recognized in the pharmaceutical industry, even beyond German borders.

FUTURE PERSPECTIVE

Our ongoing research subjects may be outlined as follows:

- Freeze drying from new organic co-solvent systems.
- Development of a scale-up road map for freeze dried products, thereby combining integral freeze dryer platform design criteria and formulation related attributes; development of a software model.
- The "ideal" placebo for freeze dried products to save development costs (expensive API) and maximize occupational safety (high potency API).
- Controlled nucleation in freeze drying.

SELECTED PUBLICATIONS

- U. Stange, C. Führling, H. Gieseler, *Pharm. Dev. Technol.* **2014**, 19, 137–147
- H. Gieseler, Encyclopedia of Pharmaceutical Science and Technology, Fourth Edition, J. Swarbrick, Ed. *Informa Healthcare* **2013**, 2903–2917
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- S. Hibler, C. Wagner, H. Gieseler, *J. Pharm. Sci.* **2012**, 101, 1189–1201

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- H. Gieseler, P. Stärtzel, *Eur. Pharm. Rev.* **2012**, 17, 63–68
- S. Hibler, H. Gieseler, *J. Pharm. Sci.* **2012**, 101, 4025–4031



THEORETICAL CHEMISTRY

PD DR. ANDREAS HESSELMANN

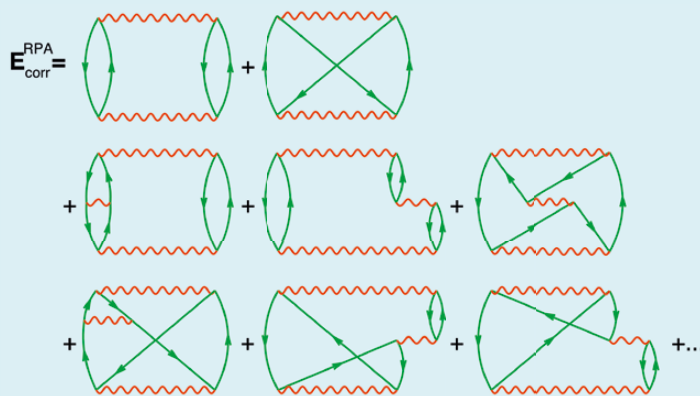
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CURRICULUM VITAE

Since 2012	Lecturer (PD) at the University of Erlangen-Nürnberg, Germany
2012	Habilitation in Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Görling), Germany
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

RESEARCH HIGHLIGHTS

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.



Density-functional theory methods are also employed to describe intramolecular correlation effects in the framework of the intermolecular Symmetry-Adapted Perturbation Theory (SAPT). This method, termed DFT-SAPT, enables a decomposition of intermolecular interaction energies into distinct physically interpretable terms like electrostatics, induction, dispersion and exchange repulsion types of interaction. In this way, in contrast to the commonly used supermolecular methods that are used to describe intermolecular interactions with quantum chemistry methods, the intermolecular perturbation theory also allows a characterisation and deeper understanding of the bonding in intermolecular complexes.

FUTURE PERSPECTIVE

Current time-dependent Kohn-Sham (KS) density functional (TDDFT) response methods still are not capable to accurately describe charge-transfer excitations or polarisabilities of long conjugated chain molecules. While these problems can e.g., be solved by using generalised KS methods employing a nonlocal (range-separated) exchange potential/kernel, often these methods are not feasible anymore for larger systems. We therefore seek for a new TDDFT method which both can describe nonlocal excitations (including charge-transfer excitations) as well as local excitations with the same accuracy.

SELECTED PUBLICATIONS

- A. Heßelmann, T. Korona, *J. Chem. Phys.* **2014**, 141, 094107
- A. Heßelmann, A. Görling, *Mol. Phys.* **2010**, 108, 359–372
- A. Heßelmann, *J. Chem. Theory Comput.* **2013**, 9, 273–283
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- 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

SELECTED REVIEWS

- A. Heßelmann, A. Görling, Random-phase approximation correlation methods for molecules and solids, *Mol. Phys.* **2011**, 109, 2473–2500

SELECTED AWARDS

- 2004 Gottschalk-Diederich-Baedeker Award



THEORETICAL CHEMISTRY

PD DR. WOLFGANG HIERINGER

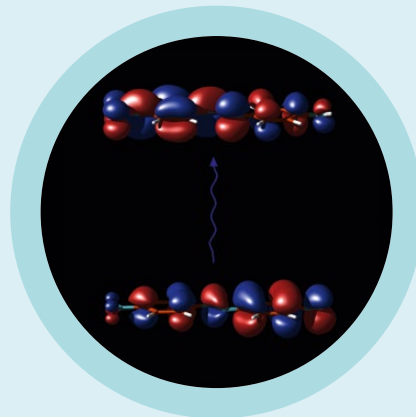
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CURRICULUM VITAE

Since 2010	Lecturer (PD), Theoretical Chemistry at the University of Erlangen-Nürnberg, Germany
2010	Habilitation in Theoretical Chemistry, University of Erlangen-Nürnberg (Prof. Görling), Germany
2004 – 2010	Habilitation, 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 quantum chemical methods, in particular density functional theory, to theoretically study complex problems in catalysis, surface science, and photophysics, with a special focus on systems containing transition metals. Recent examples deal with



the theoretical investigation of large metalloporphyrin molecules at surfaces, surface-bound organometallic coordination polymers, or organic nanotracks. We have been able to identify, for the first time, the surface analogue of the so-called *trans* effect, which has been known before only in the field coordination chemistry. We have elucidated the mechanism of the homogeneous ruthenium-catalyzed water-gas shift reaction, and contributed to the characterization of one of the very first U(II) complexes known to date using relativistic density functional methods. We also work on spectroscopic techniques such as nonlinear optics and core-level spectroscopy. Recently, we have developed new density-functional methods to both accurately and efficiently describe excitations of core-electrons in large molecules, followed by successful applications in surface science. Many of our projects involve strong collaborations with experimentally working groups of various disciplines.

FUTURE PERSPECTIVE

Our goal is to design novel functional transition metal systems with unprecedented catalytic, electronic, or optical properties using modern theoretical methods. To this end, we mainly use accurate quantum chemical methods, but we will also combine them with more efficient force-field techniques to treat environmental effects. We will furthermore continue to develop computer programs which provide the necessary functionality to achieve our goals.

SELECTED PUBLICATIONS

- S. La Pierre, A. Scheurer, F. W. Heinemann, W. Hieringer, K. Meyer, *Angew. Chem. Int. Ed.* **2014**, 53, 7158–7162
- S. Ditzel, M. Stark, F. Buchner, A. Aichert, N. Jux, N. Luckas, A. Görling, W. Hieringer, J. Hornecker, H.-P. Steinrück, H. Marbach, *J. Am. Chem. Soc.* **2014**, 136, 1609–1616
- H. Schulz, A. Görling, W. Hieringer, *Inorg. Chem.* **2013**, 52, 4786–4794
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- W. Hieringer, K. Flechtner, A. Kretschmann, K. Seufert, W. Auwärter, J. V. Barth, A. Görling, H.-P. Steinrück, J. M. Gottfried, *J. Am. Chem. Soc.* **2011**, 133, 6206–6222

SELECTED AWARDS

- 2011 Starting Grant of the Cluster of Excellence “Engineering of Advanced Materials”
- 2003 Marie Curie Reintegration Grant of the European Commission
- 2000 Marie Curie Individual Fellowship of the European Commission



MEDICINAL CHEMISTRY

PD DR. HARALD LANIG

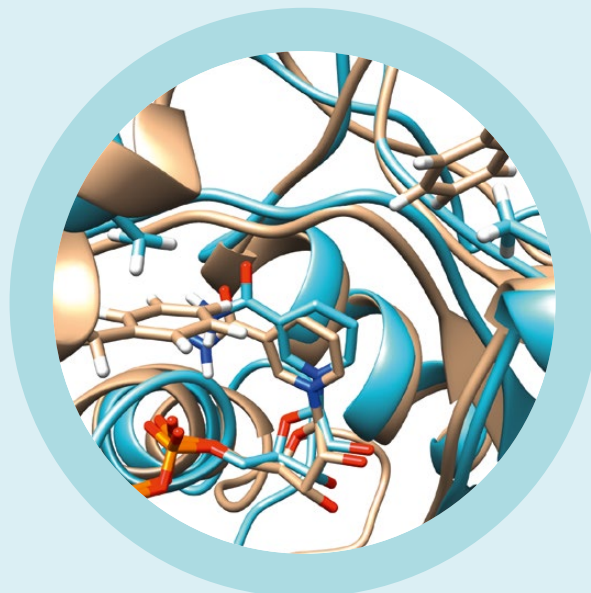
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CURRICULUM VITAE

- Since 2012** Lecturer (PD) at the University of Erlangen-Nürnberg, Germany
- 2012** Habilitation in Medicinal Chemistry, University of Erlangen-Nürnberg (Prof. Gmeiner), Germany
- 2005 – 2012** 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

RESEARCH HIGHLIGHTS

My general interest focuses on the exploration of structure and dynamics of proteins and DNA with classical simulation methods. I am applying Molecular Dynamics, Homology Modeling and Molecular Docking techniques to understand how chemical signals are processed, transduced, and converted into protein structural changes. In recent examples, the activation of G-Protein Coupled Receptors, Tetracycline Repressor variants, Collagen type II model systems,



enzymes like the Prolyl Hydroxylase PHD2 and Interleukin Receptor complexes have been investigated by modelling and simulation techniques.

FUTURE PERSPECTIVE

Based on my experience in modelling and simulation of protein structures, I am currently focusing on proteins which are able to interact with oligonucleotides (transcription factors) to understand how the interaction with DNA changes its principal properties. In another project, I am developing a structural model for Fibulin-4, a large calcium binding glycoprotein that has an important role in development and integrity of extracellular matrices and already a single mutation may cause severe diseases. In all current and future projects, I am emphasizing the collaboration with experimentalists for a successful synergy with theory in an iterative way.

SELECTED PUBLICATIONS

- R. C. Kling, N. Tschammer, H. Lanig, T. Clark, P. Gmeiner, *PLoS One* **2014**, 9, e100069
- C. R. Wick, H. Lanig, C. M. Jäger, N. Burzlaff, T. Clark, *Eur. J. Inorg. Chem.* **2012**, 4973–4985
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- U. Böiers, H. Lanig, B. Sehnert, R. Holmdahl, H. Burkhardt, *Eur. J. Immunol.* **2008**, 38, 2784–2795
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- 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

SELECTED AWARDS

- Members of the German Pharmaceutical Society and the Royal Society of Chemistry
- Chairman of the Molecular Graphics and Modelling Society—German Section
- Grant from the Bavarian Ministry of Science and Research
- Grants from Federal Ministry of Education and Research and Fonds der Chemischen Industrie



PHYSICAL CHEMISTRY

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CURRICULUM VITAE

- 2014 – 2015** Temporary Professorship (W3), interim holder of chair for Experimental Physics, University of Erlangen-Nürnberg, Germany
- Since 2010** Lecturer (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 nanoscaled struc-

tures. 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 particular we systematically explored temperature dependent processes which allow for determining the energetics of the corresponding molecular processes close to room temperature (e.g., diffusion, metalation reaction, conformational switching). 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 of the controlled conformational switching of individual porphyrin molecules close to room temperature

