

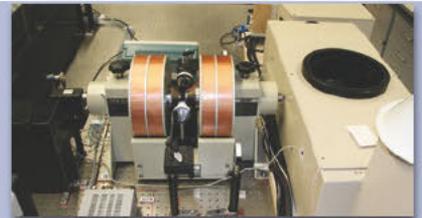
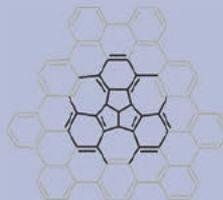
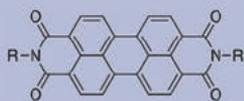
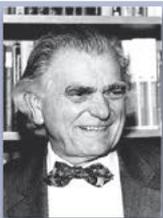
# Institut für Organische Chemie

Center for Nanosystems Chemistry

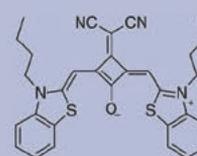
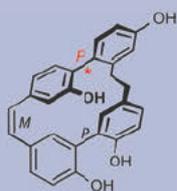
Julius-Maximilians-

**UNIVERSITÄT  
WÜRZBURG**

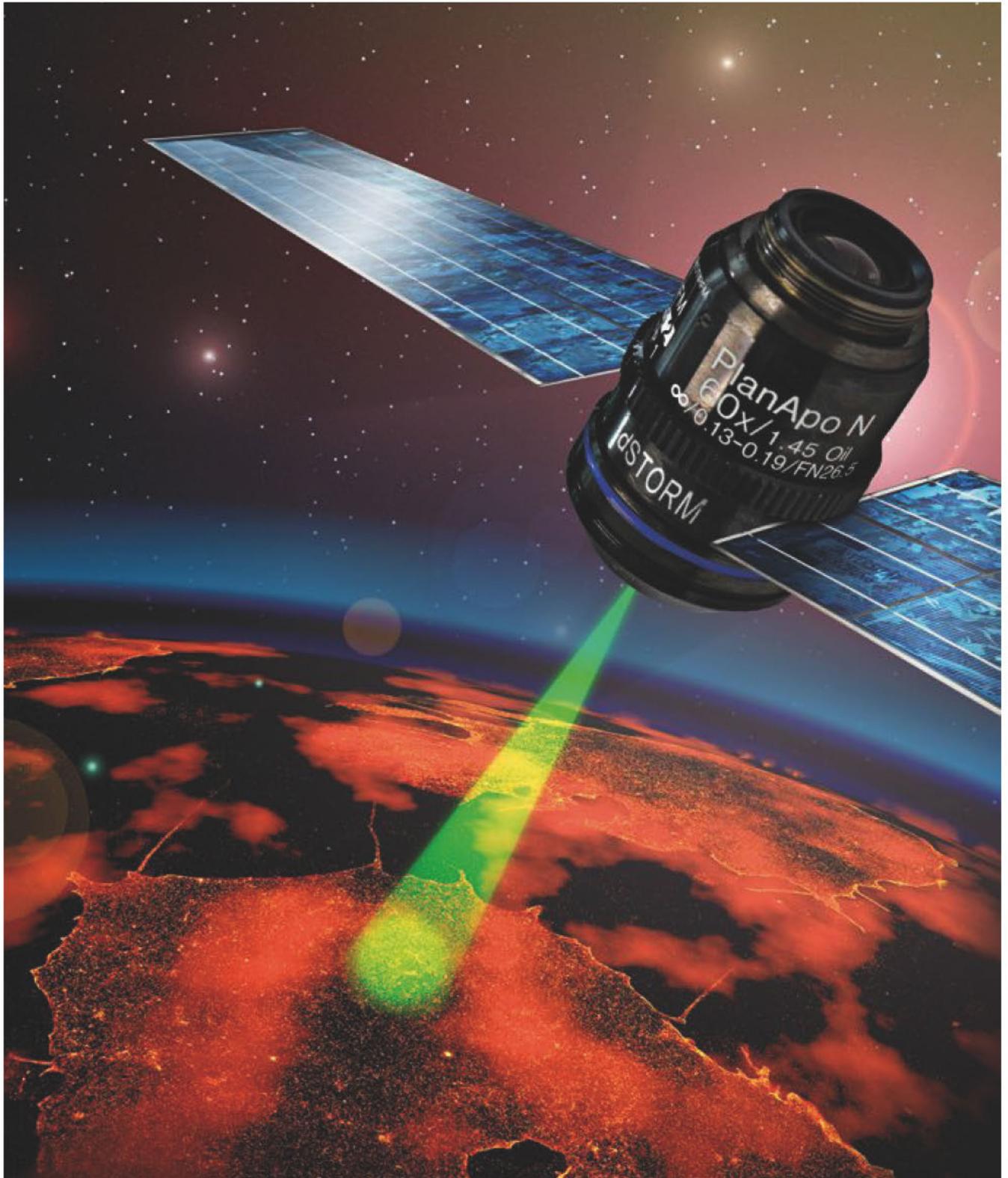




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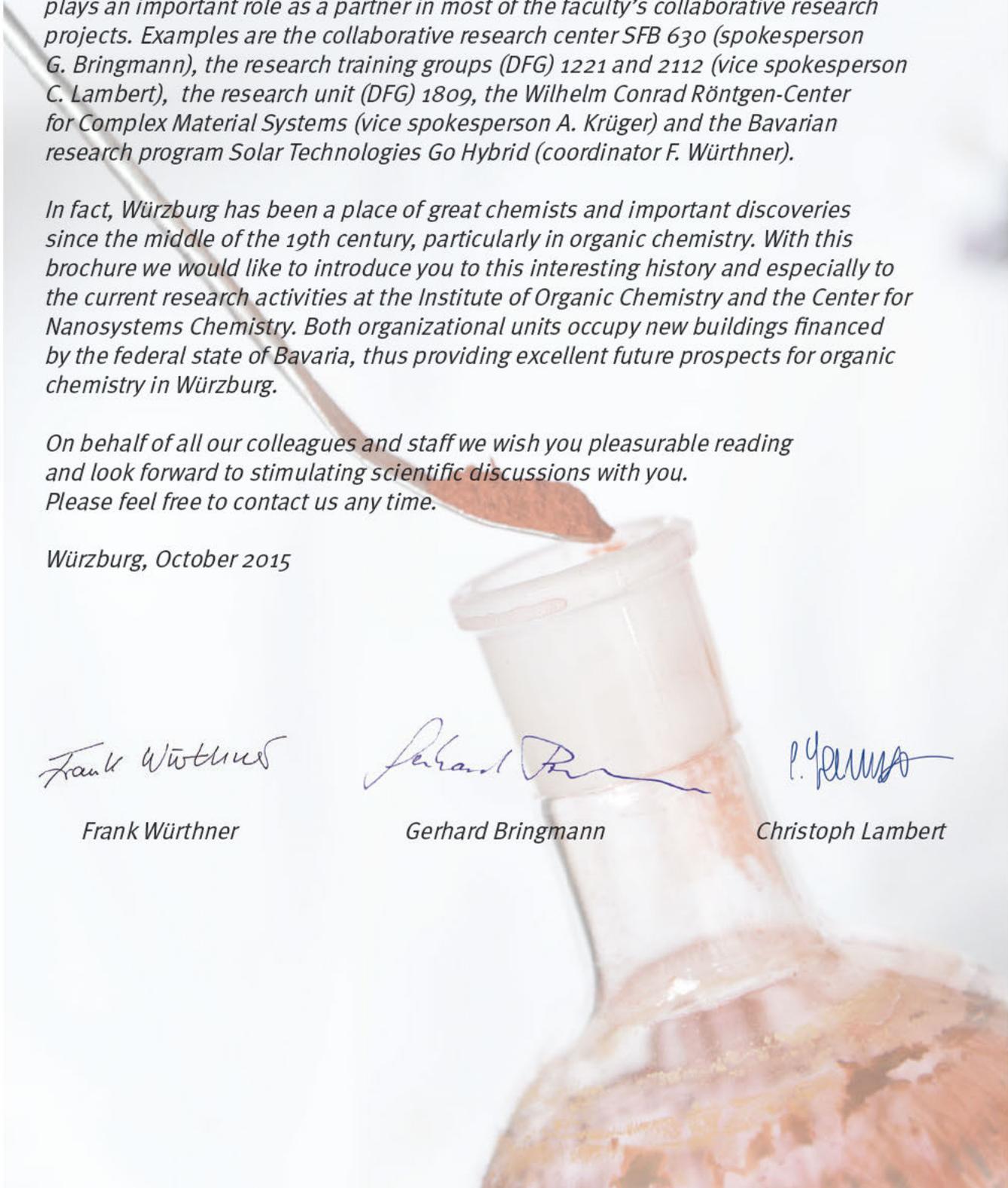
Dear Reader,

For more than ten years Würzburg's chemistry department has belonged to the top 40 in the Academic Ranking of World Universities ('Shanghai Ranking') where it currently ranks third amongst German universities. Here, the Institute of Organic Chemistry plays an important role as a partner in most of the faculty's collaborative research projects. Examples are the collaborative research center SFB 630 (spokesperson G. Bringmann), the research training groups (DFG) 1221 and 2112 (vice spokesperson C. Lambert), the research unit (DFG) 1809, the Wilhelm Conrad Röntgen-Center for Complex Material Systems (vice spokesperson A. Krüger) and the Bavarian research program Solar Technologies Go Hybrid (coordinator F. Würthner).

In fact, Würzburg has been a place of great chemists and important discoveries since the middle of the 19th century, particularly in organic chemistry. With this brochure we would like to introduce you to this interesting history and especially to the current research activities at the Institute of Organic Chemistry and the Center for Nanosystems Chemistry. Both organizational units occupy new buildings financed by the federal state of Bavaria, thus providing excellent future prospects for organic chemistry in Würzburg.

On behalf of all our colleagues and staff we wish you pleasurable reading and look forward to stimulating scientific discussions with you. Please feel free to contact us any time.

Würzburg, October 2015



Frank Würthner



Gerhard Bringmann



Christoph Lambert

### The History of Organic Chemistry in Würzburg

The history of academic education in Würzburg dates back as far as 1402 when a first short-lived university was founded. Almost 200 years later, in 1582, today's Julius-Maximilians University was re-inaugurated by Prince-Bishop Julius Echter of Mespelbrunn. It consisted of the faculties of theology, philosophy, law and medicine.

The history of chemistry as an academic discipline at the University of Würzburg begins in the 18th century when the reigning Prince-Bishop wanted the professors of medicine to give chemistry lectures and to show chemical experiments to their students. In the second half of the 18th century, physics and chemistry had become increasingly independent from medicine. Finally, in 1865, Würzburg's chemists secured their own new institute building located in the heart of the city between the residence and the cathedral.

