



Max-Planck-Institut
für Kohlenforschung

Report for the Scientific Advisory Board



2017 – 2019



**Max-Planck-Institut
für Kohlenforschung**

Max-Planck-Institut für Kohlenforschung

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Max-Planck-Institut
für Kohlenforschung

Max-Planck-Institut für Kohlenforschung

Kaiser-Wilhelm-Platz 1
45470 Mülheim an der Ruhr, Germany
Tel. +49 208 3 06 1
Fax +49 208 3 06 29 80
www.kofo.mpg.de

Managing Director: Professor Dr. Tobias Ritter

Director of the Department of Organic Synthesis
Professor Dr. Tobias Ritter
Tel. +49 208 3 06 24 14
Fax +49 208 3 06 29 72
E-mail: ritter@kofo.mpg.de

Director of the Department of Homogeneous Catalysis
Professor Dr. Benjamin List
Tel. +49 208 3 06 24 10
Fax +49 208 3 06 29 99
E-mail: list@kofo.mpg.de

Director of the Department of Heterogeneous Catalysis
Professor Dr. Ferdi Schüth
Tel. +49 208 3 06 23 73
Fax +49 208 3 06 29 95
E-mail: schueth@kofo.mpg.de

Director of the Department of Organometallic Chemistry
Professor Dr. Alois Fürstner
Tel. +49 208 3 06 23 42
Fax +49 208 3 06 29 94
E-mail: fuerstner@kofo.mpg.de

Director of the Department of Molecular Theory and Spectroscopy
Professor Dr. Frank Neese
Tel. +49 208 3 06 21 91
Fax +49 208 3 06 29 80
E-mail: frank.neese@kofo.mpg.de

Emeritus Scientific Members of the Max-Planck-Institut für Kohlenforschung

Professor Dr. Manfred Reetz

Professor Dr. Walter Thiel (*deceased August 23rd, 2019*)

**Elected Members of the Scientific Council of the Max Planck Society,
Section of Chemistry, Physics and Technology**

Dr. Michael Felderhoff

Table of Contents

1	The Max-Planck-Institut für Kohlenforschung	7
1.1	History	9
1.2	Organigram 2019	11
1.3	Members of the Scientific Advisory Board - Extended	12
1.4	Members of the Board of Governors (“Verwaltungsrat“).....	14
2	Research Programs	15
2.1	Department of Organic Synthesis (T. RITTER).....	17
2.2	Department of Homogeneous Catalysis (B. LIST).....	21
2.3	Department of Heterogeneous Catalysis (F. SCHÜTH)	25
2.4	Department of Organometallic Chemistry (A. FÜRSTNER).....	29
2.5	Department of Molecular Theory and Spectroscopy (F. NEESE).....	33
2.6	Department of Theoretical Chemistry (W. THIEL / F. NEESE).....	37
2.7	Independent Research Groups	
2.7.1	Homogeneous Catalysis and Reaction Design (B. MORANDI).....	39
2.7.2	Sustainable Catalysis for Organic Synthesis (P. CORNELLA).....	41
2.7.3	Computational Electronic Spectroscopy and Theory Development (B. HELMICH-PARIS)	43
2.7.4	Biocatalysis (M. T. REETZ).....	45
3	Scientific Service Units	47
3.1	Technical Laboratories and Central Occupational Safety (N. THEYSSEN)	49
3.2	Chromatography and Electrophoresis (P. SCHULZE).....	50
3.3	Mass Spectrometry (W. SCHRADER)	51
3.4	Nuclear Magnetic Resonance (C. FARÈS)	52
3.5	Electron Microscopy and Chemical Crystallography (C. W. LEHMANN).....	53
3.6	Library and Information Management (C. BAUMERT / A. LEHMANN).....	54
3.7	IT Group (C. BAUMERT).....	55
3.8	ORCA (F. WENNMOHS)	56
4	Training of Young Scientists	57
5	Equal Opportunities	69

6	Personnel and Finances	73
6.1	Personnel.....	74
6.1.1	Structure.....	74
6.1.2	Research Departments	75
6.1.3	Independent Junior Research Groups.....	77
6.1.4	Central Scientific Service Units	77
6.1.5	Administration and General Services.....	78
6.2	Finances.....	80
6.2.1	Research Budget	80
6.2.2	Third Party Funds.....	80
6.3	Facilities.....	100
7	Technology Transfer	101
8	Special Activities.....	105
8.1	Special Events.....	106
8.2	Public Relations	113
8.3	Local Activities of the Young Chemists Forum (JCF) of the German Chemical Society (GDCh).....	115
9	Appendices.....	119
9.1	Invited Presentations	120
9.2	Scientific Honors, Name Lectureships, Awards	139
9.3	Further Activities of Members of the Institute.....	144
9.4	Courses Taught at Universities	147
9.5	Scientific Talks Given by Guests	152
9.6	Publications	169

CHAPTER 1

The Max-Planck-Institut für Kohlenforschung

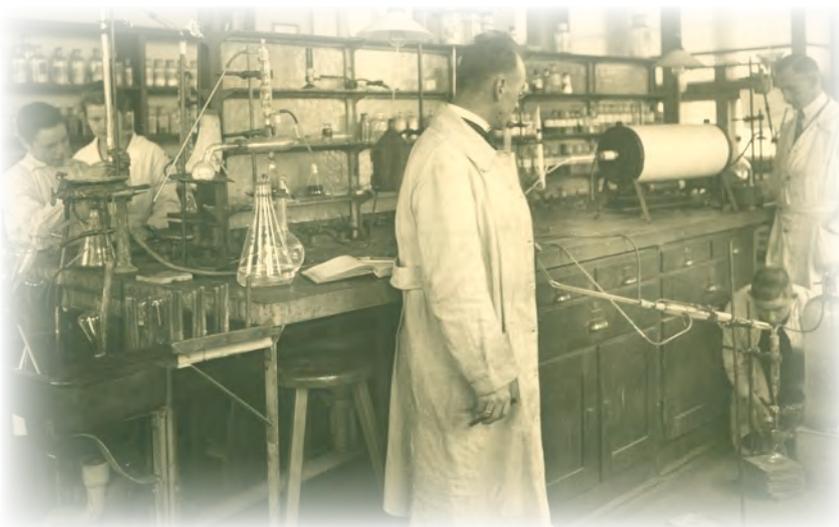
1.1 History

The Max-Planck-Institut für Kohlenforschung is one of the oldest institutes of the Max Planck Society and was founded in 1914 as the “Kaiser-Wilhelm-Institut für Kohlenforschung”. The research goal of the institute was the direct conversion of coal energy into electricity.