SELECTED PUBLICATIONS

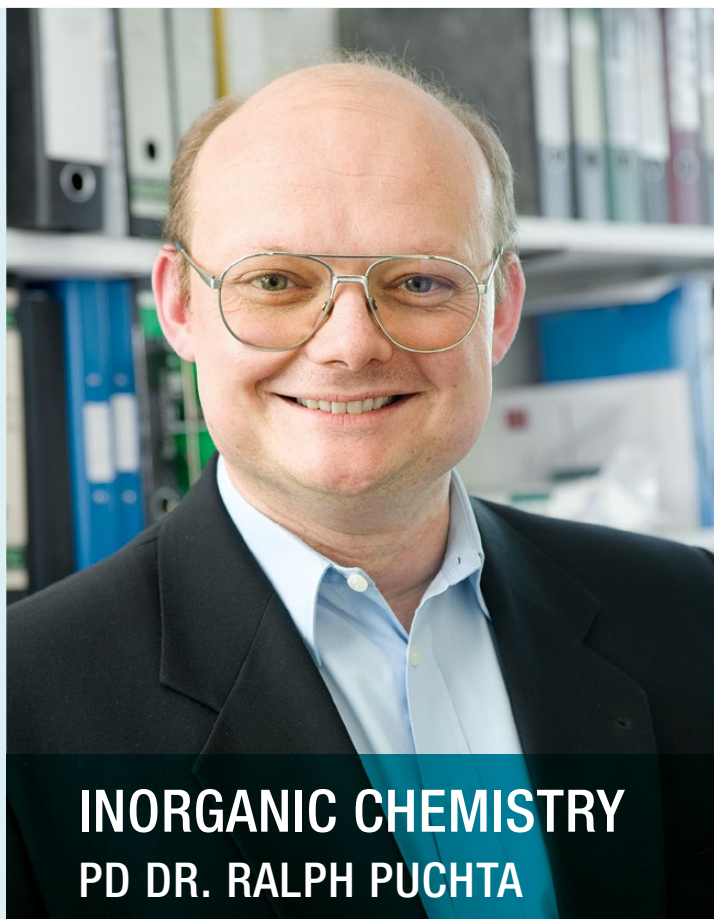
- S. Ditze, M. Stark, F. Buchner, A. Aichert, N. Jux, N. Luckas, A. Görling, W. Hieringer, J. Horneberger, H.-P. Steinrück, H. Marbach, *J. Am. Chem. Soc.* **2014**, 136, 1609–1616
- M. Stark, S. Ditze, M. Lepper, L. Zhang, H. Schlott, F. Buchner, M. Röckert, M. Chen, O. Lytken, H.-P. Steinrück, H. Marbach, *Chem. Commun.* **2014**, 50, 10225–10228
- S. Ditze, M. Stark, M. Drost, F. Buchner, H.-P. Steinrück, H. Marbach, *Angew. Chem., Int. Ed.* **2012**, 51, 10898–10901
- 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

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



INORGANIC CHEMISTRY

PD DR. RALPH PUCHTA

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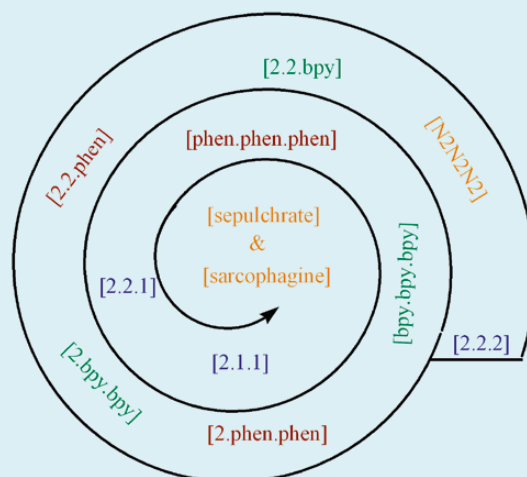
CURRICULUM VITAE

Since 2013	Lecturer (PD) at the University of Erlangen-Nürnberg, Germany
2013	Habilitation in Inorganic Chemistry, University of Erlangen-Nürnberg (Prof. van Eldik), Germany
2004 – 2013	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

RESEARCH HIGHLIGHTS

The fundamental idea of our research is the fruitful interplay of experimental and computational chemistry. Within this concept we inspect (inorganic) reaction mechanisms and (metallo) cryptate complexes.

We calculate model reactions to gain knowledge on the reactivity of metal ions. Therefore, we investigate tetrahedral coordinated Be(II) and Cu(I) complexes, while we utilize solvated Zn(II) and Al(III) complexes to study octahedral coordinated systems. These computations allow insights into explicit reactions and in parallel we gain new con-



ceptual ideas on their reactivity and possible reaction pathways.

The main aspect of our studies on (metallo)cryptate complexes is to learn more about their ion selectivity. This can be derived from tailor made model reactions, too.

FUTURE PERSPECTIVE

Our focus will be the transfer of the gained knowledge from model reactions to reactions with catalytic or bioinorganic background. Further studies of model reactions will parallel enlarge our treasure of fundamental knowledge.

The investigations on (metallo)cryptands and (metallo)cryptates lead to a clear prediction which host can select a specific ion and (hopefully) one day make Fritz Haber's dream of selective ion mining in sea (or waste water) come true under economic and ecologic conditions.

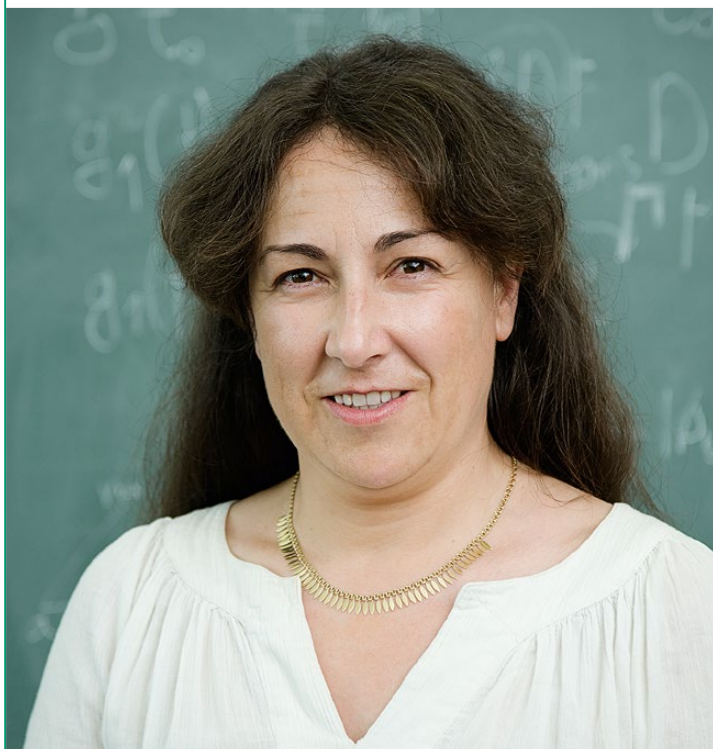
Whenever possible, we will continue our theoretical oriented studies in close cooperation with experimental scientists.

SELECTED PUBLICATIONS

- S. Begel, R. Puchta, R. van Eldik, *J. Mol. Model.* **2014**, 20, 2200
- B. M. Alzoubi, I. Weber, H. Hanauer, R. Puchta, R. van Eldik, *J. Mol. Model.* **2014**, 20, 2083
- B. M. Alzoubi, M. Walther, R. Puchta, R. van Eldik, *Eur. J. Inorg. Chem.* **2013**, 2059–2069
- S. Begel, R. Puchta, R. van Eldik, *Beilstein J. Org. Chem.* **2013**, 9, 1252–1268
- R. Puchta, B. M. Alzoubi, R. Meier, S. I. Almuhtaseb, M. Walther, R. van Eldik, *Dalton Trans.* **2012**, 41, 14151–14156
- B. M. Alzoubi, M. Walther, R. Puchta, R. van Eldik, *Dalton Trans.* **2012**, 41, 6932–6941
- M. Walther, R. Puchta, *RSC Adv.* **2012**, 2, 5815–5821
- A. Budimir, M. Walther, R. Puchta, R. van Eldik, *Anorg. Allg. Chem.* **2011**, 637, 515–522
- M. Walther, C. Dücker-Benfer, R. Puchta, *Anorg. Allg. Chem.* **2011**, 637, 1736–1740
- R. W. Saalfrank, H. Maid, A. Scheurer, R. Puchta, W. Bauer, *Eur. J. Inorg. Chem.* **2010**, 2903–2906

SELECTED REVIEWS

- R. Puchta, E. Pasgreta, R. van Eldik, *Adv. Inorg. Chem.* **2009**, 61, 523–571
- Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. von Ragué Schleyer, *Chem. Rev.* **2005**, 105, 3842–3888



THEORETICAL CHEMISTRY

PD DR. MARÍA BELÉN RUIZ RUIZ

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CURRICULUM VITAE

- Since 2010** Lecturer (PD), at the University of Erlangen-Nürnberg, Germany
- 2010** Habilitation in Theoretical Chemistry at the University of Erlangen-Nürnberg (Prof. Göring), Germany
- 2009** Visiting Professor at Autónoma 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

My research interests are the development of highly accurate quantum mechanical methods, and their applications to problems in Chemistry, Physics, Medicine and Technology. The method of Hylleraas-Configuration Interaction is a powerful predictive tool to

explain and stimulate new experiments. Using this method we can calculate very accurately the energy and various properties of the ground, low-lying excited states and weakly-bound Rydberg states of atoms and thus draw the computational spectrum of atoms and ions. Another theme of my research is the evaluation of molecular integrals over Slater orbitals. Slater orbitals are the natural basis of orbitals in quantum mechanical calculations, but their use is limited due to the difficulty to efficiently solve all integrals occurring in a molecular calculation. Therefore in the practice, Gaussian orbitals are used. However, research on integrals over Slater orbitals has continued in recent years, due to Slater orbitals are suitable for the physical description of the electronic interactions between the atoms.

FUTURE PERSPECTIVE

The wave functions of very good quality have many applications today. These applications include: (1) the study of the redistribution of the electronic density in beta-decay, bound-state beta-decay and electron capture processes; (2) the mechanism of collision processes including ionization, double ionization and electron attachment; (3) nuclear reactions such as the Boron Neutron Capture Therapy (BNCT), a promising anticancer therapy; (4) atoms and ions under confinement conditions, important in space research, quantum computers and the future of microelectronics; (5) Rydberg states under the presence of an electric field; (6) the optical spectra of Wolf-Rayet stars, the brightest objects of our universe. The addition of finite mass, isotopic shift, finite volume of the nucleus, relativistic corrections and lower order quantum electrodynamics, QED corrections, allow direct comparison of energy and properties with experimental data.