Johann Joseph **von Scherer**, who had worked with Justus von Liebig in Gießen and had been appointed the first full professor of chemistry in Würzburg in 1847, moved into that building. He carried out important studies on biological pigments and proteins and is considered one of the founders of clinical chemistry. His successor was Adolph **Strecker**, well known for his amino acid synthesis. Chemistry in Würzburg separated from the faculty of Medicine and Strecker was the first to hold a chair of chemistry at the faculty of philosophy, from 1869 until his death in 1871. Another important organic chemist on that chair was Johannes **Wislicenus** who discovered the "geometrical isomerism" in lactic acid and made major contributions to stereochemistry supporting the theories of van't Hoff. In 1885 Wislicenus was followed by the later Nobel Prize winner Emil **Fischer**. Fischer stayed seven very fruitful years in Würzburg before moving on in 1892. In Würzburg he carried out the monumental studies on sugars that would yield him the Nobel Prize in 1902, and he proposed for the first time the „Lock and Key Model“ to visualize substrate and enzyme interactions. Moreover, thanks to Fischer's reputation the ministry in Munich granted funds for the construction of a new and much bigger chemistry building.



Sketch of the Chemical Institute planned by E. Fischer

The new institute, located at the Pleicher Ring (later renamed to Röntgenring), was inaugurated in 1896. Originally planned by Emil Fischer, it was probably the best-equipped chemistry building in Germany at the end of the 19th century. Arthur Hantzsch, who was the new head of the institute, had plenty of space and excellent conditions for his research. His syntheses of pyridine and pyrrole are well known contributions to synthetic organic chemistry, but his research interests in electrochemistry and spectroscopy also pioneered physical organic chemistry. In 1903 Hantzsch left Würzburg and Julius Tafel, a scholar with E. Fischer, became head of the institute. Just like his predecessor, Tafel showed great interest in electrochemistry and electrosynthesis. The "Tafel rearrangement" and the "Tafel equation" bear his name.

Tafel's successor in 1911 was the very renowned chemist and zymologist Eduard **Buchner**, who had already been awarded the Nobel Prize in 1907 for his discovery of cell-free alcoholic fermentation. He was very happy about the excellent conditions he found in Würzburg but only three years later World War I broke out and soon the institute suffered from lack of scientists and students. In 1917 Buchner was wounded in battle and died soon after. From 1918 to 1937 the situation at the institute was stable again with several extraordinary professors of chemistry and Otto **Dimroth** serving as the institute's director. Dimroth was a very complete synthetic chemist, working on heterocycles and natural products and also including aspects of physical organic chemistry. The "Dimroth rearrangement" and the "Dimroth condenser" are prominent examples of his scientific legacy. In 1938 F. G. **Fischer** became the head of the Institute of Chemistry shortly after the natural sciences separated from the faculty of philosophy to form the new faculty of natural sciences. His research interests included physiological chemistry and natural products.

In 1961 Siegfried **Hünig** came from Marburg via Munich to Würzburg to succeed F. G. Fischer. Just like his predecessors he started in the building planned by Emil Fischer, and he still was the only chair professor and director of the Institute of Chemistry. However, progress in chemistry and developments at other universities had shown already that the old structures should be replaced. Hünig himself had seen the benefits of modern structures during a visit to the USA. Thus, he supported the establishment of independent Institutes of Inorganic and Physical Chemistry in 1965. Moreover, Hünig, now director of the Institute of Organic Chemistry, solved infrastructural problems by planning a new chemistry center on the outskirts of Würzburg where it's still located today.

Of course Hünig was not only a far-sighted strategist but also an excellent researcher. His research topics included dyes, redox systems of stable radical ions, organic metals, rearrangements and electrochromics. N,N-Diisopropylethylamine, a very non-nucleophilic base for alkylations, is frequently called Hünig's base. The second chair of organic chemistry, established in the early 1960s was held by Alfred **Rödig** until 1978. Rödig's successor was Waldemar **Adam** who came to Würzburg from the USA in 1980. With Adam the institute became much more international and new aspects of organic chemistry were introduced since he also worked on metal-catalyzed reactions and photochemistry and cooperated with inorganic chemists, nutrition chemists and medical scientists. Adam published more than 1000 papers and was among the hundred most highly cited chemists in 2001.

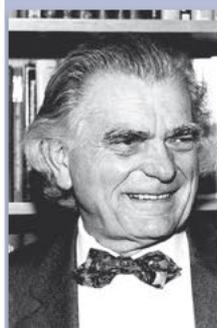
When Hünig retired in 1988 he was succeeded by Gerhard **Bringmann**, who is still in charge as one of the directors of the institute. Until 2002 the other director was Adam. After his retirement Frank **Würthner** accepted the call to the second chair of organic chemistry. In 2010 a third chair on physical organic chemistry was established and offered to Christoph **Lambert**. In addition to the three chairs, three permanent professor positions at the Institute of Organic Chemistry are currently held by Anke Krüger, Jürgen Seibel and Matthias Lehmann.



Emil Fischer  
1895



Siegfried Hünig  
1964



Waldemar Adam  
1999

## PAST, PRESENT AND FUTURE

The building planned by Hünig provided excellent research conditions for organic chemists over more than four decades. In 2013 the institute found a new home in a completely renovated building and in 2016 further laboratory and office space will become available in a new research building for the Center for Nanosystems Chemistry headed by Frank Würthner. The latter will particularly strengthen instrumental facilities with new units for materials characterization (X-ray diffraction and electron microscopy) and device fabrication, in addition to the already existing NMR spectroscopy and mass spectrometry facilities. Moreover, a great part of the additional space will be provided for independent junior research groups to continue a long-standing tradition of affording the best support to young scientists at the beginning of their independent careers.



Foundation Stone Ceremony for the  
Institute of Organic Chemistry  
on 11. March 1965  
(Photo: Main-Post/Röder)



Renovated building for the  
Institute of Organic Chemistry  
2013

Over the past five decades the following renowned chemists benefited from the excellent research conditions for junior researchers and associate professors at the Institute of Organic Chemistry before accepting the offer for a full professor position from another university:

E. Fahr (1956/75)  
F. Vögtle (1970/75)  
V. Jäger (1979/92)  
G. Erker (1985/90)  
M. Schmittel (1993/99)  
J. Hartung (1994/2002)  
U. Diederichsen (1999/2001)  
G. Fernández (2010/15)

G. Märkl (1959/71)  
H. Hopf (1975/78)  
G. Helmchen (1981/85)  
A. G. Griesbeck (1988/93)  
T. Linker (1993/98)  
C. Meier (1997/99)  
C. Schmuck (2002/08)

Th. Eicher (1963/74)  
H.-D. Martin (1975/80)  
H.-U. Reißig (1979/86)  
R. Brückner (1991/92)  
P. Bäuerle (1994/96)  
H. Ihmels (1997/2003)  
M. Breuning (2002/12)



### „Historical“ Award for the Institute of Organic Chemistry

The Institute of Organic Chemistry received one of 2014's American Chemical Society's Citation for Chemical Breakthrough awards for the outstanding work of Emil Fischer „About the Configuration of glucose and its isomers“.

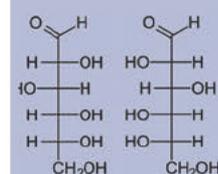
This award program honors publications, patents and books worldwide that have made breakthroughs in the field of chemistry. The criteria are very strict, which means that the advances in chemistry must have been revolutionary in concept, broad in scope, and long-term in impact.

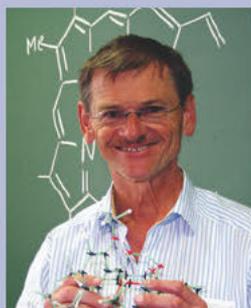
The award is given to the institution from which the award winning material was published rather than to the authors or inventors themselves, should they be alive. It was first presented in 2006 and after the University of Kiel (2011) the University of Würzburg is the second German university that has got this award.

Emil Fischer, who carried out research in Würzburg from 1885 to 1892, is one of the most well-known German chemists. His name is inseparably linked with the chemistry of sugars. Even today, each German high school student has to learn the Fischer projection formula of sugars.

Therefore is it not surprising that the award committee selected the publication of Emil Fischer „Über die Configuration des Traubenzuckers und seiner Isomeren“ („About the Configuration of glucose and its isomers“) in „Chemische Berichte“ from 1891. Also from today's perspective his research is still a brilliant feat of scientific art of experimentation and sharp mind. This becomes even more apparent when considering that at that times there were no modern spectroscopic analytical methods for the elucidation of the structure of a chemical compound such as nuclear magnetic resonance spectroscopy or infrared spectroscopy. Even the formula language of chemistry as we know it today, was still in its infancy and was far from being generally accepted.

Beside that Emil Fischer had to struggle with lack of space, primitive laboratory conditions and inadequate ventilation systems when he came to Würzburg in 1885, so that certain types of work could not be performed for technical reasons. From the outset he therefore endeavored to bring about a new institute building, which was finally granted to him in 1892 and led to the establishment of the most advanced chemistry laboratories of his time in Würzburg.





### Education and Academic Career of Prof. Dr. Dr. h.c. mult. Gerhard Bringmann

since 1987	Chair Professor, Institute of Organic Chemistry, University of Würzburg
1984	Habilitation University of Münster
1978-1979	Postdoctoral fellow with Prof. Sir D.H.R. Barton at the Institute de Chimie des Substances Naturelles of the C.N.R.S. in Gif-sur Yvette, Paris (France)
1978	Dr. rer. nat. (Chemistry), University of Münster
1970-1975	Study of Chemistry and Biology, Universities of Gießen and Münster

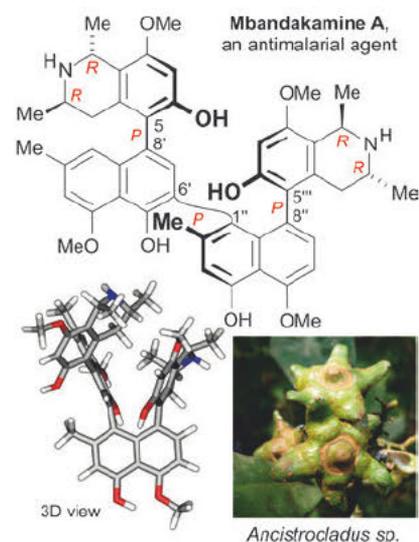
### Research Interests

Our group pursues natural products chemistry with structural, biosynthetic, and pharmacological facets. We approach this topic in a broad, highly interdisciplinary way, applying – and, in part, newly developing – novel efficient methods of analytical, synthetic, computational, and medicinal chemistry. Our special interest is devoted to stereochemical questions of all sorts of stereogenic centers (*C*- or *N*-based), axes (*C,C* or *C,N*,  $sp^2$ - $sp^2$  or  $sp^2$ - $sp^3$ ), of chiral ‘planes’ or helices, both analytically and synthetically, and we test and optimize their bioactivities. Starting from rewarding sources for novel natural products (e.g., tropical plant families), we search for novel anti-infective and anti-tumoral compounds including the online elucidation of their full absolute stereostructures, by applying our analytical triad HPLC-MS/MS-NMR-CD, assisted by quantum-chemical CD calculations (CD = circular dichroism). We elaborate synthetic pathways to the most rewarding metabolites using biomimetic or non-biomimetic strategies; as an example, we have developed the lactone method for the atropo-selective construction of highly hindered axially chiral biaryl and hetero-biaryl systems of any desired configuration.