The institute in 1914

The first director to be appointed was Franz Fischer (1877-1947). After the end of WWI, Franz Fischer and his co-workers carried out research that culminated in the Fischer-Tropsch process for coal liquefaction. Today, there is a renewed interest in Fischer-Tropsch technology with plants in Sasolburg/South Africa, Malaysia, and Qatar (using natural gas instead of coal).



Hans Tropsch in the synthesis laboratory in 1922

Franz Fischer succeeded in transforming the institute into a foundation, making it legally independent. Its legal status is still unique among the 86 institutes of the Max Planck Society.

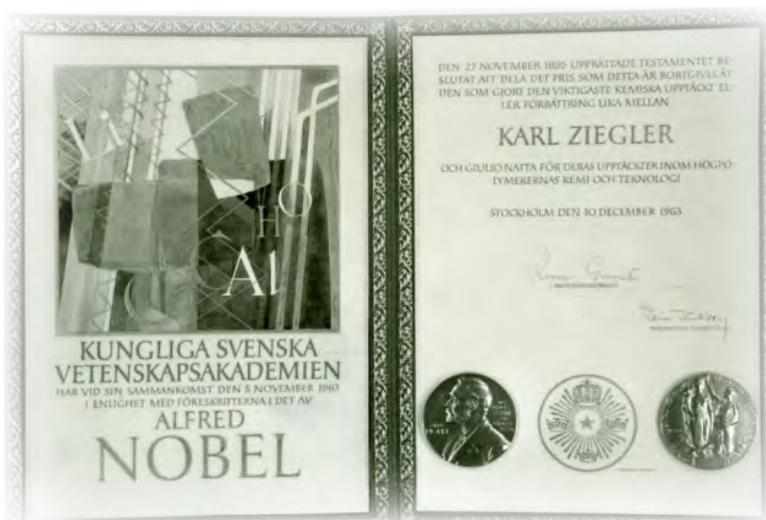
In 1943, Karl Ziegler (1898-1973) was appointed director of the Institute. He came under the condition to be allowed to carry out fundamental research, as opposed to application oriented, which he termed “general synthetic chemistry”. In 1949, Ziegler and his co-workers succeeded in developing the addition of ethylene to aluminum alkyls which became known as the “Aufbaureaktion”. The systematic investigation of this reaction led to the discovery of the Ziegler catalysts for ethylene polymerization at normal pressure and temperature. The process was patented in 1953 and led to a stunning development of the industrial production of polyethylene and polypropylene as inexpensive and versatile polymers. The royalty payments enabled the Institute to be financially independent for nearly 40 years.

In 1963, Karl Ziegler and Giulio Natta were awarded the Nobel Prize for Chemistry for “their groundbreaking discoveries in the field of chemistry and technology of high polymers.”

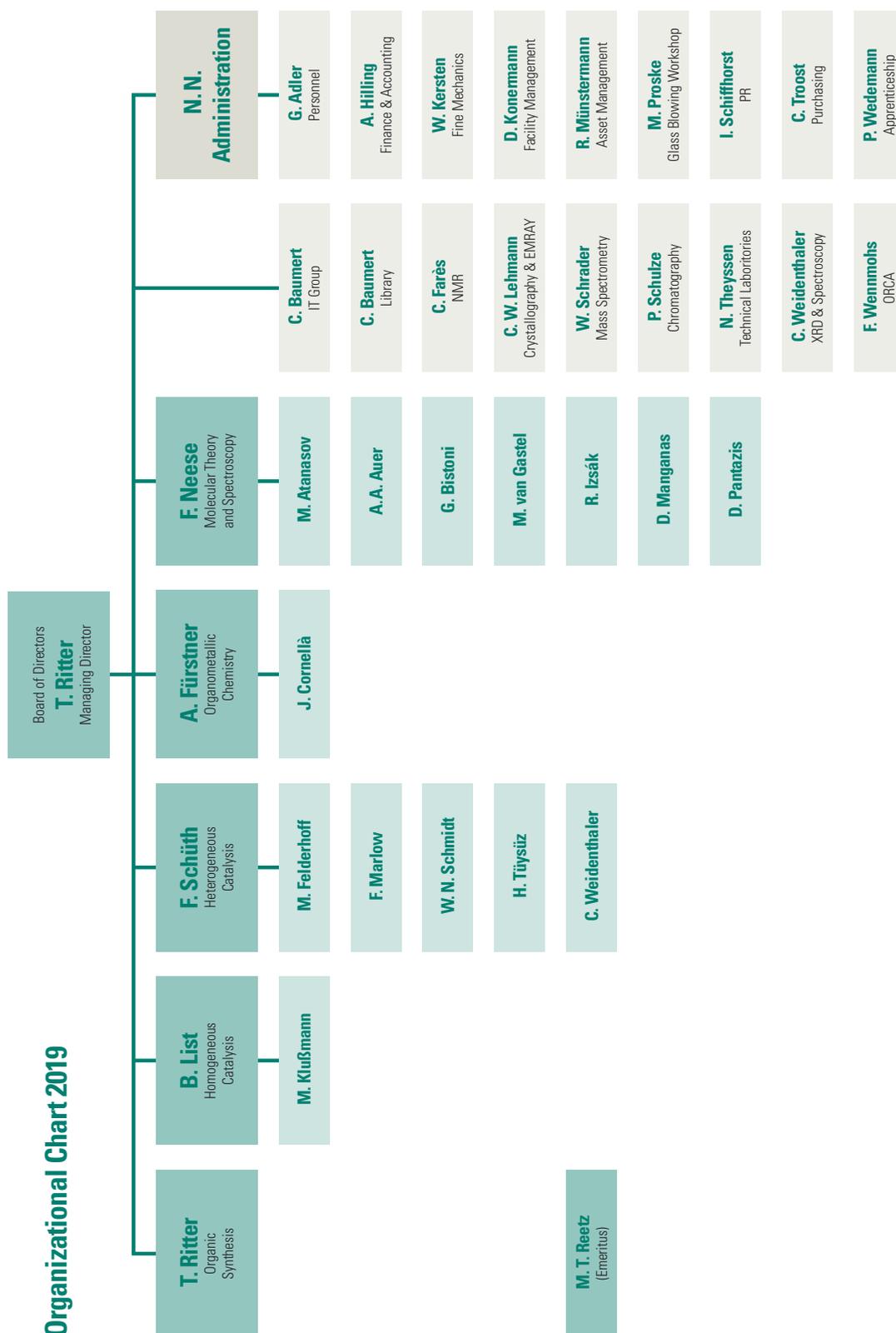
Günther Wilke (1925-2016) followed Karl Ziegler as director in 1969. He had been associated with the institute for almost 20 years before becoming its director. His researches as director concentrated on the organometallic chemistry of the transition metals (especially nickel) and their application in homogeneous catalysis.