SELECTED PUBLICATIONS

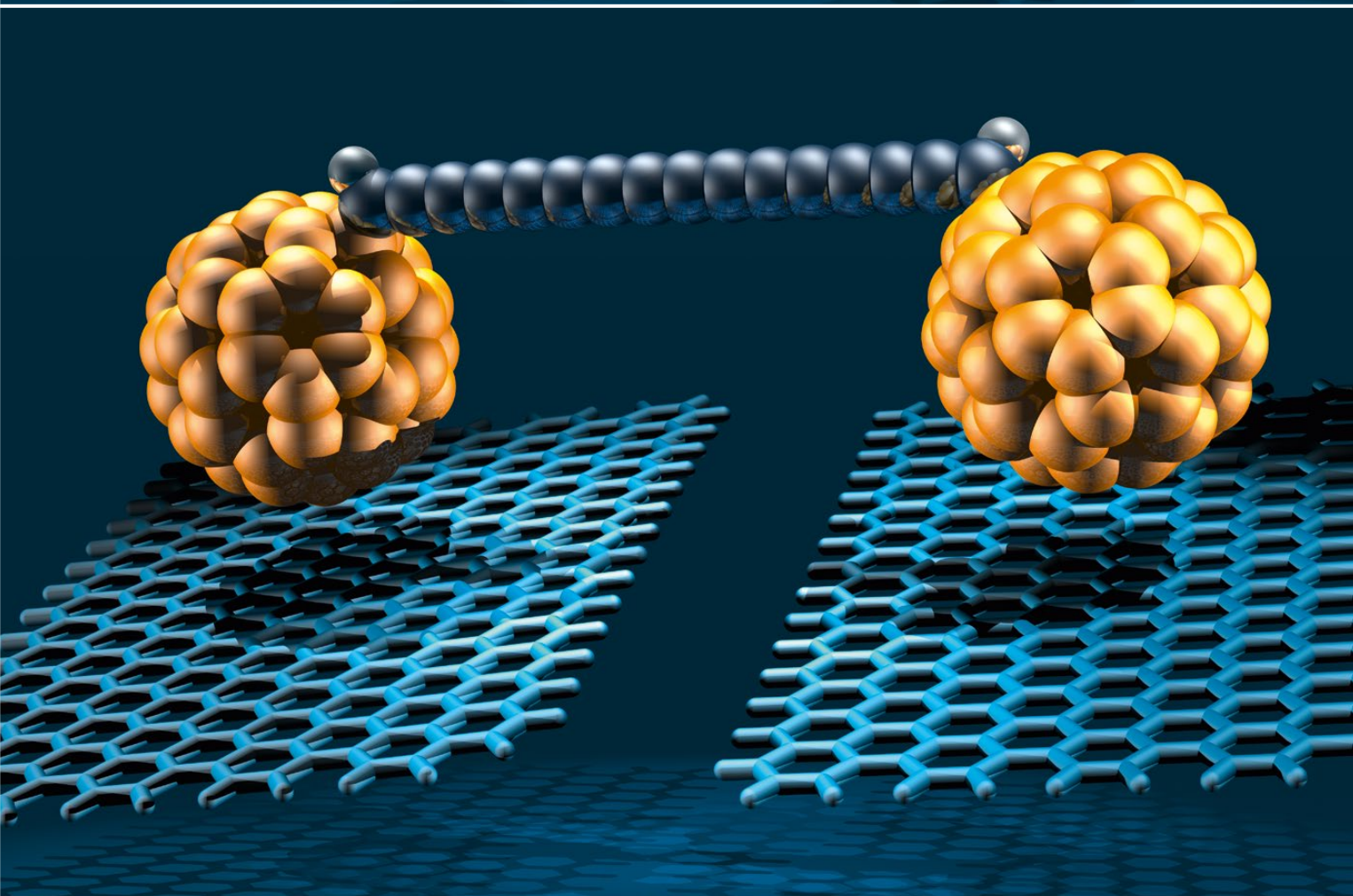
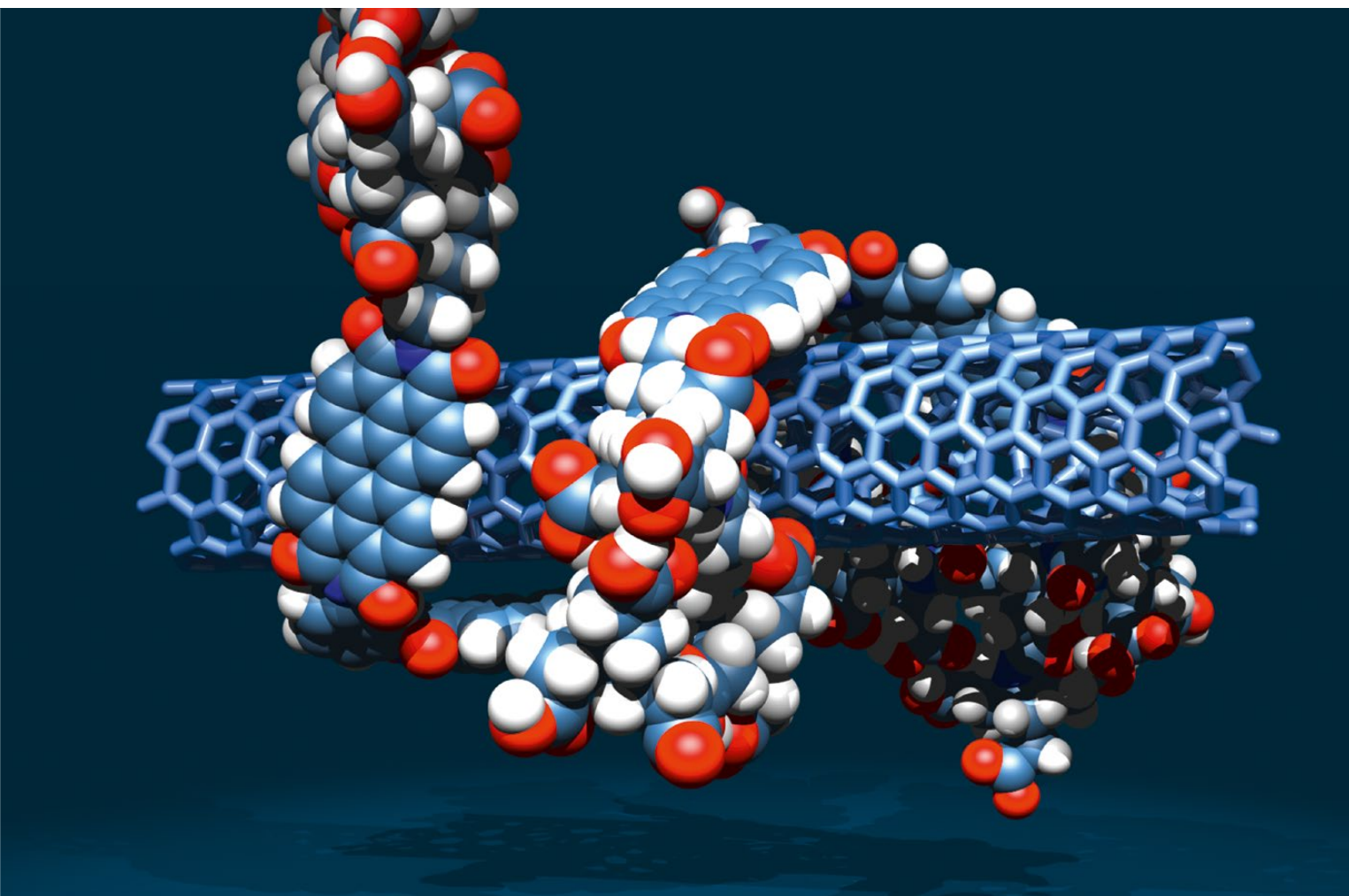
- A. M. Frolov, M. B. Ruiz, D. M. Wardlaw, *Chem. Phys. Lett.* **2014**, 608, 191–200
- M. B. Ruiz, J. T. Margraf, A. M. Frolov, *Phys. Rev. A* **2013**, 88, 012505
- M. B. Ruiz, A. M. Frolov, *Adv. Quantum Chem.* **2013**, 67, 267–290
- A. M. Frolov, M. B. Ruiz, *Phys. Rev. A* **2010**, 82, 042511
- M. B. Ruiz, *J. Math. Chem.* **2009**, 46, 24–64
- M. B. Ruiz, *J. Math. Chem.* **2009**, 46, 1322–1355

SELECTED REVIEWS

- Accurate wave functions for the atomic effect in the whole-atom-nuclear β -decay of the Li atom, M. B. Ruiz, *Mol. Phys.* **2014**, 112, 1174–1188
- P. E. Hoggan, M. B. Ruiz, T. Özdoğan, Molecular Integrals over Slater orbitals. From pioneers to recent progress, in: *Quantum Frontiers of Atoms and Molecules*, Ed. Mihai V. Putz **2010**, 63–90
- 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. Özdoğan, M. B. Ruiz, **2008**, 99–144

SELECTED AWARDS

- Employee Price of the University of Erlangen-Nürnberg for outstanding achievements
- 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





ORGANIC CHEMISTRY
DR. SIEGFRIED EIGLER

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CURRICULUM VITAE

- Since 2014** Junior group leader, Organic Chemistry, University of Erlangen Nürnberg, Germany
- 2010 – 2014** Research associate at the Central Institute for New Materials and Processes, University of Erlangen-Nürnberg, Germany
- 2006 – 2010** Project-leader, Research at DIC Berlin GmbH (DIC Corporation), Germany
- 2006** PhD, Organic Chemistry, University of Erlangen-Nürnberg, Germany

OBJECTIVES AND PERSPECTIVES

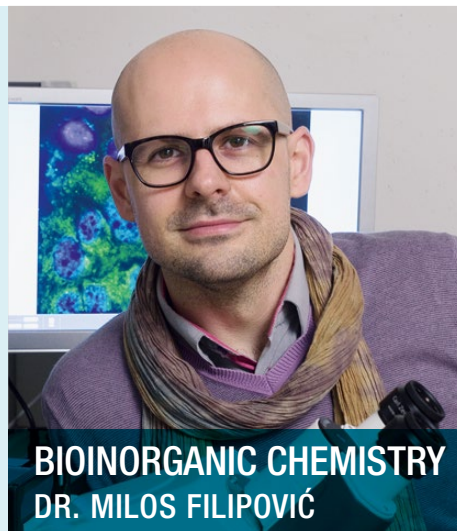
The controlled synthesis of novel graphene based materials with architectures that enable the selective binding of biomolecules will lead to highly sensitive biosensors. Our research focuses on the defect-free synthesis, structure evaluation, and controlled functionalization of oxo-functionalized graphene and graphene. We elaborate the relationship between electronic properties of graphene materials and their chemical structure. With the resulting information we will be able to develop targeted sensors.

SELECTED PUBLICATIONS AND REVIEWS

- S. Eigler, *Phys. Chem. Chem. Phys.* **2014**, 16, 19832–19835
- S. Eigler, A. Hirsch, *Angew. Chem. Int. Ed.* **2014**, 43, 7720–7738
- S. Eigler, F. Hof, M. Enzelberger-Heim, S. Grimm, P. Müller, A. Hirsch, *J. Phys. Chem. C* **2014**, 118, 7698–7704
- S. Eigler, S. Grimm, A. Hirsch, *Chem. Eur. J.* **2014**, 20, 984–989
- S. Eigler, S. Grimm, M. Enzelberger, P. Müller, A. Hirsch, *Chem. Commun.* **2013**, 49, 7391–7393
- S. Eigler, C. Dotzer, F. Hof, W. Bauer, A. Hirsch, *Chem. Eur. J.* **2013**, 19, 9490–9496
- S. Eigler, Y. Hui, Y. Ishii, A. Hirsch, *Nanoscale* **2013**, 5, 12136–12139
- S. Eigler, M. Enzelberger-Heim, S. Grimm, P. Hofmann, W. Kroener, A. Geworski, C. Dotzer, M. Röckert, J. Xiao, C. Papp, O. Lytken, H.-P. Steinrück, P. Müller, A. Hirsch, *Adv. Mater.* **2013**, 25, 3583–3587

SELECTED AWARDS

- 1st place of “innovation check” 2013 of FAU Erlangen-Nürnberg and TH Nürnberg



BIOINORGANIC CHEMISTRY
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CURRICULUM VITAE

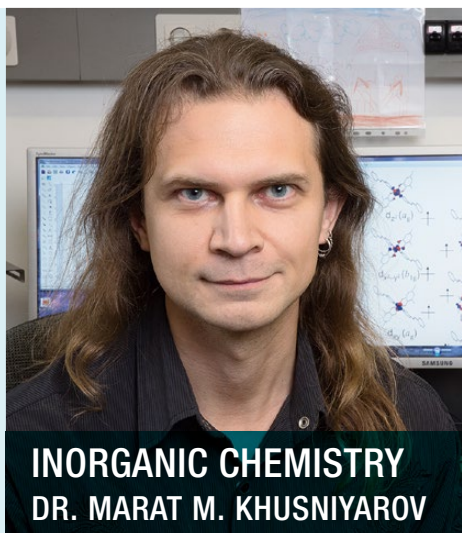
- Since 2009** Junior group leader, Bioinorganic Chemistry, University of Erlangen Nürnberg, Germany
- 2008 – 2009** Senior Research Associate, ICTM-Center for Chemistry, University of Belgrade, Serbia
- 2008** DSc, Biochemistry, University of Belgrade, Serbia

OBJECTIVES AND PERSPECTIVES

My research interests are quite wide: from understanding the basic chemical steps behind intracellular metabolic pathways to regulation and treatment of different disease states (such as diabetes, neuropathies, and heart failure). More specifically we have been addressing the signalling by small gaseous molecules, i.e., gasotransmitters. This covers the signalling by nitric oxide (NO) and hydrogen sulfide (H₂S). We are working on unraveling the (bio) chemical steps behind H₂S signaling, with particular emphasis on its intracellular crosstalk with NO (and NO metabolites). In addition, changes in oxidative post-translational modifications of cysteine residues in proteins have become interest of mine. The development of selective methods for detection of the H₂S-induced protein modifications, so called S-sulphydration, would be one of our future goals.