### Our Current Research Topics:

#### From the Plant to the Agent

*C,C*- or *N,C*-coupled monomeric, or dimeric naphthylisoquinoline alkaloids (e.g., mbandakamine A) and related compounds: spectroscopically (LC-NMR, LC-MS, LC-CD) and bioassay-guided search for new bioactive natural products with antimalarial, anti-trypanosomal, antileishmanial, anti-HIV, or antitumoral activities from Asian and African Ancistrocladaceae and Dioncophyllaceae plants: isolation, structural elucidation, semi or total synthesis, cultivation of plants and plant cell cultures; elucidation of novel biosynthetic pathways to isoquinoline alkaloids; optimization of the pharmacological and toxicological properties of anti-infective naphthylisoquinoline alkaloids and anti-tumoral naphthoquinones, including their mode of action.



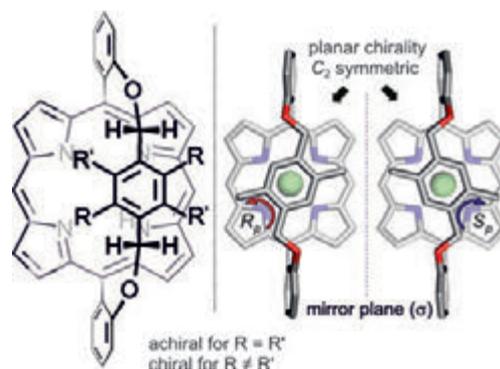
Y. Hemberger *et al.*, *Chem. Eur. J.* **2015**, *21*, 14507-14518; *Highly Antiplasmodial Non-Natural Oxidative Products of Dioncophylline A: Synthesis, Absolute Configuration, and Conformational Stability.*

G. Bringmann *et al.*, *Org. Lett.* **2013**, *15*, 2590-2593; *Mbandakamines A and B, Unsymmetrically Coupled Dimeric Naphthylisoquinoline Alkaloids, from a Congolese Ancistrocladus Species*

G. Bringmann *et al.*, *Chem. Eur. J.* **2012**, *19*, 916-923; *Jozimine A2: The First Dimeric Dioncophyllaceae-Type Naphthylisoquinoline Alkaloid, with Three Chiral Axes and High Antiplasmodial Activity.*

## Chiral Porphyrins Inspired by Nature

Synthesis of dimeric or bridged porphyrins with intrinsic axial, or planar, or helical chirality: resolution and configurational assignment of the enantiomers by LC-CD coupling in combination with quantum-chemical CD calculations; formation of a huge chirally modified cavity with useful imaginable applications; preparation of a broad variety of constitutionally symmetric and unsymmetric dimers with two different, freely combinable, mono-porphyrin subunits including bridged representatives; directed, i.e., atropo-/enantioselective synthesis of chiral mono-, bis- and triporphyrins; investigations of structural, chiroptical, photophysical, and electrochemical properties.



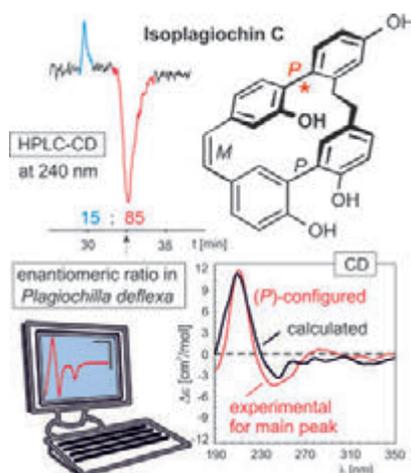
A. C. Gehrold *et al.*, *Org. Lett.* **2015**, *17*, 210-213; *Chiral and Achiral Basket-Handle Porphyrins: Short Synthesis and Stereostructures of These Versatile Building Blocks.*

T. Bruhn *et al.*, *Chem. Eur. J.* **2014**, *20*, 3998-4006; *C,C- and N,C-Coupled Dimers of 2-Aminotetraphenylporphyrins: Regiocontrolled Synthesis, Spectroscopic Properties, and Quantum-Chemical Calculations.*

C. Brückner *et al.*, *J. Am. Chem. Soc.* **2011**, *133*, 8740-8752; *Helimeric Porphyrinoids: Stereostructure and Chiral Resolution of meso-Tetraarylmorpholinochlorins.*

## Absolute Stereostructures by CD Calculations

Use of force field, semiempirical, density functional, coupled cluster, and ab-initio methods for the computational calculation of structures, dynamics, and chemical reactivities of molecules; prediction of NMR shifts; simulation of IR, Raman, and UV spectra; quantum-chemical calculations of circular dichroism (CD) spectra for the assignment of the absolute configuration of novel-type compounds with stereogenic centers, or with elements of axial, planar, or helical chirality, or combinations thereof; combination of LC-CD coupling with quantum-chemical CD calculations for the online elucidation of the absolute stereostructures of chiral compounds, directly from the peak in the chromatogram.



T. Bruhn *et al.*, *Chirality* **2013**, *25*, 243-249; *SpecDis: Quantifying the Comparison of Calculated and Experimental Electronic Circular Dichroism Spectra.*

Y. Hemberger *et al.*, *Chem. Eur. J.* **2013**, *19*, 15556-15564; *Pestalotiopens A and B: Stereochemically Challenging Flexible Sesquiterpene-Cyclopaldic Acid Hybrids from Pestalotiopsis sp.*

A. Schaumlöffel *et al.*, *Eur. J. Org. Chem.* **2012**, 6878-6887; *Configurational Assignment of Cyclic Bisbibenzyls by HPLC-CD and Quantum-Chemical CD Calculations.*

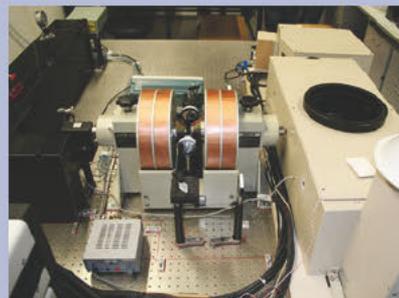


### Education and Academic Career of Prof. Dr. Christoph Lambert

since 2009	Chair (W3) of Physical Organic Chemistry, University of Würzburg
2009	Chair (W3) of Organic Chemistry, University of Bonn offered, declined
1999-2009	Professor (C3) of Organic Chemistry, University of Würzburg
1998	Habilitation in Organic Chemistry, University of Regensburg
1993-1994	Postdoc with Dr. R. Snaith, University of Cambridge, (UK)
1991-1993	Dr. rer. nat. (Chemistry), University of Erlangen-Nürnberg (with P. v. R. Schleyer)
1986-1991	Diploma (Chemistry), University of Erlangen-Nürnberg

### Research Interests

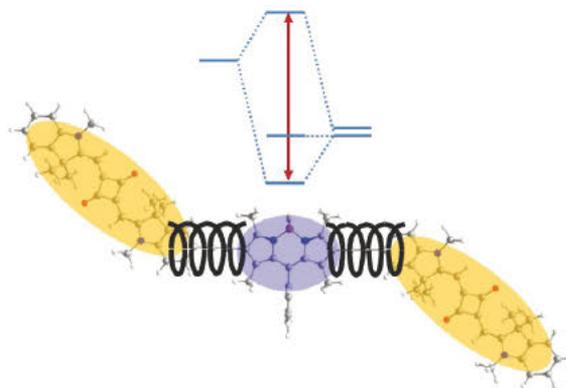
Electronic processes in functional  $\pi$ -systems are in focus of our group. We synthesise monomeric and polymeric  $\pi$ -conjugated compounds and investigate their electrochemical (cyclic voltammetry, spectroelectrochemistry in the UV/vis/NIR) and photophysical properties (steady-state absorption and emission spectroscopy, transient absorption spectroscopy in the fs- to  $\mu$ s time regime, fluorescence upconversion, magnetic-field dependent transient absorption measurements) concerning electron and energy transfer processes. A thorough understanding of these fundamental processes is a prerequisite for further development and optimisation of optoelectronic devices (e.g. OLED, OPV, OFET).



### Our Current Research Topics:

#### Low Band Gap Polymers

We synthesise squaraine dye homo- and copolymers with a low band-gap and spectrally broad absorption bands for light harvesting applications. The photophysical properties are explained using exciton coupling theory. Also low-molecular weight oligomers and conjugates with other dyes such as BODIPYs or pyrene are synthesised and investigated.

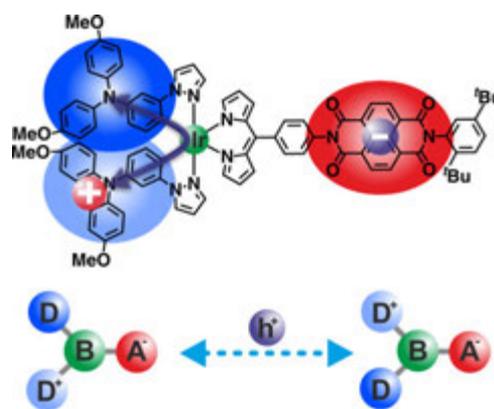


C. Lambert *et al.*, *J. Am. Chem. Soc.* **2015**, *137*, 7851-7861; *Energy Transfer Between Squaraine Polymer Sections: From Helix to Zigzag and All the Way Back.*

C. Lambert *et al.*, *J. Am. Chem. Soc.* **2015**, *137*, 3547-3557; *Coupled Oscillators for Tuning Fluorescence Properties of Squaraine Dyes.*

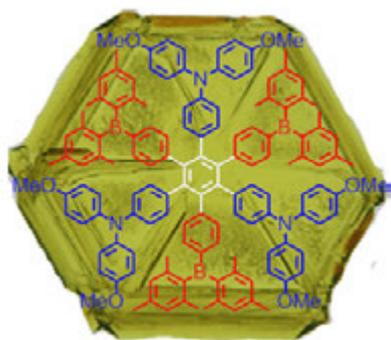
## Organic Mixed-Valence Compounds

Our research on MV compounds provides the basis for a better understanding of electron or hole transfer processes between various redox centres such as triaryl amines, perchlorinated triphenylmethyl radicals and triarylboranes. These redox centres are connected by saturated or conjugated bridges with different lengths and electronic properties. Besides (spectro)electrochemical and steady-state UV/Vis/NIR spectroscopy, dynamic EPR-spectroscopy helps us to analyse the optical and thermal electron transfer kinetics.



B. Y. Mladenova *et al.*, *J. Phys. Chem. C* **2015**, *119*, 8547-8553; *Investigations of the Degenerate Intra-molecular Charge Exchange in Symmetric Organic Mixed Valence Compounds: Solvent Dynamics of Bis(triarylamine)paracyclophane Redox Systems.*

C. Lambert *et al.*, *Chem. Commun.* **2014**, *50*, 11350-11353; *A photoinduced mixed-valence state in an organic bis-triarylamine mixed-valence compound with an iridium-metal-bridge.*



## Electron and Energy Transfer in Multidimensional Chromophores and Dendrimers

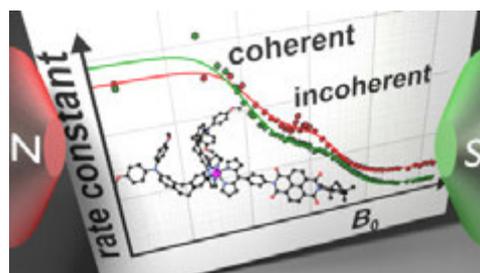
A well-defined alignment of several chromophores or redox centres as in hexaarylbenzenes (HABs) is a helpful prerequisite when studying electron or energy transfer processes because the orientation of the subunits determines many photophysical properties. Charge and energy transfer processes are investigated by steady-state and fs-time dependent fluorescence anisotropy spectroscopy.