His major achievement was the nickel-catalyzed cyclootrimerization of butadiene.

In 1993, Manfred T. Reetz was appointed Director of the institute, who changed the structure of the institute and established the five Departments Synthetic Organic Chemistry, Homogeneous Catalysis, Heterogeneous Catalysis, Organometallic Chemistry, and Theoretical Chemistry, which still exist today.



1.2 Organigram (01.11.2019)



1.3 Members of the Scientific Advisory Board - Extended

For the period 2018-2022:

GONZÁLEZ , Leticia Prof. Dr.	University of Vienna Institute of Theoretical Chemistry Währinger Straße 17 1090 VIENNA, AUSTRIA
KNOCHEL , Paul Prof. Dr.	Ludwig-Maximilians-Universität München Fakultät Chemie und Pharmazie Butenandtstr. 13 81377 MÜNCHEN, GERMANY
MILLER , Scott J. Prof. Dr.	Yale University Department of Chemistry Chemistry Research Building – 110 PO Box 208107 NEW HAVEN, CT 06520-8107, USA
PÉREZ-RAMÍREZ , Javier Prof. Dr.	ETH Zürich Institute for Chemical and Bioengineering ETH Hönggerberg HCI E125 Vladimir-Prelog-Weg 1 8093 ZÜRICH, SWITZERLAND
ROVIS , Tomislav Prof. Dr.	Columbia University Department of Chemistry 3000 Broadway NEW YORK, NY 10027, USA
SCHREINER , Peter R. Prof. Dr. Chair	Justus-Liebig-University Gießen Institut für Organische Chemie Heinrich-Buff-Ring 17 35392 GIESSEN, GERMANY
TRAUNER , Dirk Prof. Dr.	New York University Department of Chemistry 100 Washington Square East, Room 712 NEW YORK, NY 10003, USA

de VOS, Dirk Prof. Dr.	KU Leuven Centrum voor Oppervlaktechemie en Katalyse Kasteelpark Arenberg 23 – bus 2461 3001 LEUVEN, BELGIUM
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Rapporteurs:

SANCHEZ, Clément Prof. Dr.	Collège de France Chimie de la Matière Condensée Paris UMR 7574-UPMC/CNRS/Collège de France Bâtiment D 11 place Marcelin Berthelot 75231 PARIS, FRANCE
BEIN, Thomas Prof. Dr. rer. nat.	Ludwig-Maximilians-Universität München E3.033 (Haus E) Butenandtstraße 11 81377 MÜNCHEN, GERMANY

Previous members of the SAB (since 2005):

Prof. Avelino Corma (Valencia, ES); Prof. Janine Cossy (Paris, FR), Prof. Pierre H. Dixneuf (Rennes, FR); Prof. Dieter Enders (Aachen, DE); Prof. Ben L. Feringa (Groningen, NL); Prof. J. A. Gladysz (Erlangen, DE); Prof. Peter Hofmann (Heidelberg, DE); Prof. Graham Hutchings (Cardiff, UK); Prof. Jeremy Harvey (Leuven, BE), Prof. Eric N. Jacobsen (Cambridge, US); Prof. Henri Kagan (Orsay, FR); Prof. Rutger A. van Santen (Eindhoven, NL); Prof. Joachim Sauer (Berlin, DE); Prof. Richard R. Schrock (Cambridge, US);

1.4 Members of the Board of Governors ("Verwaltungsrat")

(01.11.2019)

Representative of the Ministry of Culture and Science of the State of North Rhine-Westphalia

Annette Storsberg, State Secretary at the Ministry of Culture and Science
of the State of North Rhine-Westphalia

Representative of the Municipality of Mülheim an der Ruhr

Ulrich Scholten, Lord Mayor of Mülheim an der Ruhr

Representatives of the Max Planck Society

Rüdiger Willems, Secretary General of the Max Planck Society

Prof. Dr. Klaus Müllen, Emeritus Director of the Max Planck Institute for Polymer Research

Wolfgang Schlieper, retired

Representatives of the Studiengesellschaft Kohle mbH

Prof. Dr. Stefan Buchholz, Managing Director Evonik Creavis

Prof. Dr. Michael Dröscher (Chairman), retired

Dr. Detlef Kratz, Senior Vice President Corporate Technology & Operational Excellence BASF

Honorary Members

Dr. Werner Schwilling, retired

CHAPTER 2

Research Programs

2 Research Programs

The Max-Planck-Institut für Kohlenforschung seeks to contribute scientifically to all fields of catalysis at the highest level. Our goal to illuminate, understand, and apply concepts in catalysis from diverse approaches, rooted in organic, inorganic, organometallic, bio, and theoretical chemistry, is only second to our commitment to hiring in accordance with the Harnack principle, instituted by the first president of the Kaiser Wilhelm Society: hiring the brightest minds, independent of research field. Currently, the five Departments of the Institute encompass Synthetic Organic Chemistry, Homogeneous Catalysis, Heterogeneous Catalysis, Organometallic Chemistry, and Molecular Theory and Spectroscopy, each headed by one of our directors.



Organic Synthesis
Prof. Dr. Tobias Ritter



Heterogeneous Catalysis
Prof. Dr. Ferdi Schüth



Homogeneous Catalysis
Prof. Dr. Ben List



Molecular Theory and Spectroscopy
Prof. Dr. Frank Neese

Reactions



Organometallic Chemistry
Prof. Dr. Alois Fürstner

In contrast to previous years, we have opted to significantly shorten the reports of the research programs to focus only on the most significant research result from the reporting period in the interest of clarity and brevity to provide the readers of the report with a clear overview of the most important research results out of our institute within the past three years.

2.1 Late-Stage Functionalization

Department of Organic Synthesis by Tobias Ritter

ABSTRACT: Late-stage functionalization reactions can chemo- and regioselectively functionalize complex molecules. Late-stage functionalization is desirable in areas such as pharmaceutical discovery to accelerate drug development and essential in other areas such as positron-emission tomography to avoid unproductive decay of short-lived isotopes before meaningful medically imaging. We have discovered a new reaction that can introduce a linchpin into complex small arene molecules with exquisite selectivity. Subsequently, the linchpin can be transformed into numerous groups that are important for medicinal and medical applications.