SELECTED PUBLICATIONS AND REVIEWS

- M. Eberhard, M. Dux, B. Namer, J. Lj. Miljkovic, N. Cordasic, C. Will, M. Fischer, S. A. Suarez, D. Bikel, J. de la Roche, K. Dorsch, T. I. Kichko, A. Leffler, A. Babes, A. Lampert, J. K. Lennerz, J. Jacobbi, M. A. Marti, F. Doctorovich, E. D. Högestätt, P. M. Zygmunt, I. Ivanović-Burmazović, K. Messlinger, P. Reeh, M. R. Filipović, *Nature Communications* **2014**, DOI: 10.1038/ncomms5381
- D. Zhang, I. Macinkovic, No. O. Devarie-Baez, J. Pan, C. M. Park, K. S. Carroll, M. R. Filipović, M. Xian, *Angew. Chem. Int. Ed.* **2014**, 53, 575–581
- J. Lj. Miljkovic, I. Ivanović-Burmazović, M. R. Filipović, *Angew. Chem. Int. Ed.* **2013**, 52, 12061–12064
- M. R. Filipović, J. Lj. Miljkovic, T. Nauser, M. Royzen, K. Klos, T. Shubina, W. H. Koppenol, S. J. Lippard, I. Ivanović-Burmazović, *Journal of the American Chemical Society* **2012**, 134, 12016–12027
- M. R. Filipović, J. Lj. Miljkovic, A. Allgaeuer, R. Chaurio, T. Shubina, M. Herrmann, I. Ivanović-Burmazović, *Biochemical Journal* **2012**, 441, 609–621



INORGANIC CHEMISTRY
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CURRICULUM VITAE

- Since 2009** Junior group leader, Inorganic Chemistry, University of Erlangen Nürnberg, Germany
- 2006 – 2009** Postdoctoral Fellow, Max Planck Institute for Bioinorganic Chemistry, Mülheim an der Ruhr, Germany
- 2002 – 2006** PhD, Inorganic Chemistry, Philipps-Universität Marburg, Germany
- 1997 – 2002** Chemistry studies, Department of Natural Science, Novosibirsk State University, Russia

OBJECTIVES AND PERSPECTIVES

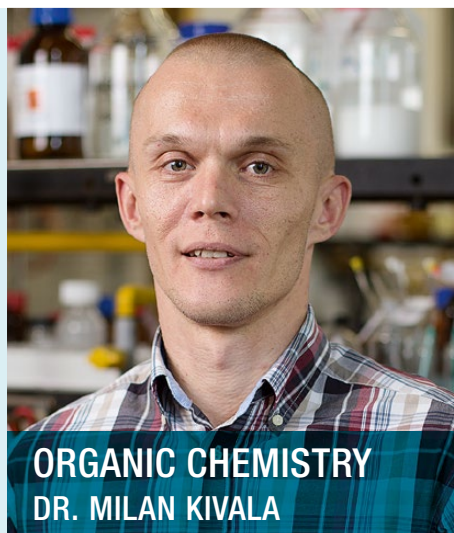
The research in our group is dedicated to the development and investigation of molecular switches and magnetic materials. Much attention is paid to the synthesis and studies of bistable metal complexes that can be reversibly switched at room temperature. To accomplish our goals strongly interdisciplinary approach comprising synthetic inorganic and organic chemistry, photochemistry, applied spectroscopy and theoretical calculations is used.

SELECTED PUBLICATIONS AND REVIEWS

- A. Witt, F. W. Heinemann, S. Sproules, M. M. Khusniyarov, *Chem. Eur. J.* **2014**, 20, 11149–11162
- M. Milek, F. W. Heinemann, M. M. Khusniyarov, *Inorg. Chem.* **2013**, 52, 11585–11592
- M. Milek, A. Witt, C. Streb, F. W. Heinemann, M. M. Khusniyarov, *Dalton Trans.* **2013**, 42, 5237–5241
- J. Meiners, M. G. Scheibel, M.-H. Lemée-Cailleau, S. A. Mason, M. B. Boeddinghaus, T. F. Fässler, E. Herdtweck, M. M. Khusniyarov, S. Schneider, *Angew. Chem. Int. Ed.* **2011**, 50, 8184–8187
- M. M. Khusniyarov, E. Bill, T. Weyhermüller, E. Bothe, K. Wieghardt, *Angew. Chem. Int. Ed.* **2011**, 50, 1652–1655
- J. J. Scepaniak, C. S. Vogel, M. M. Khusniyarov, F. W. Heinemann, K. Meyer, J. M. Smith, *Science* **2011**, 331, 1049–1052

SELECTED AWARDS

- 2014 Temporary position for principal investigator, German Research Foundation, Germany
- 2009 Liebig Fellowship, Fonds der Chemischen Industrie, Germany
- 2006 Postdoctoral Fellowship, Max Planck Society, Germany
- 2002 Diploma in Chemistry with honors, Novosibirsk State University, Russia



ORGANIC CHEMISTRY
DR. MILAN KIVALA

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CURRICULUM VITAE

- Since 2011** Junior group leader, Organic Chemistry, University of Erlangen Nürnberg, Germany
- 2009 – 2011** Postdoctoral Fellow, Max Planck Institute for Polymer Research (Prof. K. Müllen), Mainz, Germany
- 2008 – 2009** Postdoctoral Fellow, ETH Zürich (Prof. F. Diederich), Switzerland
- 2008** PhD, Organic Chemistry, ETH Zürich (Prof. F. Diederich), Switzerland

OBJECTIVES AND PERSPECTIVES

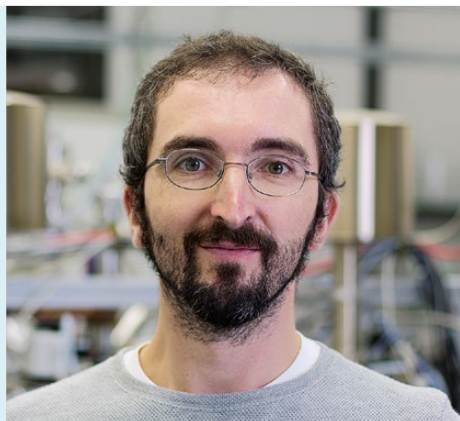
The focal point of my research program is the synthesis of unprecedented heteroatom-doped polycyclic aromatic hydrocarbons with the aim to 1) investigate the influence of various heteroatoms on their fundamental characteristics and 2) apply the resulting compounds as functional materials in organic optoelectronic devices. While my research is clearly synthesis-driven, fundamental understanding and function of the resulting compounds are essential for us. To achieve these goals, my research benefits from numerous interdisciplinary collaborations.

SELECTED PUBLICATIONS AND REVIEWS

- A. T. Haedler, S. R. Beyer, N. Hammer, R. Hildner, M. Kivala, J. Köhler, H.-W. Schmidt, *Chem. Eur. J.* **2014**, 20, 11708–11718
- P. O. Dral, M. Kivala, T. Clark, *J. Org. Chem.* **2013**, 78, 1894–1902
- M. Kivala, W. Pisula, S. Wang, A. Mavrinskiy, J.-P. Gisselbrecht, X. Feng, K. Müllen, *Chem. Eur. J.* **2013**, 19, 8117–8128
- F. Schlütter, F. Rossel, M. Kivala, V. Enkelmann, J.-P. Gisselbrecht, P. Ruffieux, R. Fasel, K. Müllen, *J. Am. Chem. Soc.* **2013**, 135, 4550–4557
- M. Kivala, F. Diederich, *Acc. Chem. Res.* **2009**, 42, 235–248
- M. Kivala, C. Boudon, J.-P. Gisselbrecht, P. Seiler, M. Gross, F. Diederich, *Angew. Chem. Int. Ed.* **2007**, 46, 6357–6360

SELECTED AWARDS

- 2014 EAM Starting Grant, DFG Exzellenzcluster 'Engineering of Advanced Materials'
- 2012 Fonds der Chemischen Industrie Grant
- 2010–2012 Humboldt Fellowship for Postdoctoral Researchers
- 2009–2010 Swiss National Science Foundation Fellowship
- 2009 ETH Medal
- 2003 Honor Award of Josef Hlávka



PHYSICAL CHEMISTRY
DR. MATHIAS LAURIN

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CURRICULUM VITAE

- Since 2012** Junior group leader, Physical Chemistry, University of Erlangen Nürnberg, Germany
- 2008 – 2012** Postdoctoral Fellow, Physical Chemistry II, University of Erlangen-Nürnberg, Germany
- 2006 – 2008** JSPS Postdoctoral fellow, Tokyo University and Keio University, Tokyo, Japan
- 2006** MPG Postdoctoral fellow, Physical Chemistry II, the University of Erlangen-Nürnberg, Germany
- 2002 – 2005** PhD studies, Department of Chemical Physics at the Fritz-Haber-Institut, Max Planck Gesellschaft, Berlin

OBJECTIVES AND PERSPECTIVES

Our group follows two complementary research directions. The closest to technical chemistry and applications provides a spectroscopic understanding of working catalysts, combined with real-time gas phase analysis. We concentrate on supported homogeneous and heterogeneous catalysts during selected reactions. On a fundamental level, we develop new concepts deriving from the characterization of the interactions between organic molecules (such as ionic liquids or porphyrins) and atomically defined oxide surfaces. Our technique of choice is infrared spectroscopy.

SELECTED PUBLICATIONS AND REVIEWS

- M. Kusche, F. Enzenberger, S. Bajus, et al., *Angew. Chem. Int. Ed.* **2013**, 52, 5028–5032
- M. Laurin, Q. Vibéplot, *J. Chem. Educ.* **2013**, 90, 944–946
- S. Schernich, M. Laurin, Ya. Lykhach, et al., *J. Phys. Chem. Lett.* **2012**, 4, 30–35
- M. Sobota, M. Happel, M. Amende, N. Paape, P. Wasserscheid, M. Laurin, J. Libuda, *Adv. Mater.* **2011**, 23, 2617–2621
- V. Johánek, M. Laurin, A. W. Grant, B. Kasemo, C. R. Henry, J. Libuda, *Science* **2004**, 304, 1639–1644

SELECTED AWARDS

- 2011 Poster prize at the 44. Katalitiker Tagung
- 2006 Japanese Society for the Promotion of Science (JSPS) Fellowship
- 2004 “Best PhD Oral Presentation” at the 3rd EFCATS School of Catalysis



PHYSICAL CHEMISTRY
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CURRICULUM VITAE

- Since 2011** Junior group leader, Physical Chemistry, University of Erlangen Nürnberg, Germany
- 2009 – 2011** Postdoctoral Fellow, Physical Chemistry II, University of Erlangen-Nürnberg, Germany
- 2007 – 2009** Postdoctoral Fellow, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
- 2007** PhD, Physical Chemistry II, University of Erlangen-Nürnberg, Germany

OBJECTIVES AND PERSPECTIVES

Our general aim is an atomic or molecular understanding of surface chemistry and surface processes on catalytically active metals. We focus on the in-situ analysis of surfaces and interfaces facilitating synchrotron radiation for (1) studying model systems, from flat surfaces to nanoclusters (2) hydrogen storage and release in liquid organic hydrogen carriers and the development of novel catalyst systems for these reactions (3) the functionalization and chemical modification of graphene for application in future information technology.

SELECTED PUBLICATIONS AND REVIEWS

- C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, *Review—The Chemical Record* **2014**, DOI: 10.1002/tcr.201402014
- C. Papp, H.-P. Steinrück, *Review—Surface Science Reports* **2013**, 68, 446–487
- C. Gleichweit, M. Amende, S. Schernich, W. Zhao, M. P. A. Lorenz, O. Höfert, N. Brückner, P. Wasserscheid, J. Libuda, H.-P. Steinrück, C. Papp, *ChemSusChem* **2013**, 6, 974–977
- J. Englert, C. Dotzer, G. Yuang, M. Schmid, C. Papp, J. M. Gottfried, H.-P. Steinrück, E. Spieker, F. Hauke, A. Hirsch, *Nature Chemistry* **2011**, 3, 279–286
- A. X. Gray, C. Papp, S. Ueda, B. Balke, Y. Yamashita, L. Plucinski, J. Minár, J. Braun, E. R. Ylvisaker, C. M. Schneider, W. E. Pickett, H. Ebert, K. Kobayashi, C. S. Fadley, *Nature Materials* **2011**, 10, 759–764
- R. Streber, C. Papp, M. P. A. Lorenz, A. Bayer, R. Denecke and H.-P. Steinrück, *Angewandte Chemie International Edition* **2009**, 48, 9743–9746

SELECTED AWARDS

- 2008–2009 Feodor-Lynen Stipend of the Alexander-von-Humboldt Foundation
- 2008 Karl-Giehl-Preis, University of Erlangen-Nürnberg



THEORETICAL CHEMISTRY
DR. TATYANA E. SHUBINA

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www.chemie.fau.de/shubina

CURRICULUM VITAE

- Since 2012** Junior group leader, Theoretical Chemistry, University of Erlangen Nürnberg, Germany
- 2007 – 2011** Postdoctoral Fellow, Computer Chemistry Center at the University of Erlangen-Nürnberg, Germany
- 2005 – 2006** Humboldt Fellow, Computer Chemistry Center at the University of Erlangen-Nürnberg, Germany
- 2003** PhD, Organic Chemistry at the National Technical University of Ukraine (KPI), Ukraine

OBJECTIVES AND PERSPECTIVES

My research centers on the application of computational chemistry to various problems in the fields of physical, organic and bioorganic chemistry.

The projects are focused on metalloporphyrins as model systems and challenges, connected with this for computational methods and on mechanistic studies related to bioorganic chemistry as well as on application of metalloporphyrins and related compounds for understanding and ultimately designing new electronic devices.