M. Steeger *et al.*, *Phys. Chem. Chem. Phys.* **2015**, *17*, 11848-11867 *On the Relation of Energy and Electron Transfer in Multidimensional Chromophores Based on Polychlorinated Triphenylmethyl Radicals and Triaryl amines.*

F. Zieschang *et al.*, *J. Phys. Chem. C* **2013**, *117*, 19816-19831; *Solvent Controlled Energy Transfer Processes in Triarylamine-Triazole based Dendrimers.*

## Photoinduced Charge Transfer Processes in Redox Cascades and Transition Metal-Complexes

We investigate donor-acceptor substituted transition metal complexes in which the transition metal complex acts as bridge and photosensitizer by time resolved and magnetic field dependent transient absorption spectroscopy. The goal is to achieve long-lived charge separated states and to use spin chemistry to influence the lifetime.



J. H. Klein *et al.*, *J. Am. Chem. Soc.* **2015**, in press; DOI: 10.1021/jacs5bo4868. *Complete Monitoring of Coherent and Incoherent Spin Flip Domains in the Recombination of Charge-Separated States of Donor-Iridium Complex-Acceptor Triads.*

F. Zieschang *et al.*, *J. Phys Chem C* **2014**, *118*, 27698-27714; *Photoinduced Electron Transfer Dynamics in Triarylamine-Naphthalene Diimide Cascades.*



### Education and Academic Career of Prof. Dr. Frank Würthner

since 2010	Chair of the Center for Nanosystems Chemistry, University of Würzburg
since 2002	Chair Professor, Institute of Organic Chemistry, University of Würzburg,
1997-2001	Habilitation, University of Ulm
1995-1996	BASF Central Research Laboratories, Ludwigshafen
1994-1995	Feodor Lynen postdoctoral fellow (AvH), Massachusetts Institute of Technology (MIT), Cambridge/MA (USA)
1993	Dr. rer. nat. (Chemistry), University of Stuttgart
1990	Diploma (Chemistry), University of Stuttgart

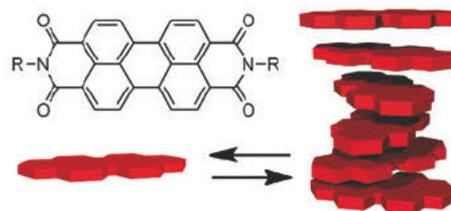
### Research Interests

Our research is devoted to the development of advanced organic materials based on functional dyes such as perylene and naphthalene bisimides, merocyanines, squaraines, chlorins and diketopyrrolopyrroles by employing supramolecular approaches. Towards this objective, we design and synthesize novel molecular building blocks and explore their self-assembly into nanoscale architectures and liquid-crystalline and crystalline solid-state materials that are applied in (opto-)electronic and photovoltaic devices as well as in photocatalytic water splitting.

### Our Current Research Topics:

#### Dye Assembly

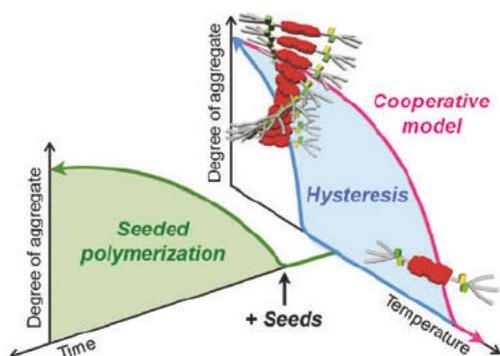
Mechanistic elucidation, including thermodynamic and kinetic analyses of self-assembly processes of functional dyes by UV/Vis/NIR absorption, fluorescence and CD spectroscopy and isothermal titration calorimetry. Structural and morphological characterization of supramolecular assemblies by 2D NMR, DLS, high-resolution MS, AFM, STM, SEM and TEM. Exploration of electrochemical and photo-physical properties of supramolecular assemblies by cyclic voltammetry, spectroelectrochemistry and time-resolved spectroscopy.



F. Würthner *et al.*, *Chem. Ref.* **2015**; DOI: 10.1021/ACS.Chemrev.5b00188 *Perylene Bisimide Dye Assemblies as Archetype Funktional Supramolecular Materials*.

C. Shao *et al.*, *Angew. Chem. Int. Ed.* **2013**, 52, 7482-7486; *Quadruple  $\pi$  Stack of Two Perylene Bisimide Tweezers: A Bimolecular Complex with Kinetic Stability*.

J. Sung *et al.*, *Nat. Commun.* **2015**, DOI:15-07331C; *Direct Observation of Ultrafast Coherent Exciton Dynamics in Helical  $\pi$  Stacks of Self-assembled Perylene Bisimides*.



#### Supramolecular Polymers and Soft Matter

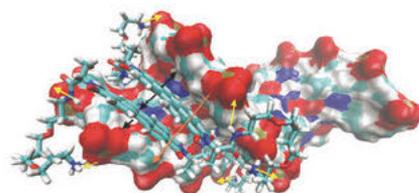
Construction of supramolecular polymers and block copolymers of functional dyes by seeded living polymerization and elucidation of their (opto) electronic properties. Development of thermotropic and lyotropic (chromonic) liquid-crystalline and gel materials based on H-bonding perylene bisimides and squaraines. Analysis of condensed phase materials by POM, DSC and XRD techniques

S. Ogi *et al.*, *J. Am. Chem. Soc.*, **2015**, 137, 3300-3307; *Mechanism of Self-Assembly Process and Seeded Supramolecular Polymerization of Perylene Bisimide Organogelator*.

D. Görl *et al.*, *Nat. Commun.* **2015**, 6, 7009; *Supramolecular block copolymers by kinetically controlled co-self-assembly of planar and core-twisted perylene bisimides*.

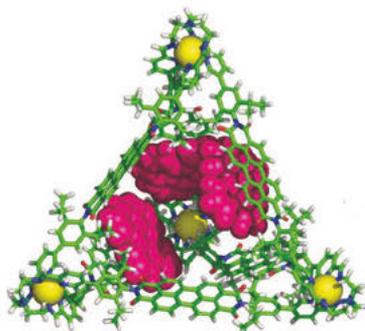
## Interaction with Biomacromolecules

Development of water-soluble fluorescent dyes and their supramolecular assemblies and exploration of their interactions with biological components like DNA, proteins, and cellular systems for sensing, imaging and therapeutic applications.



J. Gershberg et al., *Chem. Eur. J.* **2015**, 21, 7886-7895; Sensing of Double-Stranded DNA/RNA Secondary Structures by Water Soluble Homochiral Perylene Bisimide Dyes.

F-P. Gao et al., *Biomaterials* **2014**, 35, 1004-1014; Supramolecular Adducts of Squaraine and Protein for Noninvasive Tumor Imaging and Photothermal Therapy in Vivo.



## Photofunctional Macrocycles

Synthesis of multichromophoric macrocycles and elucidation of their self-organization on surfaces by e.g. scanning probe microscopy (AFM/STM) as well as characterization of their host-guest complexation and photophysical properties.

P. Spenst et al., *Angew. Chem. Int. Ed.* **2015**, 54, 10165-10168; A Perylene Bisimide Cyclophane as a "Turn-On" and "Turn-Off" Fluorescence Probe.

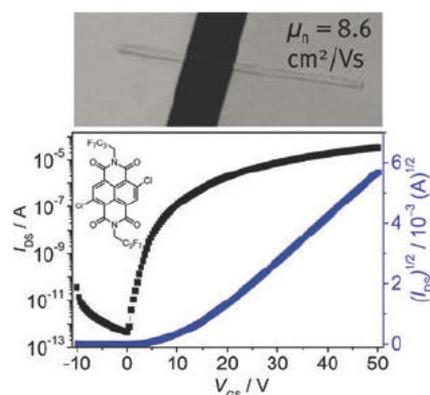
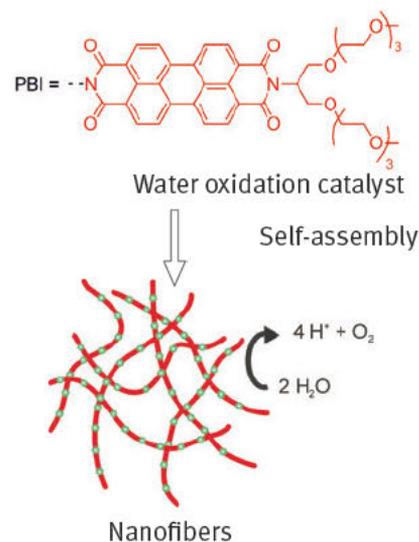
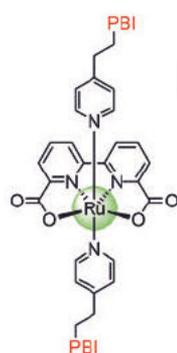
J-E. Lee et al., *ACS Nano* **2013**, 7, 5064-5076; Structure-Property Relationship of Perylene Bisimide Macrocycles Probed by Atomic Force Microscopy and Single-Molecule Fluorescence Spectroscopy.

## Supramolecular Photocatalysis

Development of multicomponent architectures containing functional dye based light harvesting antennae systems and photosensitizers as solar fuel production catalysts for the implementation into photo-reactors. Construction of metallosupramolecular architectures like one-dimensional nanofibers or two-dimensional macrocycles containing ruthenium water oxidation catalysts.

V. Kunz et al., *Chem. Commun.* **2015**, 51, 290-293; Embedding of a Ruthenium(II) Water Oxidation Catalyst into Nanofibers via Self-assembly.

P. Frischmann et al., *Chem. Soc. Rev.* **2013**, 42, 1847-1870; Powering the Future of Molecular Artificial Photosynthesis with Light-Harvesting Metallosupramolecular Dye Assemblies.



## Organic Electronics & Photovoltaics

Highly purified functional small molecules can be processed either from solution or by sublimation in vacuum to investigate their propensity as solid state materials for applications in organic thin-film transistors and organic bulk heterojunction solar cells. Structure properties relationships are established by correlation between single crystal and thin-film X-ray analysis.

A. Lv et al., *Angew. Chem. Int. Ed.* **2015**, 54, 10512-10515; Head-to-Tail Zig Zag Packing of Dipolar Merocyanine Dyes Affords High-Performance Organic Thin-Film Transistors.

T. He et al., *Nat. Commun.* **2015**, 6, 5954; Single-Crystal Field-Effect Transistors of new Cl<sub>2</sub>-NDI Polymorph Processed by Sublimation in Air.

A. Arjona-Esteban et al., *J. Am. Chem. Soc.* **2015**, 137, DOI: 10.1021/jacs.5b08386 Influence of solid state packing of dipolar merocyanine dyes on transistor and solar cell performance.