Late-stage functionalization has the potential to quickly access functional molecules of value in many areas, for example in pharmaceutical development or positron-emission tomography (PET). Late-stage functionalization is desirable because advanced, complex molecules can be used as suitable starting points, which avoids lengthy de novo syntheses from simple building blocks. However, the development of late-stage functionalization requires meeting the challenges for both, C-H functionalization reactions and functional-group-tolerant reactions. Large strides have been made in the past few decades in C-H functionalization chemistry, yet many of such reactions are not compatible with the functional complexity of complex small molecules. Likewise, important advances have been made in chemoselective functionalization of complex molecules, for example in the context of biorthogonal chemistry that can be applied to highly functionalized biomolecules, but specific functional groups must be introduced, typically at an early stage of the synthesis. Within the last reporting period we have succeeded in developing a remarkably selective C-H functionalization reaction that can function even on densely functionalized small-molecule arenes and some hetarenes. The method is unusual in the sense that for most arenes, independent of substitution pattern and directing groups, a single constitutional isomer, within the limits of conventional detection, of the functionalized product can be isolated. Subsequently, the sulfonium-based linchpin can be used as a useful synthetic handle in C-C, C-N, C-O, C-S, and C-F bond-forming reactions. We have shown for the first time that the specific arylsulfonium salts based on the heterocycle thianthrene are excellent substrates for conventional palladium-catalyzed cross-coupling chemistry, as well as provide conceptual advances in photoredox-catalyzed transformations when compared to other aryl (pseudo)halides.

As part of our ongoing program in site-selective C-H functionalization, we have attempted to identify persistent sulfur-based radicals that could add to arenes in an endergonic first step of the reaction; our design was motivated by a linear free energy relationship discovered by Brown and Stock in the 1950's that predicts reactions with a large absolute Hammett rho value to proceed inherently with high positional selectivity. A long, nascent C-S bond formed

by radical addition to an arene may result in a high rho value, and we identified the thianthrene scaffold as promising heterocycle for C-H functionalization.

After reaction optimization, arene functionalization could be executed in high selectivity, in favor of the most electron-rich position, even for substrates that are otherwise only moderately directing, such as toluene or ethylbenzene.¹ While there are isolated examples of other selective reactions, they typically introduce substituents that are not themselves synthetic linchpins and therefore synthetically of lesser value.² Some of the most useful linchpins in organic synthesis such as bromides and boronic acid derivatives still cannot be introduced selectively into most arenes. *The most important research result in the past three years from my research group is the development of the thianthrenation reaction, which is the first example of a reaction that can do both, functionalize complex small molecule arenes in high selectivity, and provide a useful handle for subsequent follow-up transformations.*

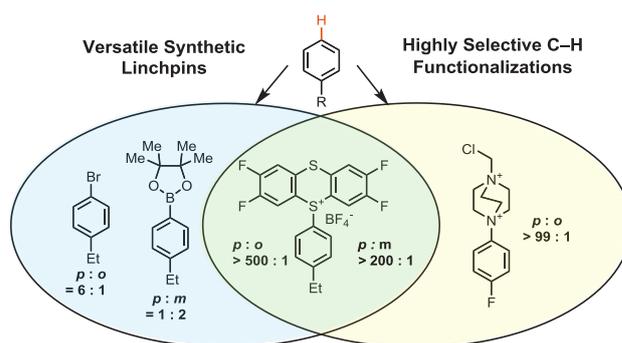
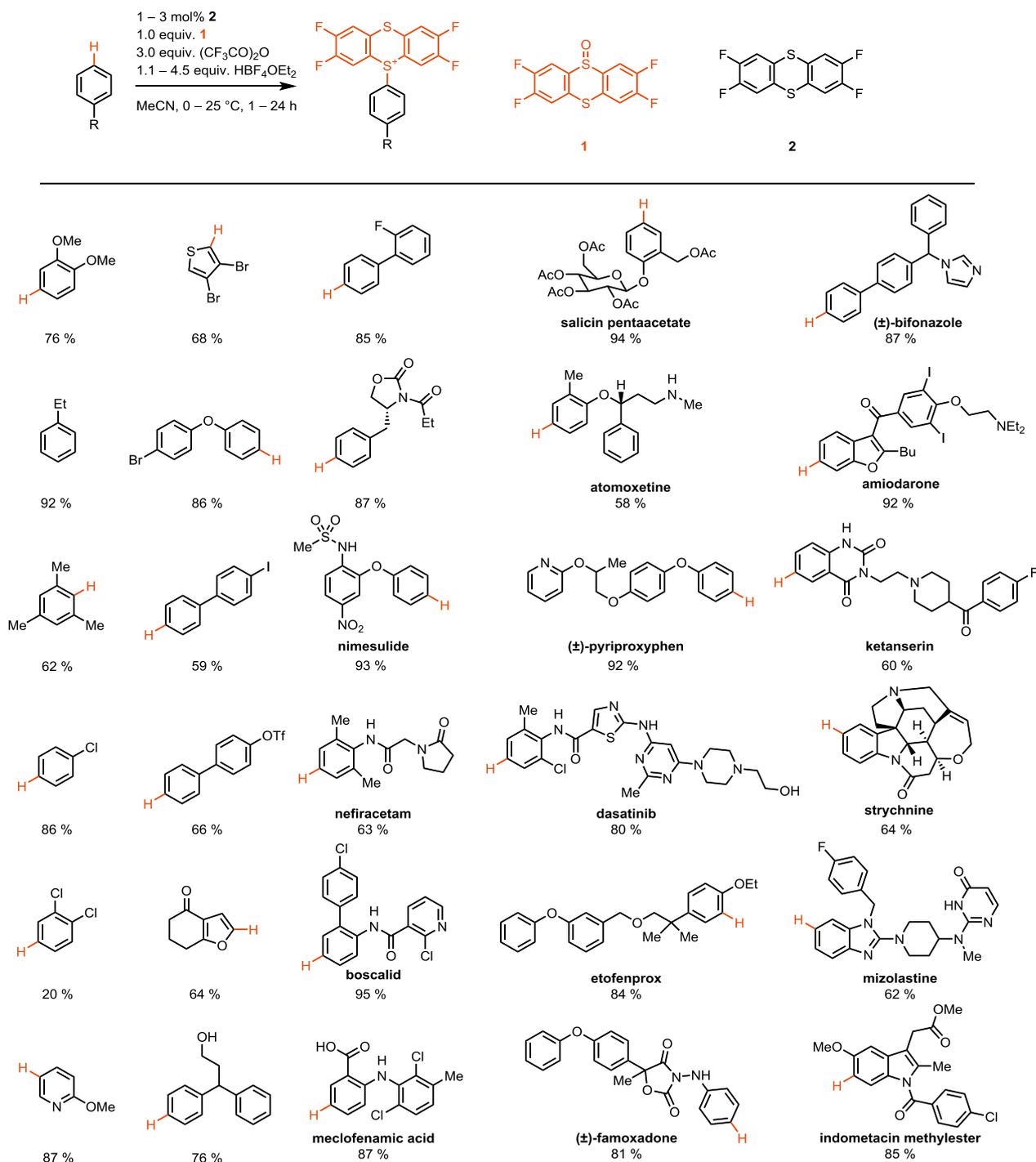


Figure 1. Highly regioselective C-H Thianthrenation.