SELECTED PUBLICATIONS AND REVIEWS

- O. Troppner, R. Lippert, T. E. Shubina, A. Zahl, N. Jux and I. Ivanović-Burmazović, *Angew. Chem. Int. Ed.* **2014**, accepted
- T. Shubina, D. I. Sharapa, C. Schubert, D. Zahn, M. Halik, P. A. Keller, S. G. Pyne, S. Jennepalli, D. M. Guldi, T. Clark, *J. Am. Chem. Soc.* **2014**, 136 (31), 10890 – 10893
- M. R. Filipović, J. Mijlkovic, T. Nausser, M. Royzen, K. Klos, T. E. Shubina, W. H. Koppenol, S. J. Lippard, I. Ivanović-Burmazović, *J. Am. Chem. Soc.* **2012**, 134, 12016 – 12027
- Y. Li, J. Xiao, T. E. Shubina, M. Chen, Z. Shi, M. Schmid, H.-P. Steinrück, J. M. Gottfried, N. Lin, *J. Am. Chem. Soc.* **2012**, 134 (14), 6401 – 6408
- T. E. Shubina, *Advances in Inorganic Chemistry* **2010**, Vol. 62, Chapter 7, 261 – 300. (Eds: R. van Eldik, J. Harvey)
- I. A. Levandovskiy, D. I. Sharapa, T. V. Shamota, V. N. Rodionov, T. E. Shubina, *Future Medicinal Chemistry* **2011**, 3(2), 223 – 241

SELECTED AWARDS

- Guest Editor for the Journal of Molecular Modeling (SI Clark)
- Member of the RSC
- Humboldt Fellowship



MEDICINAL CHEMISTRY
DR. NUSKA TSCHAMMER

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CURRICULUM VITAE

- Since 2008** Junior group leader, Medicinal Chemistry, University of Erlangen-Nürnberg, Germany
- 2004 – 2007** PhD in Biomolecular Sciences, University of Central Florida, Orlando, USA
- 1999 – 2002** Master in Chemical Technology/Chemistry of Polymers, University of Maribor, Slovenia
- 1993 – 1998** Bachelor in Biology and Chemistry, University of Maribor, Slovenia

OBJECTIVES AND PERSPECTIVES

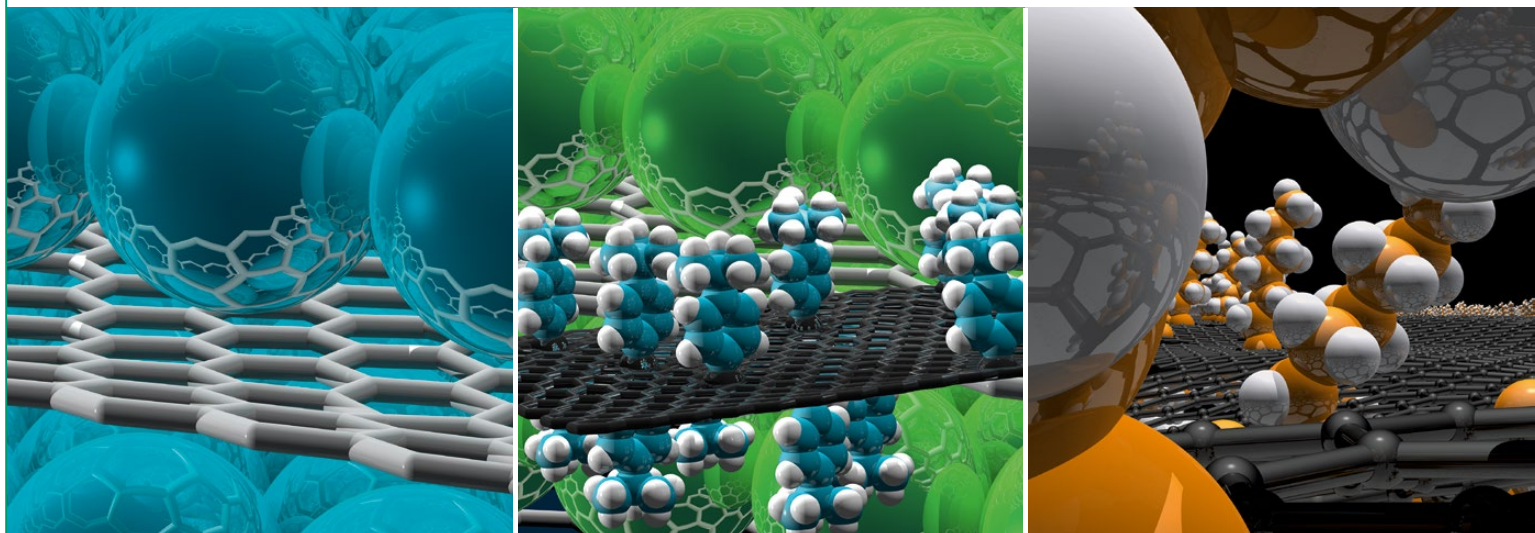
To advance the understanding of the allosteric modulation of human and viral chemokine receptors, we focus our efforts on the identification of molecular determinants involved in the allosteric modulation of these receptors. With the combination of de novo synthesis, computational approaches, molecular and pharmacological methods we are able gain detailed insight in the mechanisms of allosteric modulation. These mechanisms raise the possibility of designing novel therapeutics, which differentially activate downstream signaling pathways and thus promote desired therapeutic action with reduced unwanted effects.

SELECTED PUBLICATIONS AND REVIEWS

- V. Bernat, R. Brox, T. H. Admas, F. Heinemann, N. Tschammer, *ACS Chem. Biol.* **2014**, accepted
- N. Tschammer, *Bioorg. Med. Chem. Lett.* **2014**, 24, 3744 – 3747
- A. Kralj, E. Kurt, N. Tschammer, H. Heinrich, *ChemMedChem.* **2014**, 9, 151 – 168
- A. Kralj, M.-T. Nguyen, N. Tschammer, N. Ocampo, Q. Gesiotto, M. Heinrich, O. Phanstiel, *J. Med. Chem.* **2013**, 56, 5015032
- V. Bernat, M. Heinrich, P. Baumeister, A. Buschauer, N. Tschammer, *ChemMedChem.* **2012**, 7, 1481 – 1489
- N. Tschammer, S. Bollinger, T. Kenakin, P. Gmeiner, *Mol. Pharmacol.* **2011**, 79, 575 – 585

SELECTED AWARDS

- 2014 Womens Award of Faculty of Life Sciences, University of Erlangen
- 2004 Merit Fellowship, University of Central Florida, Orlando, USA
- Since 2012 several Grants of German Research Foundation and Bavarian Ministry of Science and Research



COLLABORATIVE RESEARCH CENTRE SFB 953: “SYNTHETIC CARBON ALLOTROPES”



Synthetic carbon allotropes such as fullerenes, carbon nanotubes and graphene currently represent one of the most promising materials families with enormous potential for high-performance applications in the fields of nanoelectronics, optoelectronics, hydrogen storage, sensors and reinforcements of polymers based on their unprecedented electronic, optical, mechanical and chemical properties.

The scientific interest of the SFB 953 “Synthetic Carbon Allotropes” is devoted to fundamental chemical and physical questions such as controlled allotrope doping with heteroatoms, development of synthesis protocols for novel carbon allotrope systems, sorting and separation of carbon nanotubes, investigation of the intrinsic chemical reactivity, and the development of carbon based architectures and devices.

Hence tremendous interdisciplinary efforts are required that systematically combine the expertise of chemists, physicists, engineers, and theoreticians, together with the contributions of high-end analytical instrumentation. The University of Erlangen-Nürnberg hosts probably the largest and most productive pioneering community in Europe or even worldwide at the forefront of carbon allotrope research. The SFB therefore constitutes the ideal forum to advance the field of synthetic carbon allotropes towards the desired goal of creating new materials for high-performance applications.

The SFB 953 is structured according to three research areas and two central projects. Research area A (Synthesis and Functionalization) provides the materials basis of the SFB. Chemical functional-

ization of existing synthetic carbon allotropes and development of new carbon modifications both lie at the forefront of this effort. The next level within the process chain is the systematic investigation of physical and materials properties and the development of concepts for device fabrication. This is guaranteed by the close interaction with Research Area B (Electronic, Optical and Structural Properties) and the two scientific central projects (Z Projects) on high-resolution electron microscopy and tandem mass spectrometry. This highly integrated and interdisciplinary approach of the SFB also necessitates a close connection with Research Area C (Theory). Both classical and quantum mechanical calculations provide the basis for an in-depth understanding of reaction mechanisms, stability as well as electronic, optical, structural and mechanical properties of synthetic carbon allotropes and their derivatives. Moreover, theory will provide some of the most valuable design principles for the exploration of hitherto unknown forms of carbon.

CONTACT

Speaker: *Prof. Dr. Andreas Hirsch*

Vice-Speaker: *Prof. Dr. Heiko B. Weber*

Administrative Coordinator: *Dr. Frank Hauke*

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RESEARCH TRAINING GROUP GRK 1910: “MEDICINAL CHEMISTRY OF SELECTIVE GPCR LIGANDS”

Approximately 30 % of the drugs on the market exert their biological activities upon binding to G-protein coupled receptors (GPCRs). Severe diseases are frequently associated with dysfunctions of GPCRs.

The Research Training Group, located at FAU and at University of Regensburg, Germany, aims to explore the ligand induced control of monoaminergic and peptidergic GPCRs. In addition to the elucidation of molecular mechanisms, we attempt to contribute to a rational development of functionally selective GPCR drugs for the treatment of chronic inflammatory, cardiovascular and CNS diseases and for diagnostic purposes. The research program is strongly interdisciplinary, covering computer assisted design of selective ligands, chemical synthesis of target compounds, the investigation of ligand-receptor interactions and the elaboration of functional selectivity by analysis of ligand-specific signaling. The

program specific qualification profile integrates chemical, radiopharmaceutical, pharmacological, molecular biological, bioanalytical and biochemical aspects of drug research. The main issues of the qualification programs are retreats, workshops, seminars and online seminars, dealing with and promoting the core research idea. All graduates will get the opportunity to work for 3–4 months in the research laboratory of a collaborator abroad to acquire new knowledge, apply modern methods and techniques and to gain international experience even before the completion of the doctorate.

CONTACT

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www.grk1910.de

RESEARCH UNIT FOR 1878: “funCOS — FUNCTIONAL MOLECULAR STRUCTURES ON COMPLEX OXIDE SURFACES”

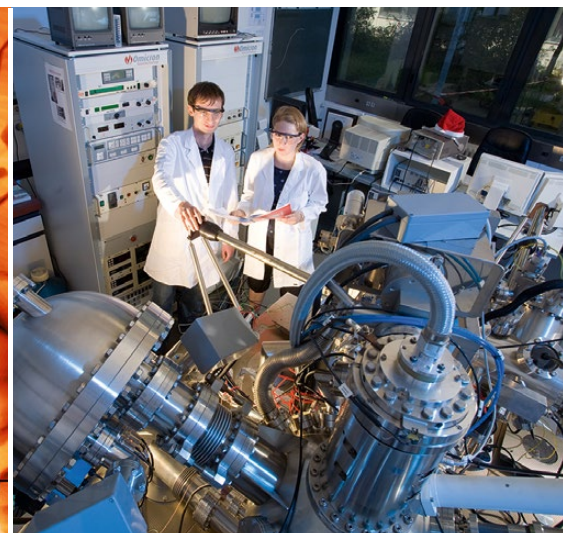
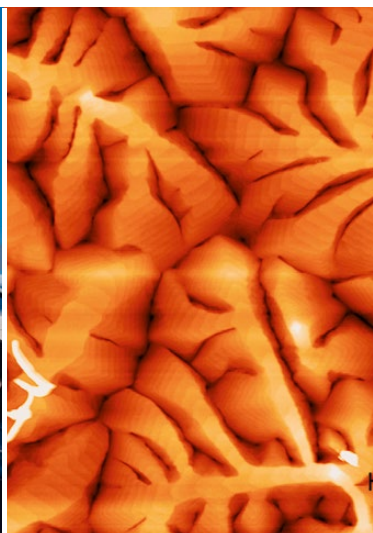
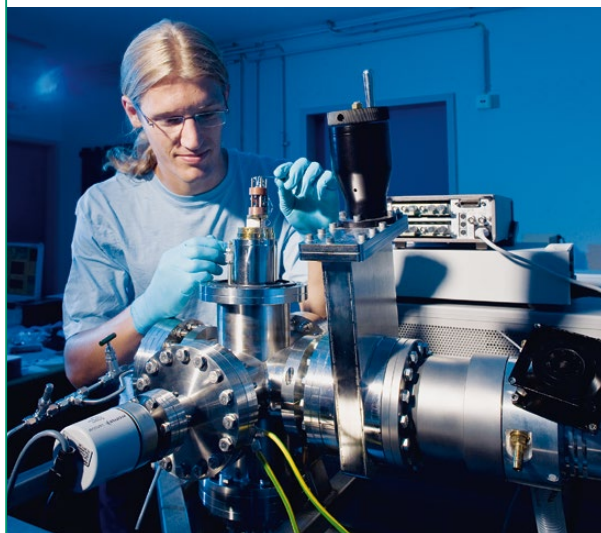


The DFG Research Unit “funCOS—Functional Molecular Structures on Complex Oxide Surfaces” (FOR 1878) was established in 2013. It comprises a total of 15 groups and project leaders from the Department of Chemistry and Pharmacy, the Department of Physics, and the Department of Materials Science. funCOS aims at a fundamental understanding of molecular films and ordered structures bound to oxide surfaces. Such systems are at the heart of emerging technologies, with potential fields of application including molecular electronics, solar energy conversion, and catalysis. In spite of the potential of these technologies, the current understanding of molecule oxide interfaces is poor at the atomic level. Whereas the surface science approach to functional organic molecules on metals has provided a wealth of knowledge on bonding mechanisms and structure formation, organic

oxide interfaces have remained largely unexplored; a situation which we denote as the ‘materials gap’ in organic thin film science. funCOS aims at closing this gap and at providing the fundamental knowledge basis required for the design of tailor-made interfaces. Eventually this knowledge should enable us to perform ‘functional landscaping’ of molecular films on oxides at the nanoscale.