### Education and Academic Career of Dr. Florian Beuerle

since 2010	Junior Research Group Leader, Institute of Organic Chemistry, University of Würzburg
2008-2010	Feodor Lynen postdoctoral fellow (AvH), Northwestern University, Evanston/IL (USA) with Prof. Dr. J. Fraser Stoddart
2008	Dr. rer. nat. (Chemistry), University of Erlangen with Prof. Dr. Andreas Hirsch
2005	Diploma (Chemistry), University of Erlangen

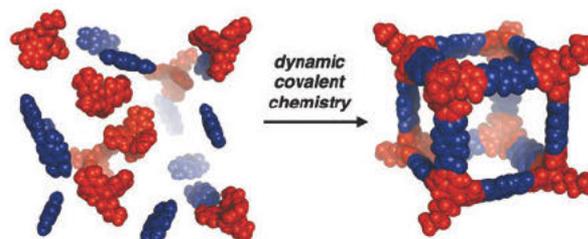
### Research Interests

Research in our group is focused on the development of functional porous materials such as metal-organic frameworks, covalent organic frameworks or organic cage compounds. In order to achieve this aim, we design and synthesize small organic building blocks possessing unusual geometries and shapes and elaborate on their self-assembly into complex molecular architectures utilizing various cross-linking motifs such as supramolecular interactions, dynamic covalent chemistry or metal coordination.

### Our Current Research Topics:

#### Covalent Organic Cage Compounds

Design and Synthesis of covalent organic cage compounds built by self-assembly of tribenzotriquinacene (TBTQ) building blocks through dynamic covalent reactions such as boronate ester formation or imine condensation. Size and shape of the cages can be controlled by molecular design of the organic building blocks. Structural characterization of cage compounds by 1D and 2D NMR, MS, UV/Vis.

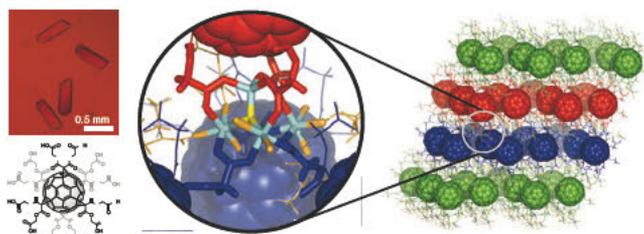


S. Klotzbach *et al.* *Chem. Commun.* **2014**, 50, 12454-12457; *Dynamic covalent assembly of tribenzotriquinacenes into molecular cubes.*

S. Klotzbach *et al.*, *Angew. Chem. Int. Ed.* **2015**, 54, 10356-10360; *Shape-Controlled Synthesis and Self-Sorting of Covalent Organic Cage Compounds*

#### Metal-Organic Frameworks

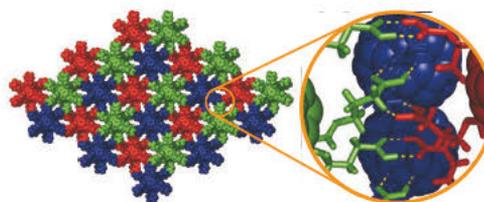
Design and Synthesis of highly functionalized [60]fullerene derivatives with octahedral addition pattern and their incorporation as organic connectivity centers in metal-organic frameworks. Materials are synthesized by various crystallization techniques or solvothermal reactions. Characterization by X-ray, PXRD, sorption measurements, TGA, elemental analysis, UV/Vis, NMR, MS.



K. Müller-Buschbaum *et al.*, *Microporous Mesoporous Mater.* **2015**, 216, 171-199; *MOF based luminescence tuning and chemical/physical sensing.*

## Supramolecular Frameworks

Utilization of weak supramolecular interactions such as hydrogen bonding or boron-nitrogen dative bonds for the self-assembly of supramolecular cage compounds or extended frameworks. Organic synthesis of small molecule precursors and analysis of supramolecular assemblies by X-ray, 1D and 2D NMR, MS, UV/Vis, ITC.



A. Kraft *et al.*, *Eur. J. Org. Chem.* **2014**, 48, 10401-10403; *Arranging Fullerenes through Hydrogen Bonding.*

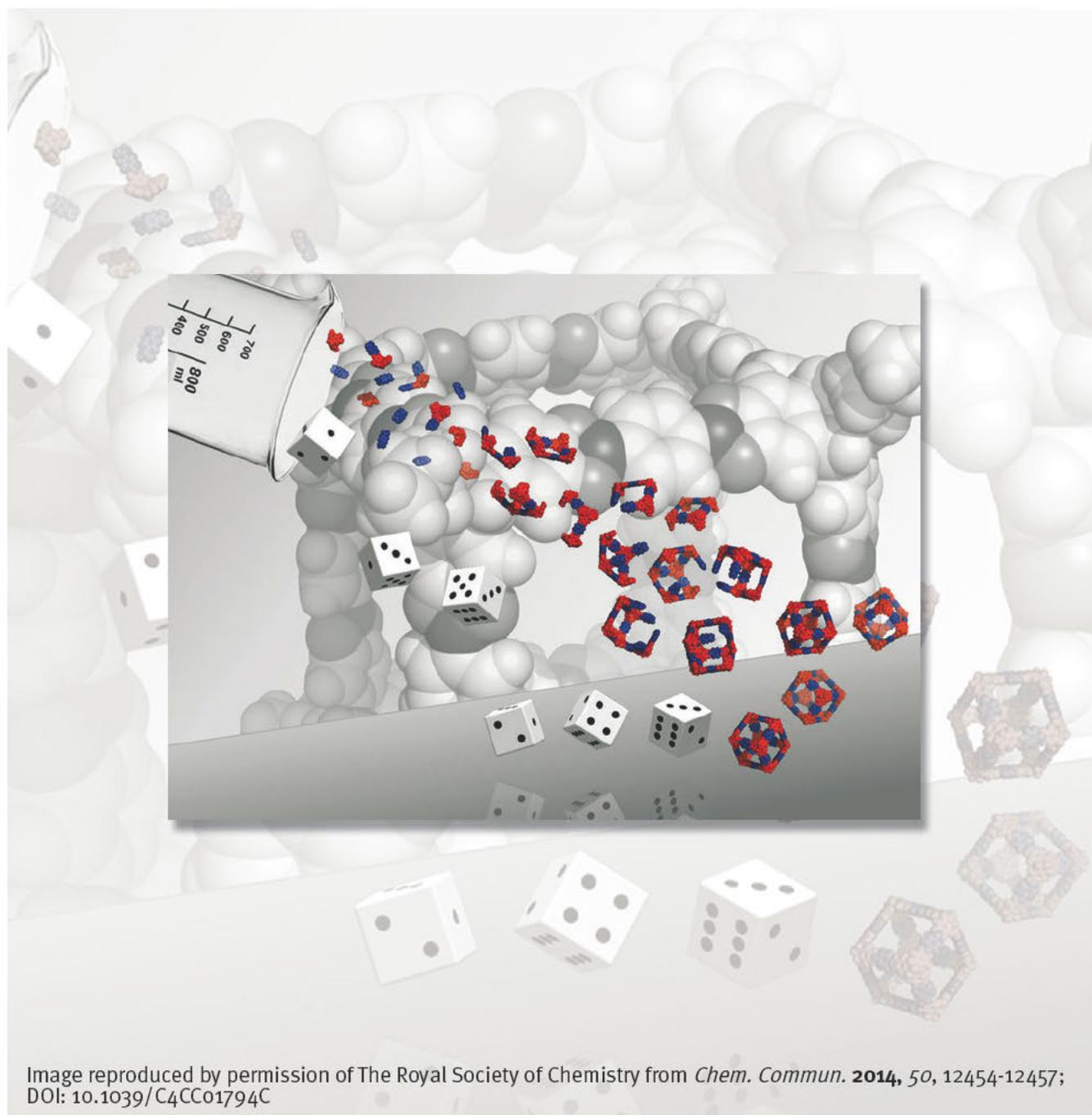


Image reproduced by permission of The Royal Society of Chemistry from *Chem. Commun.* **2014**, 50, 12454-12457; DOI: 10.1039/C4CC01794C



### Education and Academic Career of Prof. Dr. Anke Krueger

Since 2008	Professor of Organic Chemistry, Institute of Organic Chemistry, University of Würzburg
2007-2008	Junior Professor of Organic Chemistry, Institute of Organic Chemistry, Kiel University
2003-2006	Liebig Fellow, Institute of Organic Chemistry, Kiel University
2000-2002	Feodor Lynen (AvH)/JSPS fellow, Toyohashi University of Technology (Japan)
2000	Dr. rer. nat. (Chemistry), Technical University of Braunschweig
1997	Diploma (Chemistry), Technical University of Braunschweig

### Research Interests

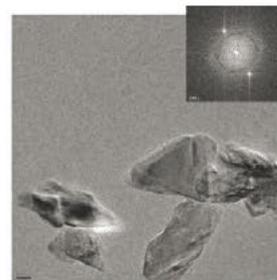
Our research is centered around the properties of carbon-rich materials and compounds. We work on the production of nanoscale carbon materials such as diamond nanoparticles, their characterization and functionalization. For this goal we develop novel functionalization techniques for carbon materials and apply these in the derivatization of diamond and other nanoparticles. Functional nanodiamond can be used for applications such as bio-imaging using non-bleaching lattice defects, composite materials for biomedical applications, catalysis and coatings with unique mechanical, electronic and thermal properties. Furthermore, we work on the synthesis and properties of carbon-rich molecules such as non-planar aromatic compounds and investigate their spectroscopic and electronic properties. Since 2015 Anke Krueger is Coordinator of the European Project DIACAT.



### Our Current Research Topics:

#### Nanoparticles and Nanocolloids

Development of methods for the production of diamond and other nanoparticles with controlled surface structure and defect density using wetchemical and mechanochemical techniques. Exploration of the properties of nanodiamond particles with different dopants such as boron, silicon and nitrogen and their application for quantum engineering, photocatalysis and imaging.



S. Heyer *et al.*, *ACS Nano* **2014**, *8*, 5757-5764; *Towards Deep Blue Nano Hope Diamonds: Heavily Boron-doped Diamond Nanoparticles.*

A. Muzha *et al.*, *Appl. Phys. Lett.* **2014**, *105*, 243112; *Room-temperature near-infrared silicon carbide nanocrystalline emitters based on optically aligned spin defects.*

E. Neu *et al.*, *Appl. Phys. Lett.* **2011**, *98*, 243107; *Narrowband fluorescent nanodiamonds produced from chemical vapor deposition films.*

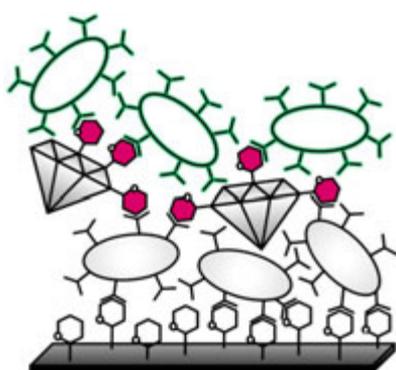
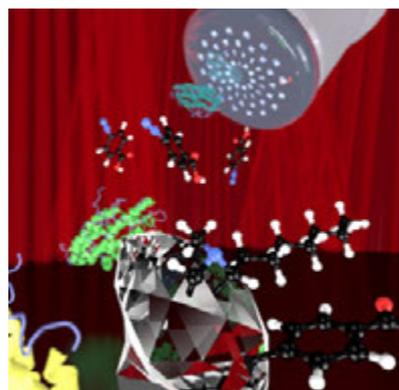
## Surface Chemistry of Carbon Nanomaterials

Exploring the surface reactivity of carbon nanomaterials. Development of novel reactions for the controlled derivatization of diamond using reactions enabling the immobilization of more complex moieties in a controlled manner.