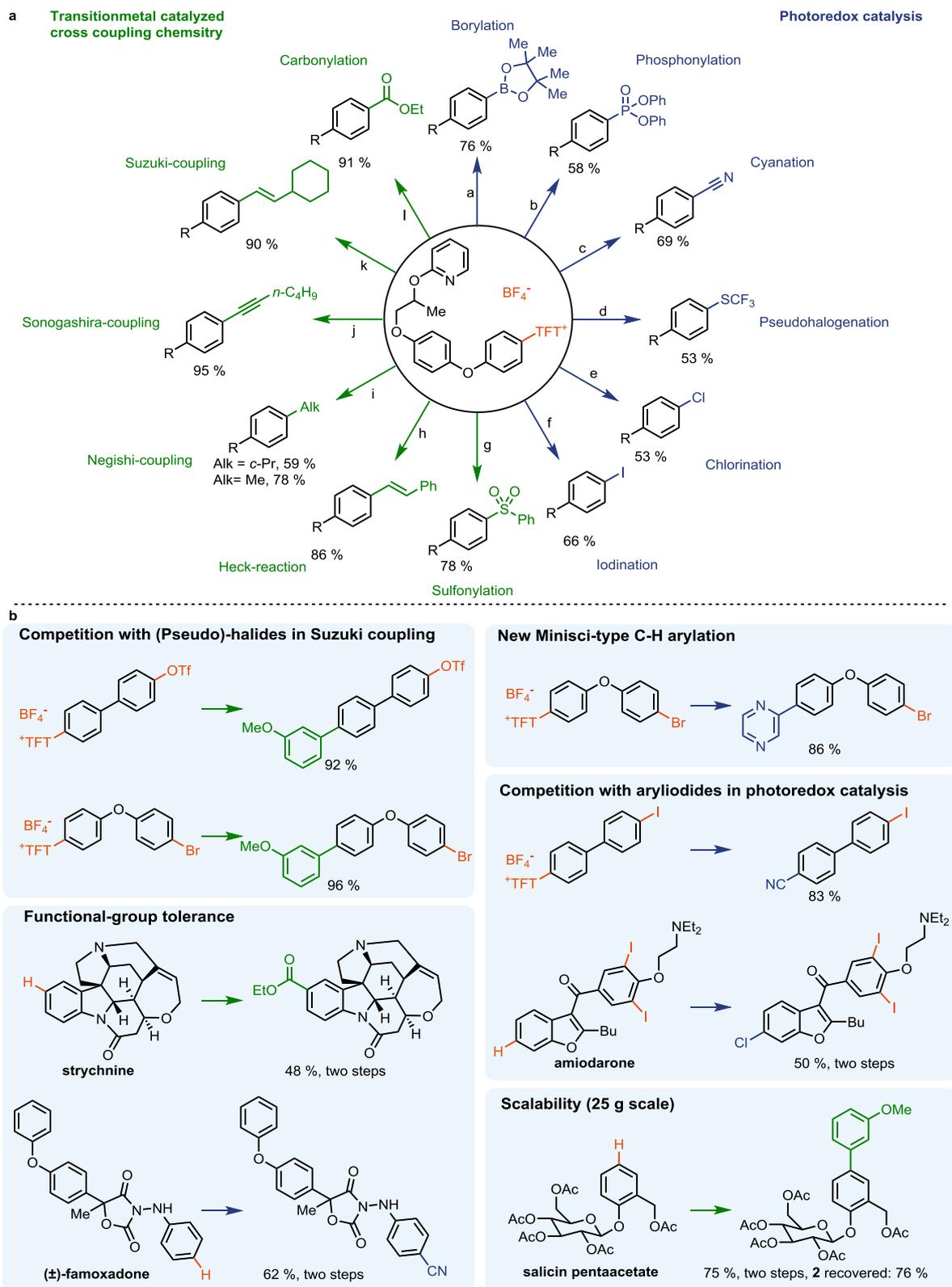
Thianthrenation can proceed on a variety of small molecule- (hetarenes) as shown in table 1; in all cases a single constitutional isomer was observed. The reaction is successful on most electron-rich arenes but fails on arenes more electron-poor than dichlorobenzene. Only electron-rich heterocycles such as thiophene can be converted effectively, electron-poor heterocycles such as pyridine require strongly electron-donating substituents. A primary kinetic isotope effect of the transformation is consistent with rate-limiting

Table 1. Late-Stage Thianthrenation of (het)arenes.



deprotonation of a dicationic Wheland intermediate, and an unusually large rho value of -11 establishes the electrophilic nature of the transformation. Given the current mechanism data, the source of selectivity seems more subtle than what was originally designed. Radical addition is not necessarily relevant; a dicationic thianthrenium intermediate may add to the arene reversibly before rate-limiting deprotonation, which is subject of current investigations, but the current hypothesis favors an electrophilic aromatic substitution mechanism in which the aromatic thianthrenium

dication reacts with the arene directly. Selectivity in this case would be determined by the relative energies of the different Wheland intermediates, assuming that the transition states of the subsequent rate-limiting deprotonations of the different Wheland intermediates are of similar magnitude. The different energies of the Wheland intermediates can be rationalized by maximization of charge separation. Equipped with this analysis, we predicted that other dicationic electrophiles should elicit similarly selective substitution reactions, which, preliminarily, seems to be the case.

Scheme 1. Cross-Coupling Reactions and Photoredox Reactions of Arylthianthrenium salts.


The thianthrenium group is useful as a leaving group in palladium-catalyzed cross coupling reactions, as well as in photoredox-mediated reactions (Scheme 1). All evaluated conventional carbon-carbon cross coupling reactions proceed well. Remarkably, the

thianthrene group outcompetes bromide and triflate leaving groups, with catalysts under reaction conditions originally developed for halides and triflate. Such reactivity enables chemoselective cross coupling even in the presence of other halides.