CONTACT

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www.funcos.fau.de



CLUSTER OF EXCELLENCE ENGINEERING OF ADVANCED MATERIALS (EAM)



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 9 disciplines (Applied Mathematics, Chemical Engineering, Chemistry, Computer Science, Electrical Engineering, Materials Science and Engineering, Medicine, Mechanical Engineering, and Physics) collaborate in more than 75 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 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:

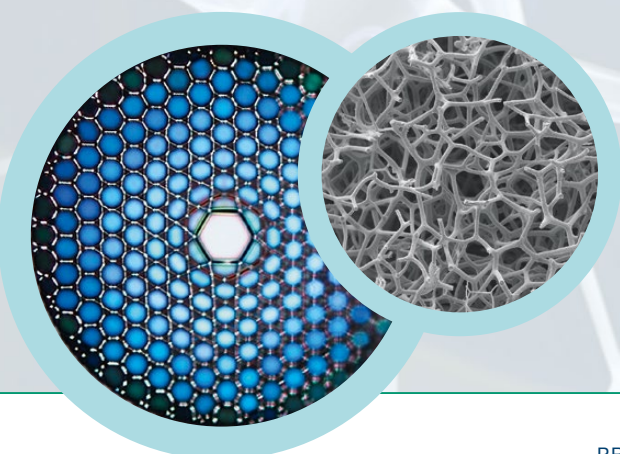
- Engineering of nanoelectronic materials
- Engineering of photonic and optical materials
- Engineering of catalytic materials
- Engineering of lightweight materials

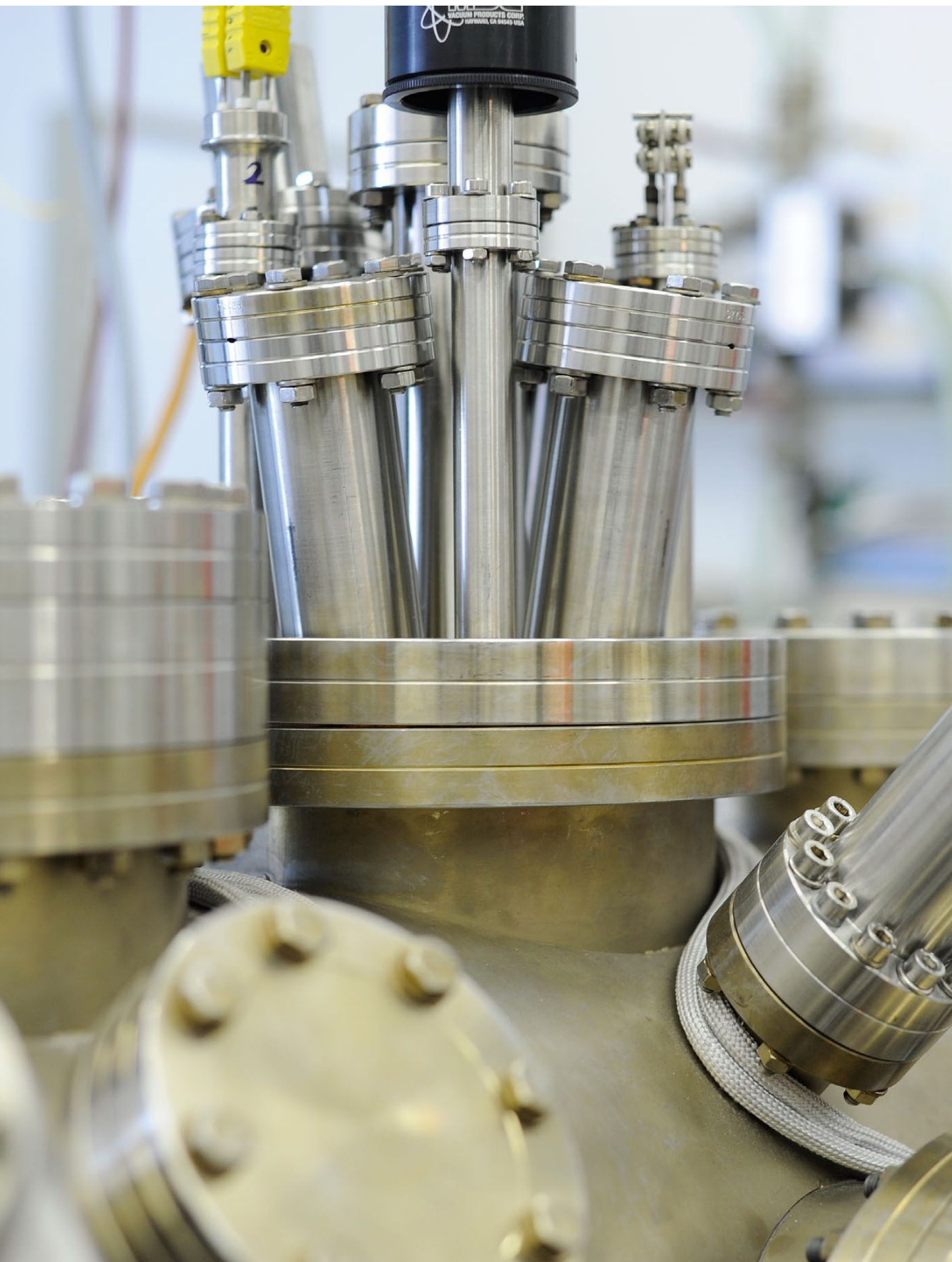
INTERDISCIPLINARY NETWORK OF PARTNERS

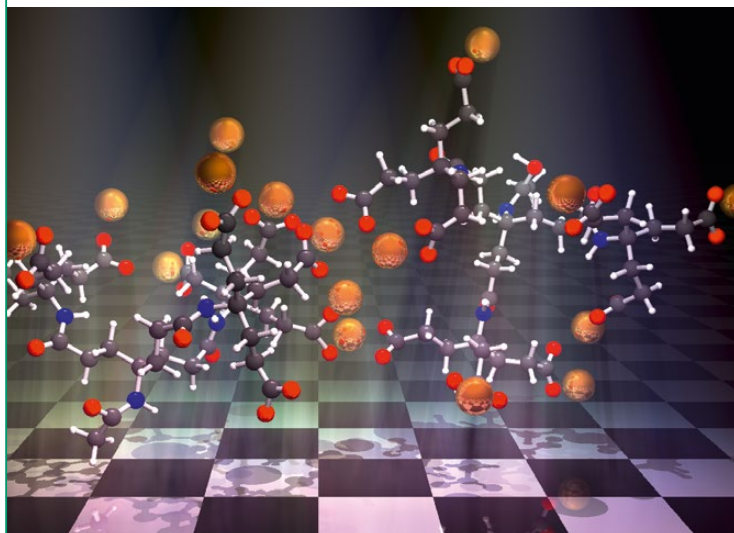
The Cluster of Excellence was established at the University of Erlangen-Nürnberg in November 2007 within the framework of the Excellence Initiative. The funding by DFG amounts to 70 million Euros for ten years with additional substantial support by the University and the state of Bavaria. EAM is based on existing and visible excellences within the University of Erlangen-Nürnberg Erlangen 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), New Materials Fürth GmbH, Bavarian Center for Applied Energy Research (ZAE), and other notable academic and industrial research partners.

CONTACT

Cluster Coordinator: *Prof. Dr. Wolfgang Peukert*
Cluster Co-Coordinator: *Prof. Dr. Peter Wasserscheid*
eam-administration@fau.de, www.eam.fau.de







COMPUTER CHEMISTRY CENTER (CCC)

The Computer-Chemie-Centrum (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 Prof. Dr. T. Clark (CCC/Organic Chemistry, Prof. Dr. B. Meyer (Interdisciplinary Center for Molecular Materials, ICMM) and Prof. Dr. D. Zahn (Theoretical Chemistry) with a total of approximately 50 researchers. Prof. (emeritus) P. von Ragué Schleyer also spends part of each year in CCC.

The research topics treated at CCC range from protein and DNA simulations and computational drug design through 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 SFB 953 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. Dr. A. Görling is the Chairman of the Kollegiale Leitung of CCC and Prof. Dr. T. Clark is its Technical Director.

CONTACT

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www.chemie.fau.de/ccc



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 and to understand the interaction of new bioactive small molecules with their target proteins and physiological function.

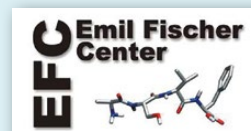
The Emil Fischer Center operates the core unit for bioanalytics, where the scientific and technical competence on targeted and non-targeted metabolome analysis as well as targeted proteome analysis is focused. The bioanalytical expertise covers further techniques of molecular biology and functional assays.

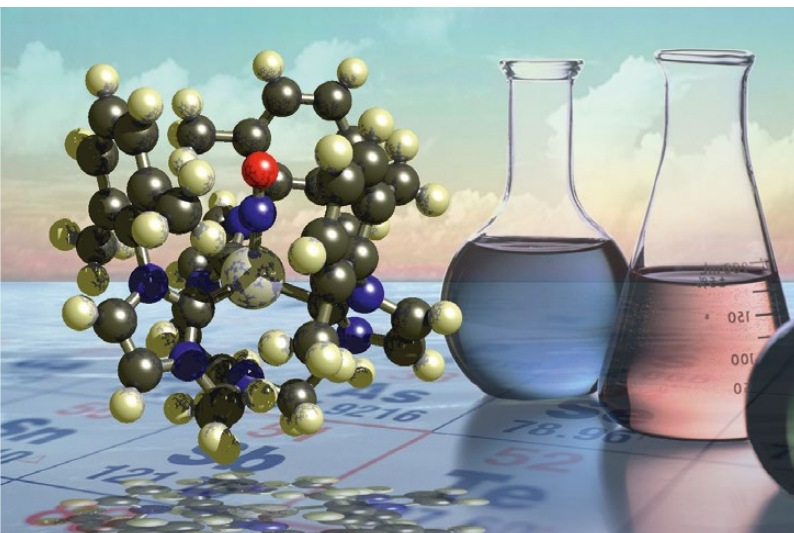
Furthermore, the Emil Fischer Center coordinates the interdisciplinary education of students in the field of pharmacy, food chemistry and molecular medicine. Excellent post graduates are trained in the Emil Fischer Graduate Programme, which is operated by the Emil Fischer Center.

Research at the Emil Fischer Center and the Emil Fischer Graduate Programme is supported by several organizations and research collaborations, such as the DFG graduate program 1910 as well as the collaborative research center SFB 796, the FAU Emerging Field Initiative, the BMBF, EU, Elite Network of Bavaria, and the Bayerische Forschungsförderung.

CONTACT

Prof. Dr. Monika Pischetsrieder
monika.pischetsrieder@fau.de
www.efc.fau.de





ERLANGEN CATALYSIS RESOURCE CENTER (ECRC)

With the inauguration of ECRC in 2008, 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. 14 research groups from the Department of Chemistry and Pharmacy (DCP) and the Department of Chemical and Biological Engineering (CBE) participate in the center representing an active and highly interdisciplinary community of chemists and engineers working in the fields of homogeneous, heterogeneous and biocatalysis as well as chemical reaction engineering and surface science. ECRC represents a center for the integrated investigation of complex catalytic materials and processes aiming at the combination of catalyst and process design. Research within the center 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 (“operando”) conditions,
- the development of new reactor concepts,
- process intensification.

Moreover, ECRC 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.