G. Jarre *et al.*, *Beilstein J. Org. Chem.* **2014**, *10*, 2729-2737; *Synthesis of nanodiamond derivatives carrying amino functions and quantification by a modified Kaiser test.*

G. Jarre *et al.*, *Chem. Commun.* **2011**, *47*, 544-546; *Playing the surface game - Diels Alder reactions on diamond nanoparticles.*

T. Meinhardt *et al.*, *Adv. Funct. Mater.* **2011**, *21*, 494-500; *Pushing the functionality of diamond nanoparticles to new horizons - orthogonally functionalized nanodiamond using click chemistry.*



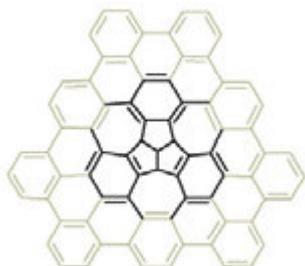
## Nanodiamond Composite Materials

Synthesis of diamond composite materials for applications such as bone implant materials, functional coatings and supercapacitors.

Y. Sun *et al.*, *Macromol. Mater. Eng.* **2015**, *300*, 436-447; *Reinforced degradable biocomposite by homogenously distributed functionalized nanodiamond particles.*

S. Suliman *et al.*, *J. Control. Release* **2015**, *197*, 148-157; *Release and bioactivity of bone morphogenetic protein-2 are affected by scaffold binding technique in vitro and in vivo.*

Z. Xing *et al.*, *Tissue Engin.* **2013**, *19*, 1783-1791; *Biological effects of functionalizing copolymer scaffolds with nano-diamond particles.*



M. S. Schuurman *et al.*, *Chem. Eur. J.* **2015**, in press; DOI: 10.1002/chem.201501624; *The Photodissociation Dynamics of Cyclopropenyliene, c-C<sub>3</sub>H<sub>2</sub>*

P. Constantinidis *et al.*, *J. Phys. Chem. A* **2014**, *118*, 2915-2921; *Electronic Spectroscopy of 1-Phenylethynyl-Naphthalene*

Y. Kirchwehm *et al.*, *Chem. Commun.* **2012**, *48*, 1502-150; *Ortho-methylated tribenzotriquinacenes – paving the way to curved carbon networks*

## Biofunctionalization of Carbon Nanomaterials

Synthesis of functional conjugates of nanodiamond with bioactive compounds such as saccharides, enzymes, antibodies etc. and exploration of their properties for imaging, detection and drug delivery.

C. Fessele *et al.*, *Eur. J. Org. Chem.* **2015**, 5519-5525; *Thiourea-bridged Nanodiamond Glycoconjugates as Inhibitors of Bacterial Adhesion.*

M. Hartmann *et al.*, *Chem. Eur. J.* **2012**, *18*, 6485-6492; *Saccharide-modified nanodiamond conjugates for the efficient detection and removal of pathogenic bacteria.*

G. Dördelmann *et al.*, *Chem. Commun.* **2012**, *48*, 11528-11530; *Cu-AAC click functionalization of azide-modified nanodiamond with a photoactivatable CO releasing molecule (PhotoCORM) based on [Mn(CO)<sub>3</sub>(tpm)]<sup>+</sup>.*



## Carbon-Rich Molecules

Synthesis of carbon-rich molecules such as non-planar aromatic molecules and precursors for highly energetic molecular species for their spectroscopic investigation and for the gain of deeper understanding of the molecular structure and electronic properties of nanocarbon surfaces.



### Education and Academic Career of Prof. Dr. Matthias Lehmann

since 2011	Professor, Institute of Organic Chemistry, University of Würzburg
2010-2011	Heisenberg fellowship, University of Würzburg
2009 - 2010	apl. Professor, Chemnitz University of Technology
2003 - 2009	Juniorprofessor, Chemnitz University of Technology
2000-2003	Postdoctoral researcher, Université Libre de Bruxelles (BEL)
1999-2000	Postdoctoral researcher, Universidad de Zaragoza (ESP)
1999	Dr. rer. nat. (Chemistry), University of Mainz
1995	Diploma (Chemistry), University of Mainz

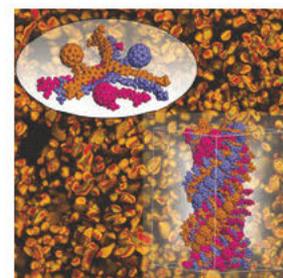
### Research Interests

Our research aims the design of novel liquid crystalline (LC) materials consisting of compounds with nonconventional shapes such as stars, V-shaped or board-shaped molecules. The star topology is generated by symmetric attachment of three to six arms to a core unit. We achieve the control of the self-assembly in LC materials by the variation of the core, the arm scaffold, and the peripheral chains. Detailed understanding of the stacking procedures in the solid-state by nanosegregation and space-filling allows the incorporation and positioning of functional building blocks. This converts the compounds in complex functional LC materials, which can be applied in organic electronics. Board- and V-shaped mesogens are investigated with respect to the formation of the highly elusive biaxial nematic mesophase. Biaxial nematogens are proposed as new materials for future fast-switching LC-Displays.

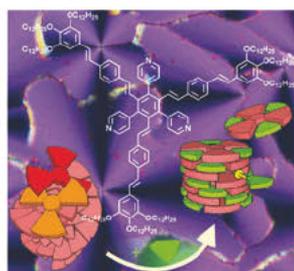
### Our Current Research Topics:

#### Star-shaped Hybrid Materials – Donor-Acceptor Dyades and Triades

Shape-persistent stars with arms consisting of conjugated oligomers possess empty space which is filled by covalently bound fullerenes and other nanoparticles via spacers to form hybrid materials between organic and inorganic materials. These may be a combination of donors and acceptors (dyades). The structures are uncovered by X-ray scattering (SAXS, MAXS, WAXS, GISAXS), modelling (Materials Studio) and X-ray simulation. The optical properties are studied by UV-Vis- and fluorescence spectroscopy. Depending on the core unit also triades can be designed, which are potential interesting materials for photovoltaic applications.



M. Lehmann, M. Hügel, *Angew. Chem. Int. Ed.* **2015**, *54*, 4110-4114; *A Perfect Match: Fullerene Guests in Star-Shaped Oligophenylenevinylene Mesogens*, German Version: *Angew. Chem.* **2015**, *127*, 4183-4187.



#### Supramolecular Crowded Stars

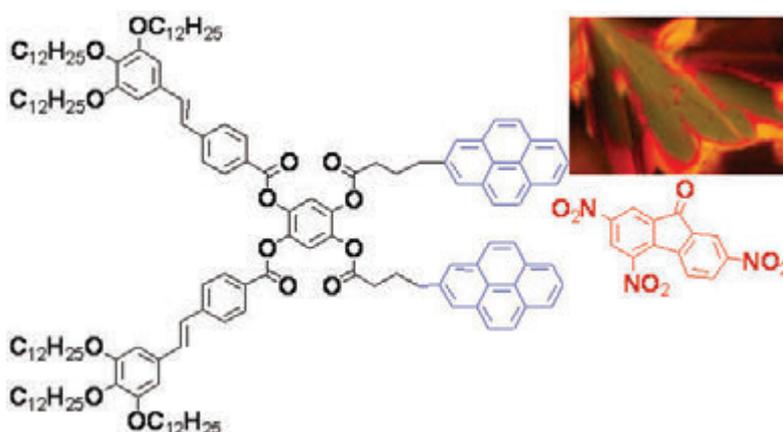
Space-filling of void in shape-persistent molecular structures forming LC materials is a novel exciting research topic in liquid crystals science. For hexasubstituted benzene derivatives every second substituent is a long arm scaffold generating the free space, whereas the other substituents are small functionalised phenyl building blocks. With this design LC-Endoreceptors are developed, which can uptake at maximum three guests. We study how the guests influence the self-assembly and the physical properties by polarised optical microscopy (contact samples), DSC (phase diagrams), FT-IR microscopy and X-ray scattering. The space is controlled by the length of the conjugated oligomer arms, thus even the size of the guests and their functionality can be adjusted for future applications.

M. Lehmann, P. Maier, *Angew. Chem. Int. Ed.* **2015**, *54*, 9710-9714; *Shape-Persistent, Sterically Crowded Star Mesogens: From Exceptional Columnar Dimer Stacks to Supermesogens*; German Version: *Angew. Chem.* **2015**, *127*, 9846-9850.

### Semiflexibel Stars with Stilbene, Acene and Pyrene Chromophores

Semiflexible oligobenzoate stars fold to various conformers in order to optimise the packing into liquid crystal phases. Thus E- and cone-shaped conformers are formed and self-assemble in lamellar, columnar, cubic bicontinuous and cubic micellar phases. The preorganisation, for example in four-arm stars, is used to control the folding and generates

Janus-type liquid crystals with stilbene, acene or pyrene moieties showing host-guest chemistry with electron deficient chromophores leading to novel LC structures.



M. Lehmann, "Star-Shaped Mesogens" in Handbook of Liquid Crystals, 2nd edition, Vol. 5, Chapter 5 (eds. J. W. Goodby et al.), ISBN 978-3-527-32773-7, Wiley-VCH, Weinheim, 2014.

### Solid-State Assisted Synthesis

The control over the formation of mesophases on a nanoscale is achieved by nanosegregation of various building blocks and also by the attachment of incompatible flexible chains (alkyl, oligoethyleneoxy, semiperfluorinated chains). The change of the number and especially the nature of chains requires a completely new optimisation of all isolation procedures, which is often challenging. The solid-state assisted synthesis

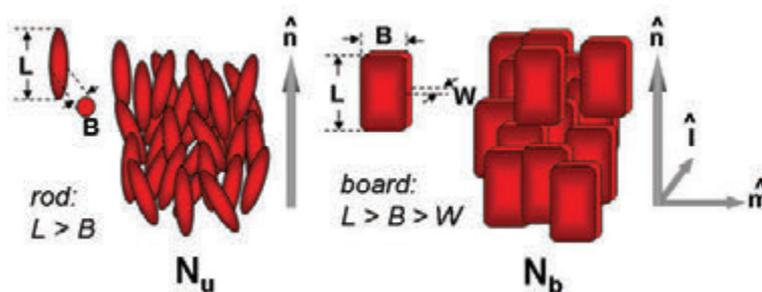
introduces the chain-building blocks in the final step and purification has to be done only once after the cleavage from the resin. It is therefore often superior over the conventional liquid phase synthesis, especially when building blocks, such as oligoethyleneoxy chains, have to be introduced.