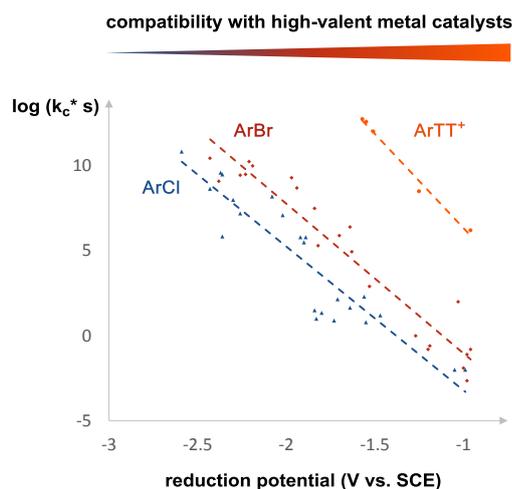
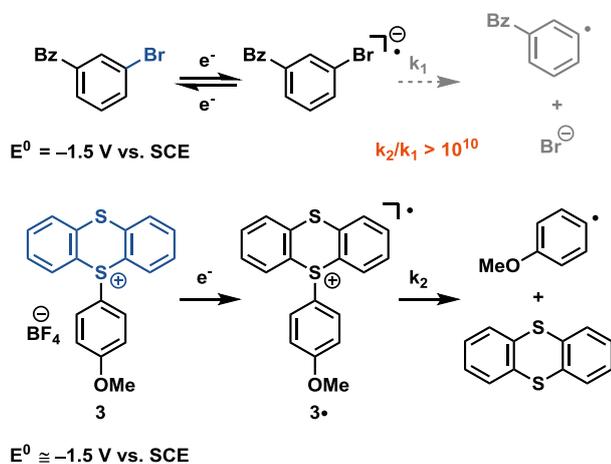


Figure 2. Conceptual Advantage of Arylthianthrenium salts of aryl halides in photoredox catalysis.

In palladium-catalyzed cross coupling, the thianthrene group behaves as an excellent, but conceptually identical, leaving group when compared to halides or other pseudohalides. For photoredox catalysis, the thianthrene group displays a fundamental advantage when compared to other (pseudo)halides. Figure 2 shows a linear relationship between the reduction potential and the log of the rate constant for mesolytic cleavage, and rationalizes that arylthianthreniums are better suited to engage in aryl radical formation through photoredox catalysis.

Scheme 2. Mesolytic Cleavage after single Electron Reduction.



It is intuitive why the reduction potential of aryl thianthreniums is lower when compared to aryl halides with identical aryl substituents owing to the positive charge. Therefore, reduction of all investigated arylthianthrenium salts is accessible to conventional photoredox catalysts ($\geq 1.7 \text{ V}$), whereas reduction of aryl halides is often plagued by fast back electron transfer. It is less obvious why mesolytic cleavage of the radical anions, which forms the synthetically useful aryl radicals, generated by single electron reduction of arylthianthrenium salts, proceeds at least ten billion times faster for aryl thianthreniums than for aryl bromides with similar reduction potential, and thereby successfully avoids unproductive back electron-transfer that is observed in aryl halides (Scheme 2).

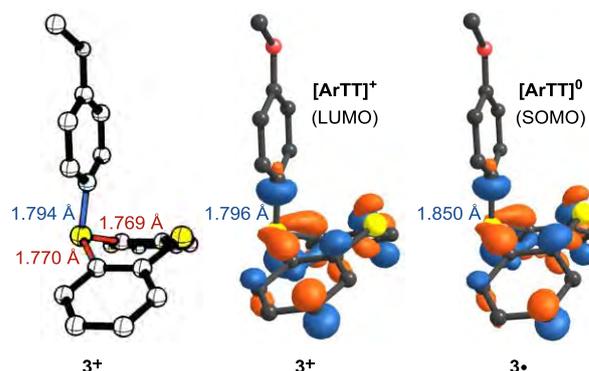


Figure 3. X-ray structure of **3** with 50% ellipsoids; H atoms and counteranion not shown for clarity, as well as computed LUMO and SOMO of **3** and **3•**, respectively.

An orbital analysis reveals that the SOMO of radical **3•**, the compound obtained following single electron reduction of **3+**, as well as the LUMO of **3+**, have an antibonding interaction along the carbon sulfur bond that must break for arene radical synthesis (Figure 3). Due to the π system of the thianthrene heterocycle, as well as the flagpole conformation of the aryl substituent, the appropriate population of the σ^* orbital is energetically more favorable than in arenes with monoatomic leaving groups such as aryl halides, which results in a substantial rate increase for mesolytic cleavage.

The ability to more effectively access aryl radicals through photoredox catalysis enabled the combination with copper-based redox catalysis in a way that has not been possible with other electrophiles, and resulted in the successful development of C–CF₃,³ C–N,⁴ C–O,⁵ and C–F⁶ bond forming reactions. Analysis of the reaction mechanism and further development based on the lessons learned enabled us to develop a selective C–H to C–¹⁸F fluorination reaction that shows promise due to its reliable and simple reaction setup for PET tracer synthesis in hospital settings. Attempts to translate our new fluorination technology to human imaging are currently underway.

Funding Sources

We acknowledge funding from the Max-Planck-Institut für Kohlenforschung and UCB Biopharma for funding for this project.

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2.2 Unprecedented Reactivity and Selectivity: The IDPi Breakthrough

Department of Homogeneous Catalysis by Ben List

ABSTRACT: Since moving to the Max-Planck-Institut für Kohlenforschung, a central aim of our research has been to develop high performance organocatalysts that rival the reactivity and selectivity of the very best enzymes and transition metal catalysts available to today's chemists. Over the years our research advanced from proline's combined enamine and Brønsted acid activation to more purely acidic motifs. During this time, we began to realize that high acidity and structural confinement are the pivotal elements in asymmetric acid catalysis. As a consequence, our research recently culminated in the imidodiphosphorimidate (IDPi) catalyst class, introduced already at the end of the previous reporting period. By combining extreme acidity and a highly confined active site, IDPi catalysts have met with remarkable success, as powerful Brønsted acid catalysts and as "silylium" Lewis acid precatalysts in several previously inaccessible transformations. Substrates as challenging to activate as simple olefins were readily transformed, ketones were employed as electrophiles in aldolizations allowing sub-ppm level catalysis, whereas enolates of the smallest donor aldehyde, acetaldehyde, did not polymerize but selectively added a single time to a variety of acceptor aldehydes.