ECRC is managed by an executive board elected by the members of the center which presently consists of two scientists from CBE (Prof. Dr. P. Wasserscheid and Prof. Dr. K. E. Wirth) and two scientists from DCP (Prof. Dr. K. Meyer and Prof. J. Libuda) and the Professor of Catalysis within ECRC (Prof. Dr. M. Hartmann as permanent member and current speaker).

CONTACT

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martin.hartmann@fau.de
www.ecrc.fau.de



INSTITUTE OF ADVANCED MATERIALS AND PROCESSES (ZMP)

The Institute of Advanced Materials and Processes (ZMP) is an interdisciplinary research center with more than 80 coworkers originating from chemistry, materials science and engineering. In June 2006 no more than 20 persons moved into the friendly and innovative environment at the “city of Fürth” and step by step breathed life into the concept of interdisciplinary research of 4 chairs from the school of engineering, 5 chairs of the Faculty of Engineering and one chair of the Department of Chemistry and Pharmacy (Organic Chemistry II). ZMP is administered by a cooperative headship formed by the seven professors involved (Profs. R. Singer, M. Göken, P. Greil, C. Körner, A. Hirsch, M. Schmidt and P. Wasserscheid) and an executive board (Dr. F. Hauke, Dr. M. Lodes). In 2013, the ZMP was expanded by the application Center VerTec.

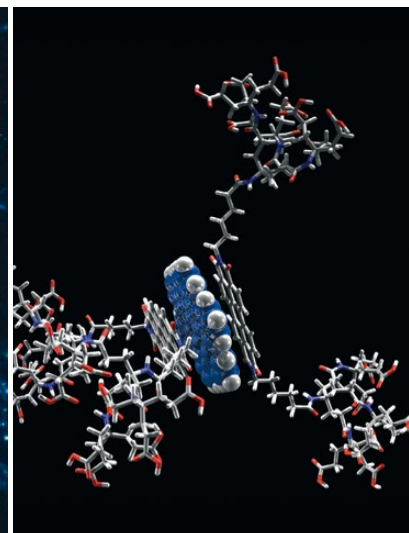
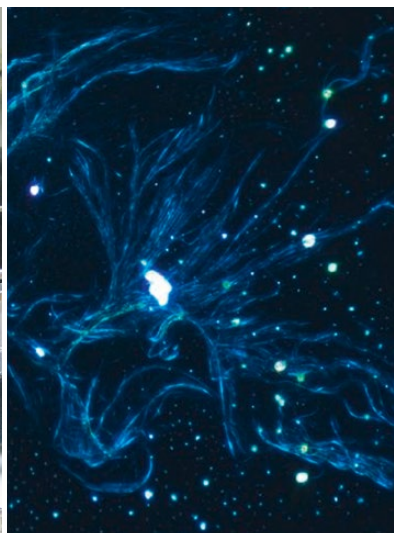
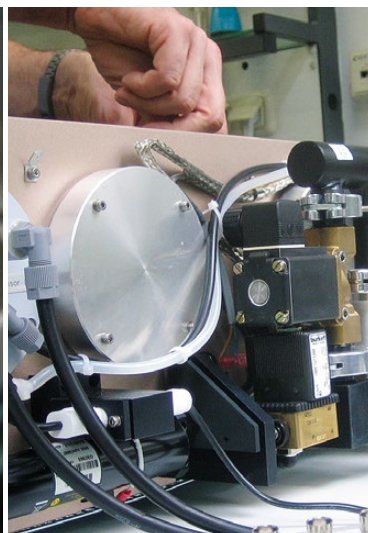
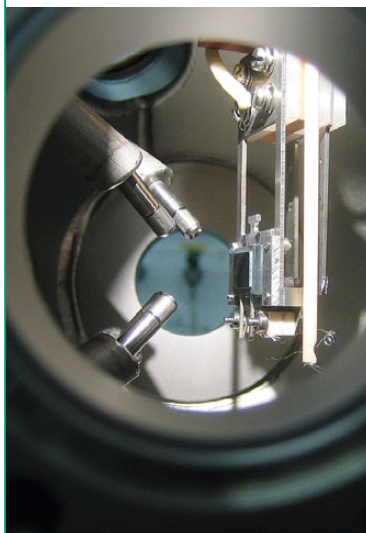
The focus of research is the construction of revolutionary light weight materials and includes the fundamental investigation of novel compound classes, the development of visionary concepts and processes as well as the application of the insights gained for the construction of prototypes. The contribution from the Department of Chemistry and Pharmacy is the functionalization 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 aspect is further reflected by the joint efforts of researchers also involved in other research centers of FAU such as the Cluster of Excellence Engineering of Advanced Materials (EAM), the Interdisciplinary Center for Molecular Materials (ICMM), the Graduate School Molecular Science (GSMS) and the Collaborative Research Center SFB 953 “Synthetic Carbon Allotropes”.

CONTACT

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www.zmp.fau.de





INTERDISCIPLINARY CENTER FOR INTERFACE-CONTROLLED PROCESSES (ICICP)

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 20 groups from the Departments of Physics, Chemistry and Pharmacy, Chemical and Biological Engineering, and Materials Science and Engineering actively participate. The research of these groups focuses on three areas: (i) the preparation and characterization of interface-modified geometric structures, (ii) theoretical and experimental investigations of structure-property relationships in interface-modified structures and their applications, (iii) interfaces of particulate systems and interface-stabilized nanoparticles. An intrinsic strength of the center is the complementary expertise of the participating groups. Bundling this know-how, ICICP has contributed to the evolution of a lively and interdisciplinary research environment, in which numerous joint activities have been initiated. Since 2013, most ICICP groups are actively cooperating within the DFG Research Unit FOR 1878 "funCOS—Functional Molecular Structures on Complex Oxide Surfaces".

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

CONTACT

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INTERDISCIPLINARY CENTER FOR MOLECULAR MATERIALS (ICMM)

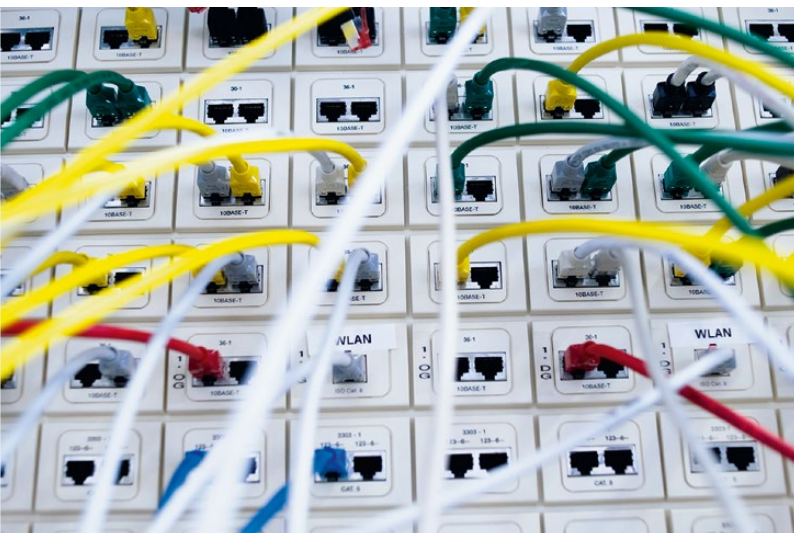
Molecular materials represent a fundamental and interdisciplinary research area at the interface between chemistry, physics and materials science. At the same time they provide the basis for a variety of future technologies. Materials based on defined molecular building blocks are characterized by tuneable performances, which is of great importance for high-end applications in nanoelectronics, medicine and energy conversion technologies. ICMM serves as a platform for interdisciplinary research projects in the field of molecular materials and nanotechnology. Currently, ICMM houses 20 research groups. Their complementary research expertise spans from the synthesis and the supramolecular organization of new molecular architectures including fullerenes, carbon nanotubes, polyynes, porphyrins 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 ICMM is supported by a variety of organizations such as DFG, BMBF, EU and the Bayerische Forschungsförderung.

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 established 12 years ago at the FAU as a consecutive Bachelor/Master curriculum, as well as recruitment of excellent international graduate students and post-docs guarantees a continuous supply of highly qualified researchers for ICMM.

CONTACT

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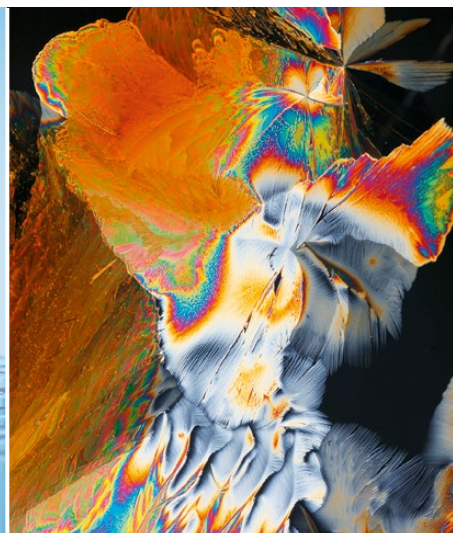
ZENTRALINSTITUT FÜR SCIENTIFIC COMPUTING (ZISC)

The Zentralinstitut für Scientific Computing (ZISC) arose from Research Area A3 (Multiscale Modeling and Simulation) of the Excellence Cluster Engineering of Advanced Materials. ZISC is the umbrella organization for all modeling and simulation activities within FAU. The Computer-Chemie-Centrum (CCC) is the largest single center within ZISC and the computational groups in the Department of Chemistry und Pharmacy play a major role in ZISC. Prof. Dr. B. Meyer and Prof. Dr. D. Zahn are members of ZISC, Prof. Dr. A. Görling is a member of the board of ZISC and Prof. Dr. T. Clark is deputy speaker. ZISC organizes workshops on subjects such as parallelization and performance optimization of computer programs and coordinates cooperative research projects. ZISC is home to the Procter & Gamble Simulation Center. The ZISC management collects and coordinates short trial modeling and simulation projects within Procter & Gamble and distributes them to the relevant research groups within FAU. The aim of such projects is that, after a proof-of-principle stage, they develop into fully-fledged joint research projects between Procter & Gamble and the groups collected within ZISC.

CONTACT

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EMIL FISCHER GRADUATE PROGRAMME OF PHARMACEUTICAL SCIENCES AND MOLECULAR MEDICINE



Training future generations of scientists to discover promising new drugs and target proteins in novel ways:

The program 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 and molecular medicine.

CONTACT

Coordinator: *Prof. Dr. Markus Heinrich*

Administrative office: *Petra Neubarth*

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www.efs.fau.de

GRADUATE SCHOOL ADVANCED MATERIALS AND PROCESSES



The Graduate School Advanced Materials and Processes (GS AMP) has been established within the framework of the Cluster of Excellence Engineering of Advanced Materials in 2009. It offers a program for graduates who are interested in research on topics related to the Cluster of Excellence.

The vision of the GS AMP is to support the evolution of young doctoral researchers into a new generation of scientists capable to pursue careers at an executive level. Successful research in natural and engineering sciences in interdisciplinary and international teams requires creative scientists who can provide cross-disciplinary and intercultural competences. The central aspect is the unique excellence of the individual doctoral project, imbedded into a training program in multidisciplinary research, international networking and soft skills development. GS AMP graduates work on innovative nanoelectronic, catalytic, optic and photonic, as well as lightweight materials focusing either on functional particle systems, nanoanalysis and micro-

scopy or multiscale modeling and simulation. 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 often in close cooperation with industrial partners.

With special activities as the EAM Winter/Summer School, the EAM Young Researchers Day and lectures on EAM topics, the GS AMP successfully creates a fruitful and productive environment for an excellent education of the future generation of interdisciplinary scientists.