M. Lehmann, K. Bahndorf, *Liq. Cryst.* 2015; DOI: 10.1080/02678292.2015.1056264; *Solid-State Assisted Synthesis of Oligobenzoates*.

### Biaxial Nematogens

Nematic phases of rod-shaped molecules possess only orientational long range order of usually one molecular axis ( $N_u$ ). The molecular centres of gravity are distributed like in an isotropic liquid and thus show the lowest viscosity in the series of mesophases. Therefore they are

applied in LC-displays. Molecules with three molecular axis of different size and a defined aspect ratio may align all three axis in a nematic phase, which is called the biaxial nematic ( $N_b$ ), for which much faster switching times are proposed. For this aim novel V- and board-shaped nematogens are prepared and their biaxial properties are studied by conoscopy and X-ray scattering.



M. Lehmann, V. Goertz "Design of Biaxial Nematic Mesogens" in Handbook of Liquid Crystals, 2nd edition, Vol. 3, Chapter 10 (eds. J. W. Goodby et al.), ISBN 978-3-527-32773-7, Wiley-VCH, Weinheim, 2014



### Education and Academic Career of Prof. Dr. Jürgen Seibel

since 2009	Professor of Organic Chemistry, University of Würzburg
2007-2009	Group leader at Helmholtz Centre for Infection biology, Braunschweig
2002-2006	Habilitation in Bioorganic Chemistry, University of Braunschweig
2000 – 2002	Postdoctoral Fellow, The Department of Chemistry, The Dyson Perrins Laboratory, University of Oxford
2000	Dr. rer.nat. (Chemistry), University Göttingen
2000	Diploma (Chemistry), University of Göttingen

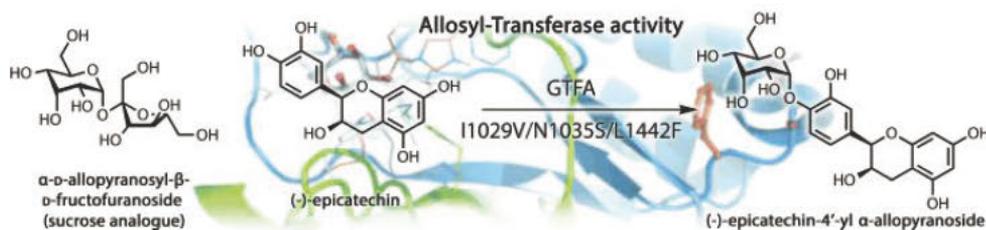
### Research Interests

The main focus of our research is centered around the exploding field of glycosciences including the development of chemical and enzymatic syntheses, biocatalysis, protein engineering and drug delivery. The motivation of our work arises from fundamental interest in the biomolecular mechanisms of life. The advancing field of glycomics is driven by the development of new analysis and synthesis techniques and novel strategies i.e. for metabolic glyco-labeling. Thus beside the main topic “tailoring chemo-enzymatic glycosyltransfer reactions” we follow other research areas. Those include screening methods like carbohydrate-based micro-arrays and metabolic glyco-engineering as a strategy to visualize biological recognition processes for the development of carbohydrate-based vaccines, chemical synthetic methods for oligosaccharide and glycoconjugate production, and the design of inhibitors against glycosyltransferases which are involved in cancer or infectious diseases.

### Our Current Research Topics:

#### Tailor-Made Glycosyltransfer-Reactions

The redesign of enzymes for new substrates and/or functions is a key endeavor of biocatalysis and the enzymatic synthesis of carbohydrates has been proven to be non-trivial in this regard. In our group we aim to extend the range of oligosaccharide synthesis of glucansucrases with enzyme and substrate engineering. Oligosaccharides (OS) and polysaccharides (PS) have found manifold interest in the field of food, pharmaceuticals and cosmetics due to their different specific properties. Large amounts of sucrose isomers and derivatives, as well as major amounts of oligosaccharides are commercialized in Europe and worldwide as sweeteners, prebiotics and ingredients of functional foods. Increasing attention has been devoted to the sophisticated roles of OS and glycosylated compounds, at cell- or membrane surfaces, and their function, e.g. in infection and cancer proliferation. The challenge for synthesis is obvious. We follow a convenient approach using cheap and readily available substrates and enzymes for the synthesis of OS and PS.



U. T. Bornscheuer *et al.*, *Angew. Chem. Int. Ed.* **2014**, *53*, 10876-10893; *Enzymatic degradation of (ligno-)celluloses.*

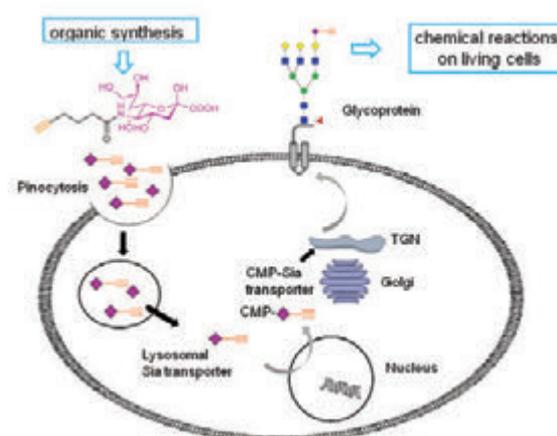
M. E. Ortiz-Soto, J. Seibel, *Cur. Org. Chem.* **2014**, *18*, 964-986; *Biotechnological Synthesis and Transformation of Valuable Sugars in the Food and Pharmaceutical Industry.*

## Metabolic Glycoengineering by Bioorthogonal Chemistry

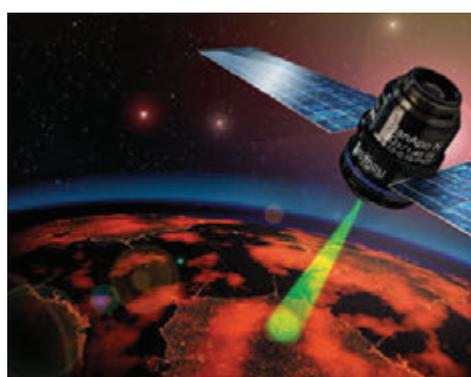
Metabolic labeling of cell surfaces is established in order to study and characterize cell signaling and cell-cell interactions to examine inflammation and infection processes. The metabolic incorporation of functionalized carbohydrates is performed with HEp-2, T24 and SKN-MC cells. These cells are chosen to evaluate this method as a general tool for a variety of biochemical applications. Moreover, the cell lines are easy to culture. The carbohydrates are modified by introducing an azide or alkyne group and are subsequently incubated with the cell lines indicated. The modified carbohydrates pass the natural carbohydrate biosynthetic pathway and are incorporated into the post-translational glycan patterns of proteins.

S. Letschert *et al.*, *Angew. Chem. Int. Ed.* **2014**, *53*, 10921-10924, *Super-Resolution Imaging of Plasma Membrane Glycans.* (hot paper)

E. Memmel, *et al.*, *Chem. Commun.* **2013**, *49*, 7301-7303; *Metabolic glycoengineering of Staphylococcus aureus reduces its adherence to human T24 bladder carcinoma cells.*



Copper-free labeling of cell-surface glycans



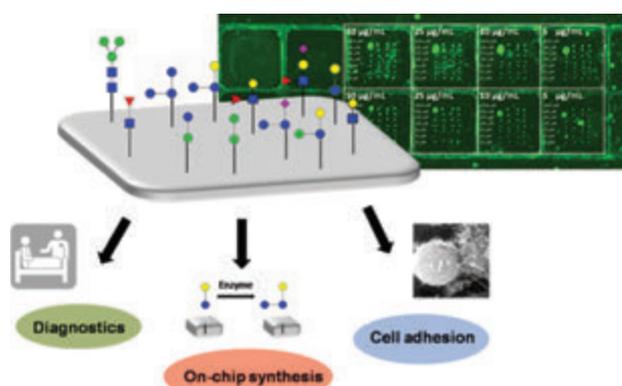
## Functional Analysis of Oligosaccharides by Carbohydrate Micro-Arrays

Despite of their prominent role in various biological processes, carbohydrate interactions are yet poorly investigated and understood. Chemical synthesis problems and usually low affinities to carbohydrate-binding proteins with  $K_D$  being in the milli-molar range cause substantial analysis problems. To overcome these difficulties, we develop a carbohydrate micro-array. The chip technology is common and commercially available for DNA and RNA analysis but not for glycan structures except of

a few special kits. Screening of glycan arrays represents a powerful, high-throughput approach for various applications. We introduced the principle of the enzymatic synthesis by glucansucrases on micro-arrays to study and evaluate alternative substrates, enzyme properties and the synthesized carbohydrates. Those studies lead to the identification of new properties of glycosyltransferases which were not observed previously and cannot be identified by sequence alignment. Maltose and primary alcohols are glucosylated using the bacterial glucosyltransferase dextranucrase.

C. Fleck *et al.*, *Eur. J. Org. Chem.* **2015**, 1696-1710; *Synthesis and Evaluation of Neoglycoconjugates Based on Adamantyl Scaffolds.*

D. Claes *et al.*, *ChemBioChem* **2014**, *15*, 2450-2457; *High-Affinity Carbohydrate Binding by Trimeric Benzoboroxoles Measured on Carbohydrate Arrays.*



**Dr. Michael Büchner**

obtained his Ph.D. degree in 2000 from the University of Bielefeld after completion of his research with Prof. Dr. H.-Fr. Grützmacher. From 2001–2003 he was postdoctoral fellow at the Fraunhofer IME in Aachen, where he established the mass spectrometry facility in proteomics. Since this time, he became a senior research associate in the Institute of Organic Chemistry. He is the head of the mass spectrometry facility and safety inspector in the Institute of Organic Chemistry.

**Mass Spectrometry**

Three mass spectrometers are operated in the Institute of Organic Chemistry. The applications are the characterization of compounds of supramolecular chemistry, functional materials and natural products. The Bruker Daltonics micOTOF focus II is equipped with an electrospray ionisation and an atmospheric pressure chemical ionisation source. The mass accuracy of this mass spectrometer is  $< 3$  ppm (RMS). LC/MS is used and benefits from the high mass accuracy. The Bruker Daltonics autoflex II is using the matrix assisted laser desorption ionisation technique. In the reflectron mode, ions from  $m/z$  0 – 3500 can be easily investigated with a resolution of 15.000. In the linear mode, ions like polymers or supramolecular compounds can be investigated. The Finnigan MAT90 is a double focusing sector field mass spectrometer and mainly used for routine electron impact mass spectra ( $m/z$  15 – 1000) and accurate mass measurements ( $< 2$  ppm RMS).

V. Dehm *et al.*, *Chem. Sci.* **2011**, *2*, 2094–2100; Foldamer with a spiral perylene bisimide staircase aggregate structure.