1. IDPi in Organic Lewis Acid Catalysis

To overcome barriers concerning reactivity and selectivity in organocatalysis, imidodiphosphorimidate (IDPi) catalysts were designed by combining the high catalytic activity of disulfonimide (DSI) catalysts with the steric confinement of imidodiphosphate (IDP) catalysts. This advancement was enabled by applying the "Yagupolskii trick", consisting of the tremendous acidifying effect upon the replacement of O atoms by NTf groups in benzoic acid, to the IDP motif (Figure 1). The profoundly enhanced acidity [$pK_a = 4.5$ to ≤ 2.0 in MeCN (depending on substituents R and R')] of the imidodiphosphorimidates created in this approach made them promising candidates for the exploration of new reactivities in asymmetric organic Lewis acid catalysis.^[1]

Asymmetric Catalysis via Cyclic, Aliphatic Oxocarbenium Ions

Substituted oxacycles constitute carbohydrates and occur in numerous other classes of drugs and natural products. This motif is frequently accessed through S_N1 -type substitution reactions involving cyclic oxocarbenium ions. Stereoselective intermolecular substitution reactions of this type so far have involved further stabilizing functionalities which additionally facilitate enantiofacial differentiation. Enantioselective nucleophilic addition reactions to simple aliphatic, cyclic oxocarbenium ions affording substituted tetrahydrofurans and -pyrans had remained an unsolved challenge though. This challenge could be solved by IDPi catalysts which not only exhibited exceptionally high catalytic activity even under cryogenic conditions, but further provided tetrahydrofurans in outstanding enantiomeric ratios of up to 99:1 (Scheme 1a).^[2]

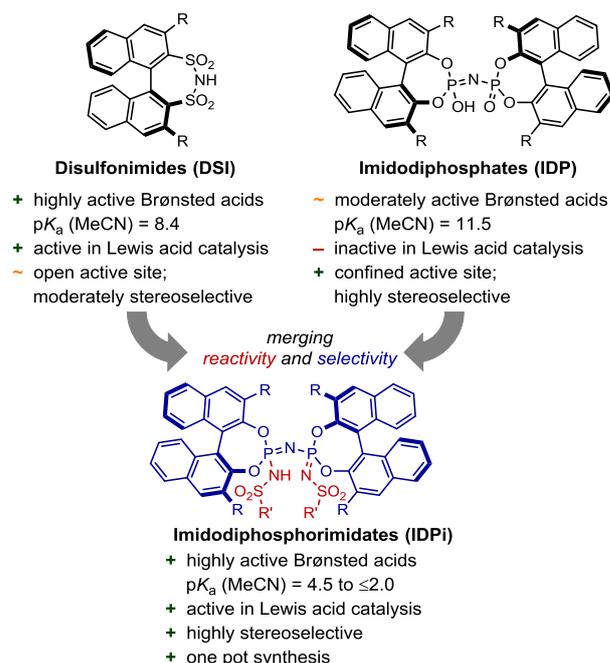
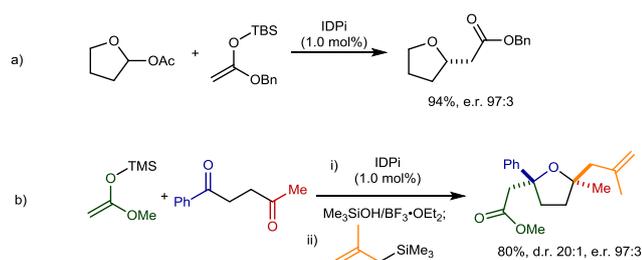


Figure 1. Imidodiphosphorimidate (IDPi) catalysts: merging reactivity and selectivity.

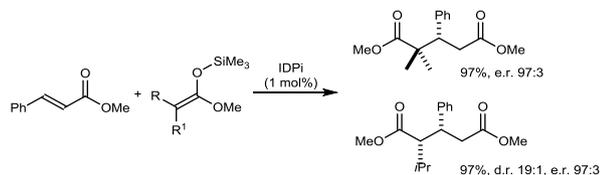
We also expanded enantioselective addition reactions to cyclic oxocarbenium ions to the synthesis of difficult to access 2,2-disubstituted and higher decorated tetrahydrofurans and tetrahydropyrans, starting from 1,4- and 1,5-ketoaldehydes or diketones (Scheme 1b).^[3]



Scheme 1. Examples for the IDPi-catalyzed synthesis of substituted tetrahydrofurans.

A General Mukaiyama–Michael Reaction of Silyl Ketene Acetals with α,β -Unsaturated Methyl Esters

α,β -Unsaturated esters as electrophiles in enantioselective Mukaiyama–Michael reactions not only suffer from difficult enantiofacial discriminations but also from an inherently low electrophilicity. As a consequence, asymmetric Michael reactions have thus far been largely limited to enals and enones as electrophiles, or to alkylidene malonates. In contrast, examples with simple α,β -unsaturated esters have remained rare, and more commonly the critical ester moiety has been replaced by more electrophilic analogues, thereby significantly diminishing the step- and atom economy. Catalytic asymmetric Mukaiyama–Michael additions to alkyl cinnamates have to our knowledge been unprecedented. Intriguingly, IDPi catalysts afforded various diesters in reactions of SKAs with alkyl cinnamates in excellent yields and enantiomeric ratios of up to 99:1., using as little as 1.0 mol% catalyst loading (Scheme 2). Other α,β -unsaturated esters were well tolerated and furnished the desired products in high yields and enantioselectivities.^[4]

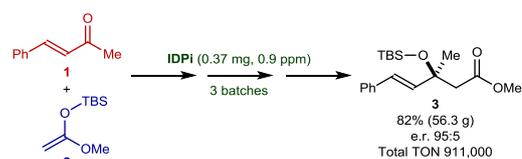


Scheme 2. Examples for the IDPi-catalyzed Mukaiyama–Michael addition to methyl esters.

Approaching sub-ppm-level Asymmetric Organocatalysis With A Mukaiyama Aldol Addition

Few reactions have caught as much attention by organic chemists as the aldol reaction, judged by the myriad of auxiliary- and catalyst-based stereoselective methods developed in the past decades. Ketone acceptors have however remained a challenging class of substrates in catalytic enantioselective variants of this transformation due to the reduced steric dissimilarity of the carbonyl-bound substituents in ketones as compared to aldehydes and the generally lower reactivity of ketones as electrophiles (as compared to aldehydes). The List group showed that IDPi catalysts successfully overcame previous limitations. Aldol products were obtained rapidly in >90% yield and with an e.r. of >95:5 by using only 0.05 mol% (= 500 ppm) catalyst

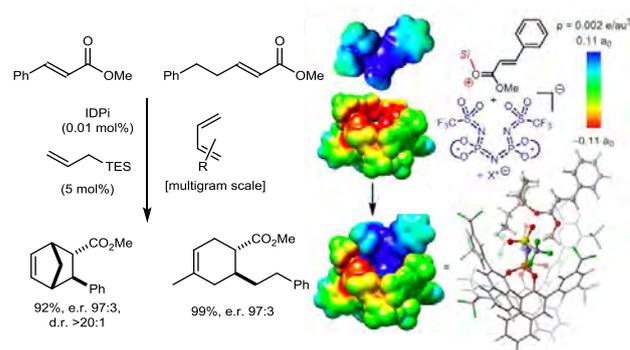
loading. A range of aryl alkyl ketones, dialkyl ketones and enones were shown to perform very well with IDPi catalysts, with catalyst loadings as low as 50–500 ppm.^[5] Moreover, to explore the limits of organocatalysis, the reaction furnishing aldol **3** was performed on a multi-decagram scale (Scheme 3). As little as 0.37 mg ($1.9 \cdot 10^{-4}$ mmol, 0.9 ppm) of IDPi catalyst fully converted three batches of ketone **1** (each 10.0 g, 68.4 mmol) and silyl ketene acetal **2** (14.2 g, 75.2 mmol, 1.1 equiv) in Et₂O (8.55 mL), ultimately reaching 95% conversion of all subjected ketone **1** and allowing for the isolation of aldol **3** in 82% yield and an e.r. of 95:5, corresponding to an outstanding total turnover number (TON) of $9.11 \cdot 10^5$.^[5] Such low catalyst loadings have been unprecedented in asymmetric, catalytic C–C bond forming reactions.