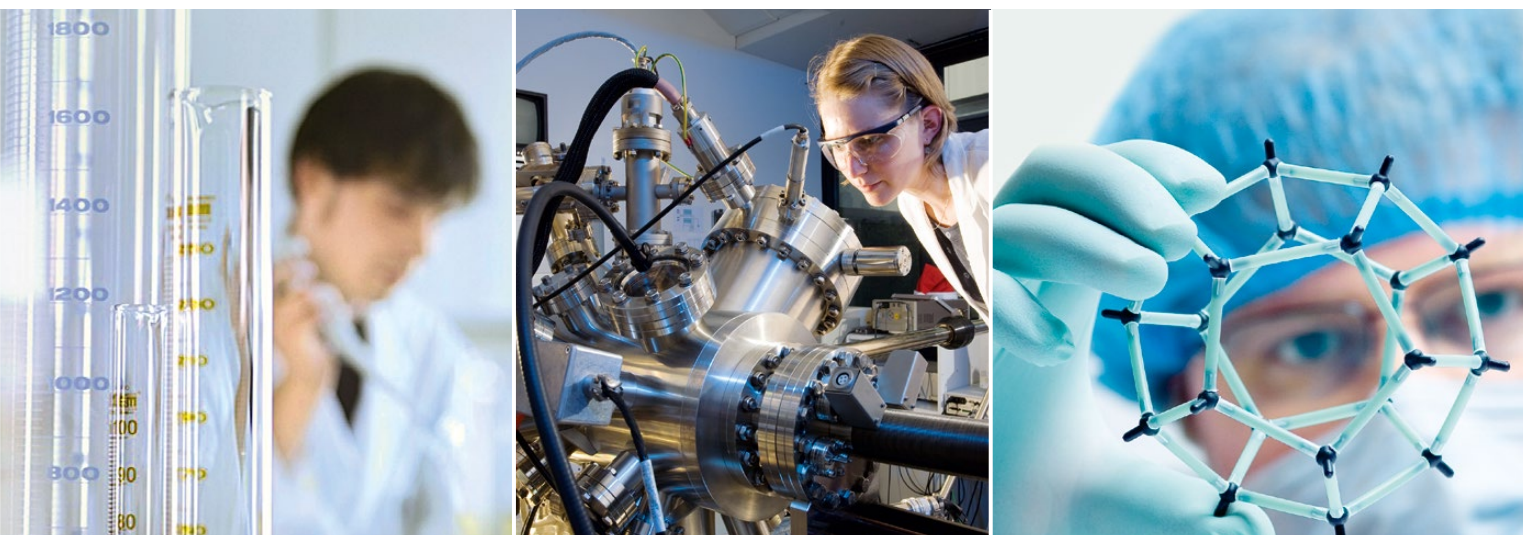
CONTACT

Speaker: *Professor Dr.-Ing. Hannsjörg Freund*

Program Director: *Dr. Marlene Reuschel*

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www.eam.fau.de/graduate-school



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, 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 lar-

ge series of seminal publications in first-class journals. Thus, we have prepared the ideal environment for the GSMS to develop into a world-leading center for academic education in Molecular Science.

Currently, 60 students are enlisted in the GSMS program with 24 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 skill 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.

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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 more than 500 partner universities all over the world. 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.

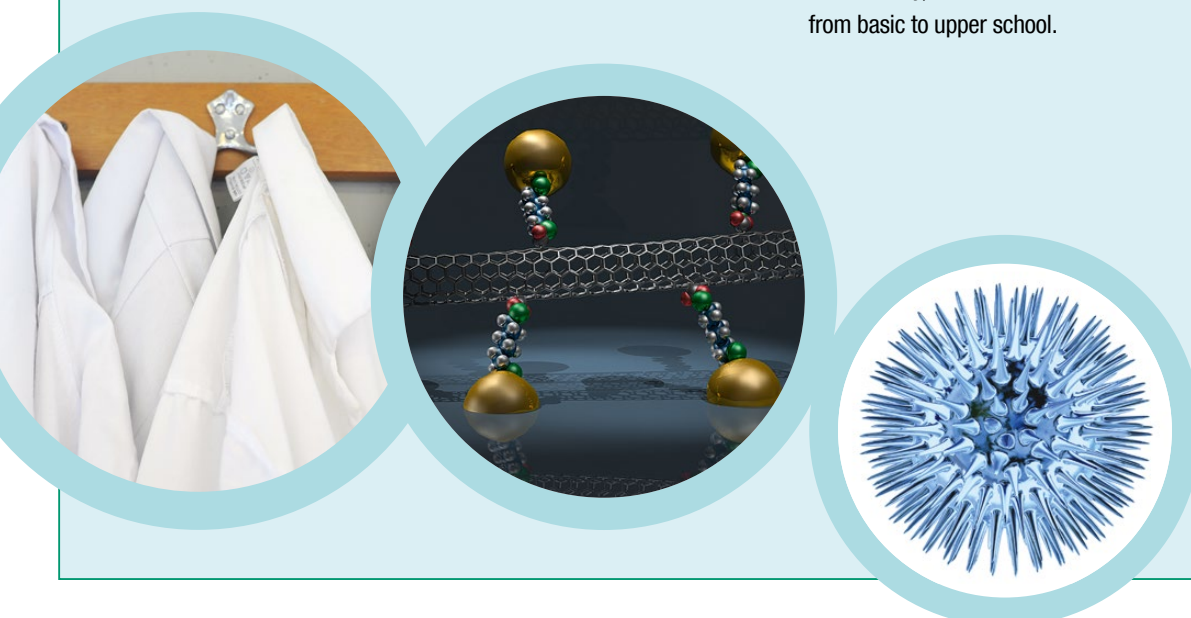
The University offers an enormous variety of subjects in more than 242 different degree courses. Even at undergraduate level students have many opportunities to experience advanced levels of research which enable them to benefit from the interdisciplinary, international and practically-oriented range of courses on offer.

The **Department of Chemistry and Pharmacy** is responsible for 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 1,800 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. programs ranging from medical to engineering sciences: every year more than 2,000 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 basic to upper school.





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

The established study course Chemistry is based on a wide-ranging basic and advanced education in the key subjects of chemistry. Students educated at FAU receive substantial chemical knowledge in all aspects 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. Basic principles are taught during the Bachelor program 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 program also includes a 6-month research project (master thesis) which usually concludes the course of study. The Master's degree program is taught in English.

Chemical expertise is relevant in many different fields related to energy, nutrition, health, mobility and communication. Chemical and pharmaceutical industry, research institutes, universities and the public sector are only a few employers who offer interesting job opportunities for our highly educated alumni.

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

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

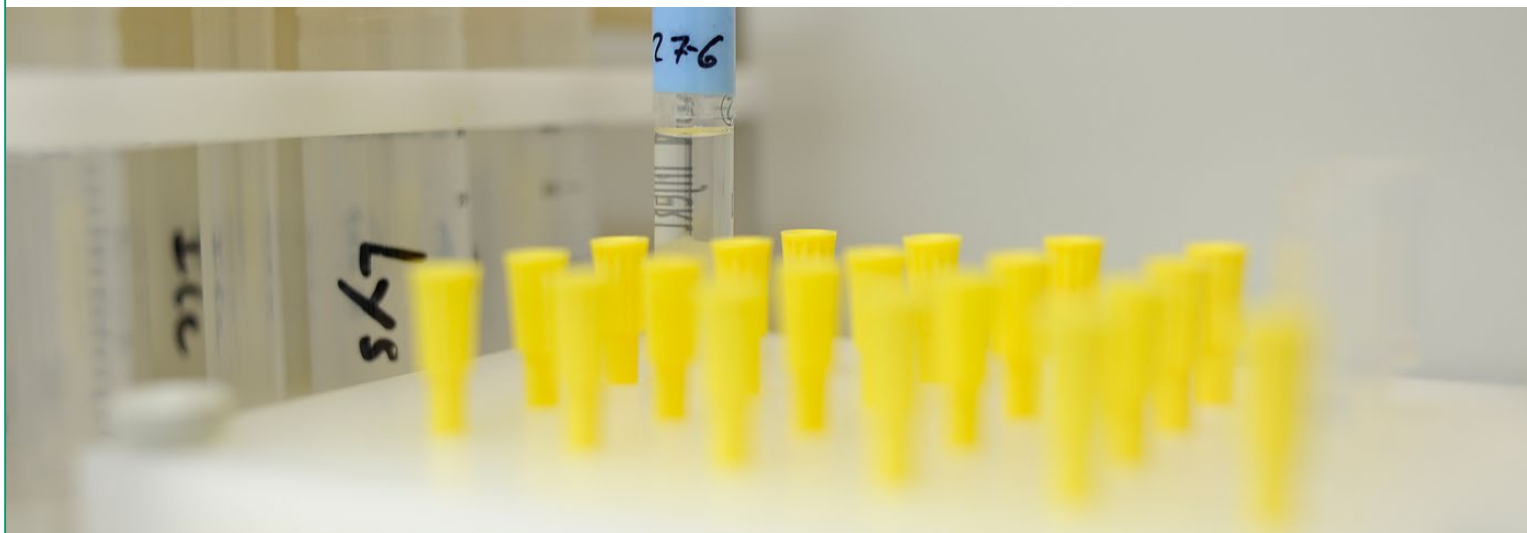
Current molecular sciences are profoundly interdisciplinary. Taking this into account, the Bachelor and Master degree programs Molecular Science are both science and technology oriented course programs including biochemistry, molecular biology, medicine, materials sciences, and pharmacy. The Bachelor program of six semesters consists of basic studies (which are related to the Chemistry degree 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 master modules Drug Discovery or Nano Science.

Molecular Science goes far beyond the general understanding of chemistry. The implementation of a two-year 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. The Master's degree program is taught in English. 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 materials sciences 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.

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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 of application.

Our four-year 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 discipline, 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 jobs 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 and private 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
PROF. DR. ANDREAS KOMETZ

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CURRICULUM VITAE

- 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** Secondary school teacher and class teacher, Hoyerswerda, Germany

Chemistry education, especially chemistry didactics, 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 faculty of the Teaching Methodology 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 its 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 its application at schools. Other fields of research contents “chemistry in context” as well as “media and experiments”.

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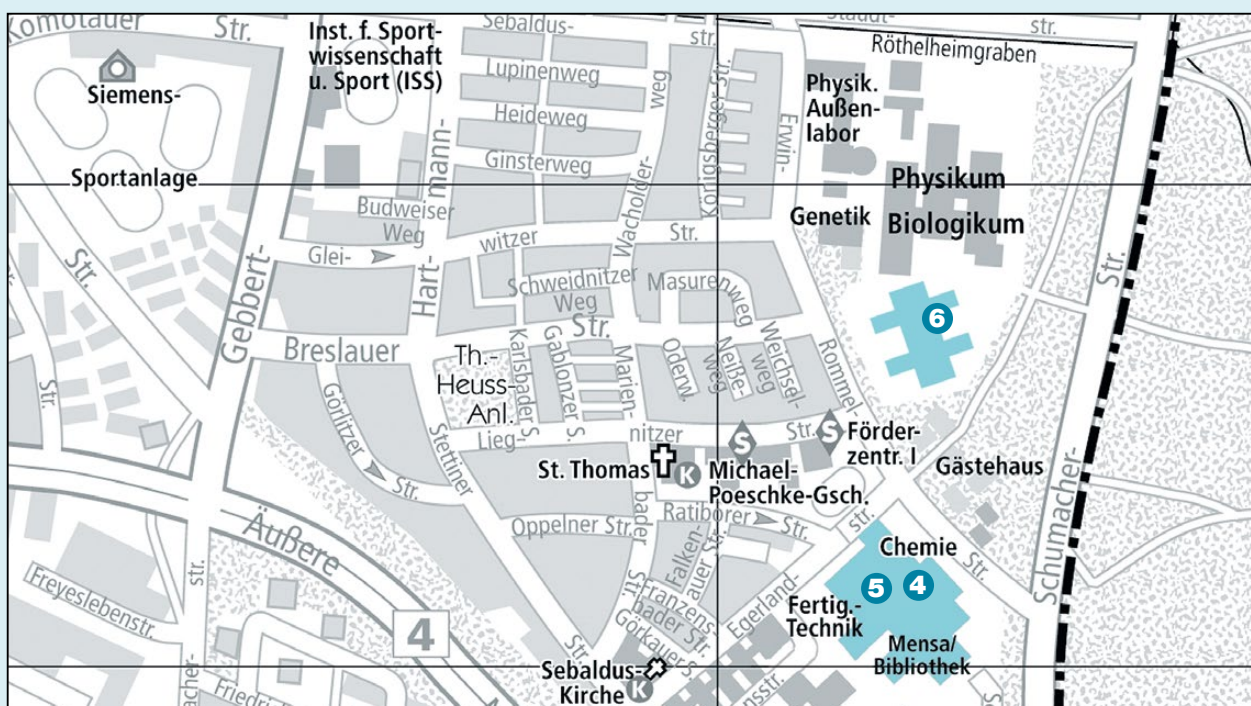


- 1 Pharmacy/Food Chemistry**, Schuhstr. 19, 91052 Erlangen
- 2 Organic Chemistry**, Henkestr. 42, 91054 Erlangen
- 3 Computer Chemistry Center**, Nägelsbachstr. 25, 91052 Erlangen
- 4 Inorganic Chemistry**, Egerlandstr. 1, 91058 Erlangen
- 5 Physical/Theoretical Chemistry**, Egerlandstr. 3, 91058 Erlangen
- 6 "Chemikum"**, under construction

ERLANGEN CITY



SOUTH CAMPUS



Site plan created by Ingenieurbüro für Kartographie Bernhard Spachmüller





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