**Dr. Matthias Grüne**

obtained his Ph.D. degree in 1992 from the University of Münster (Ph.D. award, with Prof. Dr. W. Müller-Warmuth). After research work at the C.N.R.S. Bordeaux-Talence (1993), the Institute of Molecular Biotechnology and the University of Jena (1994–1997), and the Max Planck Institute for Neurological Research in Cologne (1997–1999), he became head of the NMR Department of the Institute of Organic Chemistry in 1999.

**Nuclear Magnetic Resonance Spectroscopy**

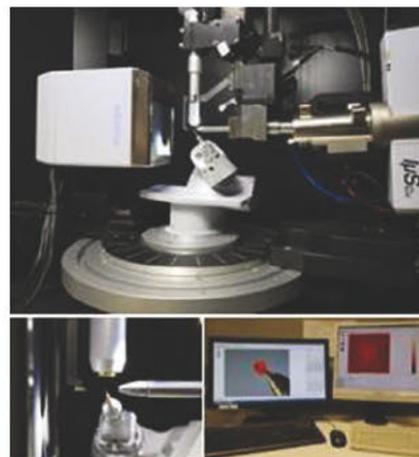
Four Bruker Avance III HD NMR spectrometers ( $2 \times 600$  MHz and  $2 \times 400$  MHz) are operated in the Institute of Organic Chemistry. One of the 600 MHz instruments is equipped with a highly sensitive cryoprobe (possibility of HPLC-NMR coupling) and thus represents a key instrument for the structure elucidation of natural products and other samples with low concentration. The second 600 MHz spectrometer is optimized to investigate topics in the field of supramolecular chemistry and functional materials. For this purpose, it contains special accessories for experiments in extended temperature ranges, for the determination of diffusion coefficients, and for the analysis of solids. The two 400 MHz instruments are used for routine NMR measurements and for variable temperature studies.

B. Fimmel *et al.*, *Chem. Eur. J.* **2015**, *21*, 615–630; Phenylene Ethynylene-Tethered Perylene Bisimide Folda-Dimer and Folda-Trimer: Investigations of Folding Features in Ground and Excited States.



### Dr. David Schmidt

obtained his Ph.D. degree in 2013 from the University of Würzburg after completion of his research with Prof. Dr. U. Radius. Since this time he joined the group of Prof. Dr. F. Würthner where he became a permanent research associate in 2014. His research is focused on the investigation of reduced PBI dye molecules and the fabrication of (metal)organic PBI architectures for photocatalytic applications.



### X-Ray Diffraction Analysis

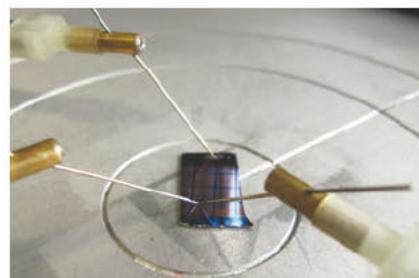
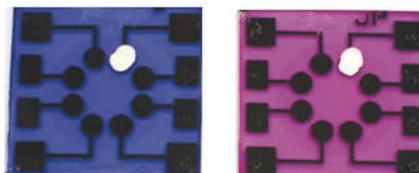
The Institute of Organic Chemistry is equipped with two X-ray diffractometers for the analysis and characterization of complex (liquid) crystalline materials. A Bruker D8 Quest single crystal diffractometer (Photon100 CMOS detector) and a Bruker Nanostar SAXS/WAXS instrument (Vantec2000 detector). Additionally, we have access to a Bruker D8 Discover powder diffractometer (LynxEye oD/1D detector) and a Bruker D8 Discover high-resolution X-ray diffractometer (LynxEye oD/1D detector).

D. Schmidt *et al.*, *Angew. Chem. Int. Ed.* **2015**, *54*, 3611-3614, *Ambient Stable Zwitterionic Perylene Bisimide-Centered Radical*.



### Dr. Matthias Stolte

obtained his Ph.D. degree in 2008 from the University of Kaiserslautern under the guidance of Prof. Dr. H.-G. Kuball. Since this time he joined the group of Prof. Dr. F. Würthner where he became a senior research associate in 2010. His research is focused on the guided supramolecular assembly of small molecules into functional solid state materials and their application in organic electronic devices.



### Organic Electronics & Photovoltaics

Purification of new functional small molecules by gradient sublimation as well as their processing in high vacuum chambers or by solution-based deposition tools into active layers are the goals of this facility of the Institute of Organic Chemistry. (Opto) Electrical characterizations of these crystalline solid state materials within single crystal field-effect transistors, organic thin-film transistors and organic bulk heterojunction solar cells enable the rationalization of structure property relationships for their implementation in complementary logical circuits and organic photovoltaics.

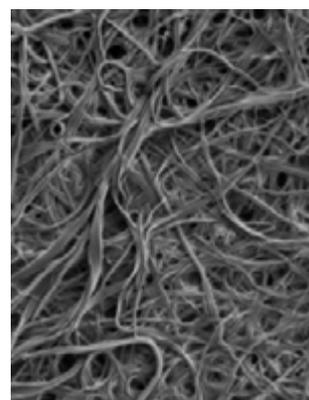
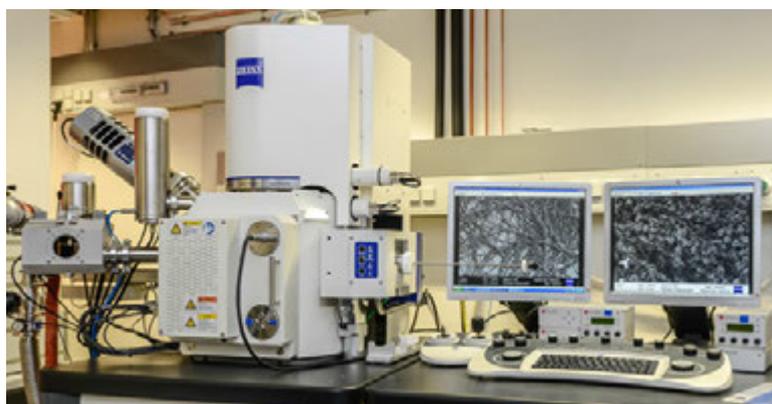
A. Liess *et al.*, *Adv. Funct. Mater.* **2015**, *25*, 44-57, *Organic Thin Film Transistors Based on Highly Dipolar Donor Acceptor Polymethine Dyes*.

### Concept and Realization of CNC

Approximately 100 years ago the chemist Emil Fischer (Nobel Prize 1902) conducted his revolutionary research in the field of sugar chemistry at the University of Würzburg (1885-1892). One of his many proposals, the Lock and Key Model, became the basis for understanding supra- and biomolecular recognition processes. Today, understanding intermolecular self-association of molecules, similar to a chemical lock and key process, helps explain the development and function of living matter and allows for the rational design of functional materials.

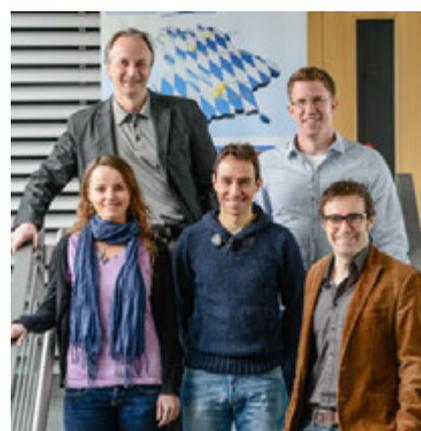


To address challenges in the development of this chemistry beyond the molecule, in particular in the area of materials science, the CNC was established as a purely research focused supplementary unit of the Institute of Organic Chemistry in 2010 and equipped with modern instruments for materials analytics including a scanning electron microscope (SEM), an atomic force microscope (AFM), two X-ray diffraction instruments and instrumentation for the preparation and characterization of organic transistor devices. Next, in 2012 substantial funds were provided by the State of Bavaria for a 1500 m<sup>2</sup> research building which will be finished in 2016 and accommodate the meanwhile expanded materials analytics sections and several independent junior research groups.



Scanning electron microscope (left) and image of self-assembled supramolecular fibers (right).

According to our mission, scientists at CNC in Würzburg study how specifically tailored molecules organize into larger supramolecular assemblies and further into hierarchically structured nanomaterials. The unique properties that emerge in such complex materials as a result of the interplay of single components are investigated from a fundamental point of view but also developed towards new applications. Recent research activities are bundled within various research programs such as the Bavarian collaborative research program *Solar Technologies Go Hybrid* (SolTech) and the Key Lab of *Supramolecular Polymers* within the *Bavarian Polymer Institute* (BPI), or constitute individual grants like the Sofja-Kovalevskaja grant on *Metal-Ion Mediated Self-Assembly of Multivalent  $\pi$ -Amphiphiles* of Dr. Gustavo Fernández and the Liebig Habilitation grant on *Mesoporous Covalent Organic Materials* of Dr. Florian Beuerle.



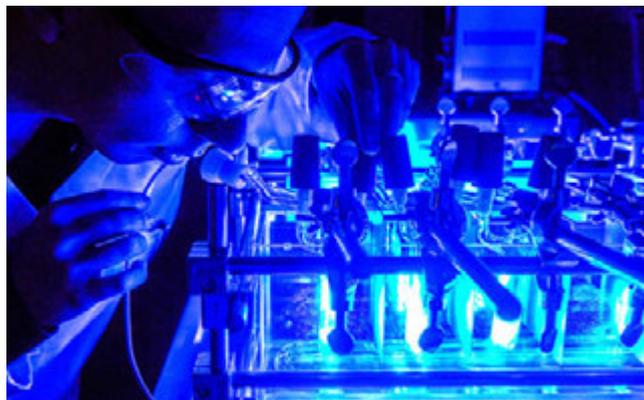
Prof. Würthner with the CNC junior group leaders (from left to right) Agnieszka Nowak-Król, Gustavo Fernández, Matthias Stolte, and Florian Beuerle in 2015

### SolTech Key Lab Supramolecular Materials for Photovoltaics and Photocatalysis

The conversion of solar energy into electrical energy is very costly with today's silicon-based solar cells. The Bavarian collaborative project *Solar Technologies Go Hybrid* (SolTech) explores alternative material systems for converting solar energy into electricity and fuels. As one of the five key laboratories of the interdisciplinary Bavarian energy research project SolTech, the CNC at the University of Würzburg develops and examines new supramolecular materials and advanced material systems for photovoltaics and photocatalysis.



Further information: [www.soltech-go-hybrid.de](http://www.soltech-go-hybrid.de)



Investigations on photocatalytic water splitting

### Key Lab Supramolecular Polymers at the Bavarian Polymer Institute (BPI)

The Bavarian Polymer Institute (BPI) is a joint research institute of the Universities of Bayreuth, Erlangen-Nürnberg and Würzburg. Supported by the Bavarian State each university hosts key laboratories for specific research in the field of polymer science and technology. The CNC hosts the key lab on *Supramolecular Polymers* which focusses on the mechanistic understanding of the formation of this newest type of polymer and applications of supramolecular polymers in optoelectronics, biomolecular imaging, as hydrogels in the life sciences, and as liquid crystals.



Further information: [www.nanosystems-chemistry.uni-wuerzburg.de](http://www.nanosystems-chemistry.uni-wuerzburg.de)



Building of the Center for Nanosystems Chemistry in September 2015.



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