Scheme 3. Sub-ppm level catalysis in the aldolization of ketone **1**.

Diels–Alder Reaction of α,β -Unsaturated Methyl Esters

Despite tremendous advances in enantioselective catalysis of the Diels–Alder reaction, the employment of simple α,β -unsaturated esters, one of the most abundant and useful classes of dienophiles, has been severely limited in scope due to their low reactivity. IDPi catalysts offer a solution to this problem by converting a large variety of poorly reactive α,β -unsaturated methyl esters with different dienes to the cycloaddition products in excellent yields, enantio- and diastereoselectivities using very low catalyst loadings of only 0.1–3 mol%. In collaboration with the Neese group the reaction profile and the chiral ion pair were also investigated computationally to understand the origin of enantioselectivity (Scheme 4).^[6]

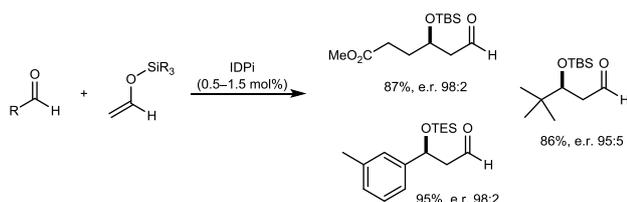


Scheme 4. IDPi-catalyzed Diels–Alder reaction.

Asymmetric Aldolizations of Vinyloxysilanes

The most challenging donors are undoubtedly those that produce another reactive acceptor unit in the course of the reaction, i.e. aldehydes, as these processes tend to yield oligomers and feature limited stability of the aldol products.

The employment of the smallest donor aldehyde, acetaldehyde, however has remained problematic and an enantioselective variant of single and double aldolizations of aromatic and aliphatic acceptor aldehydes so far elusive. IDPi catalysts cleanly converted benzaldehyde and derivatives thereof, such as *o*-tolualdehyde and *m*-anisaldehyde, with the simple TES or TBS enolates of acetaldehyde into the aldol products in very high yields and at remarkable enantiomeric ratios. Intriguingly, even aliphatic aldehydes were efficiently transformed and furnished the desired single aldolization products in high yields and good to excellent e.r. (Scheme 5).^[7]



Scheme 5. Examples for the IDPi-catalyzed Mukaiyama aldol reaction with acetaldehyde enolsilanes.

2. IDPi in Brønsted Acid Catalysis

The design of ever more acidic chiral Brønsted acids for both enantioselective Brønsted and “silylium” Lewis acid catalysis has been key to expanding the scope of substrate classes to more challenging and less basic ones.

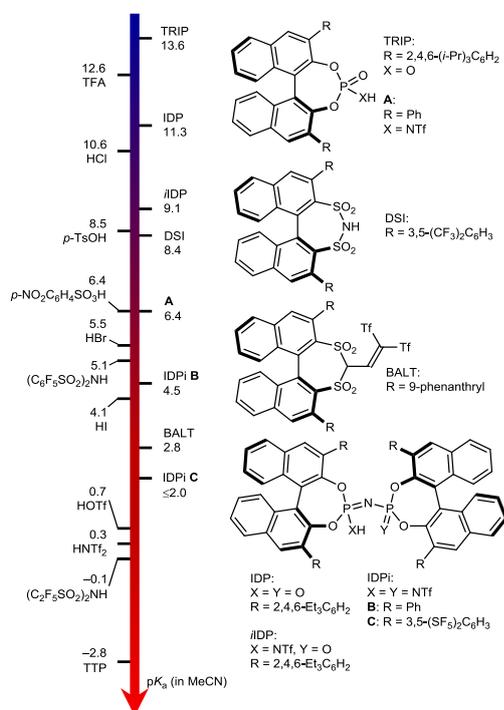
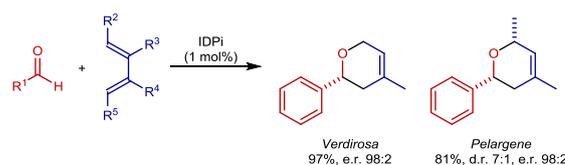


Figure 2. Experimental pK_a values of chiral and achiral Brønsted acids in MeCN.^[1] TTP = 1,1,3,3-tetratrylpropene.

While phosphoric acids like TRIP ($pK_a = 13.6$ in MeCN) are widely limited to readily activated imines, the significantly more acidic disulfonimides (DSI, $pK_a = 8.4$ in MeCN; cf. pK_a (p-TsOH) = 8.5 in MeCN; Figure 2) expanded the boundaries to the activation of aldehydes for numerous C–C bond-forming addition reactions.^[8] For the addition of particularly unreactive nucleophiles or the activation of even less basic substrates, including olefins,^[9] no sufficiently active catalyst class existed so far, resulting either in low substrate conversion and/or in undesired side-reactions driven by the Brønsted basicity of the counteranion.^[5,10] By comparison, the basicities of the newly developed binaphthyl-allyl-tetrasulfones (BALT; $pK_a = 2.8$ in MeCN) and IDPis (pK_a (B) = 4.5, pK_a (C) ≤ 2.0 in MeCN) are profoundly reduced, allowing the selective conversion of such unreactive substrates as α,β -unsaturated esters,^[11] readily enolizable ketones as electrophile^[5] and even simple olefins.^[9]

A General Catalytic Asymmetric [4+2]-Cycloaddition of Dienes with Aldehydes

The [4+2]-cycloaddition of dienes with aldehydes gained influence over decades for its efficiency and synthetic utility in the quick assembly of pyran substructures and the possibility to generate contiguous stereogenic centers, granting access to valuable enantiopure compounds. We recently found that IDPi catalysts possess appropriate features to catalyze this transformation using aromatic and even simple aliphatic aldehydes with high reactivity and selectivity.^[12] The superior acidity and enhanced confinement of IDPi enabled simple 2,3-dimethyl-1,3-butadiene to react with aromatic and even simple aliphatic aldehydes that proved inaccessible even with TfOH.^[13] Examples displaying the reactivity of other simple and in this transformation previously unprecedented dienes with a range of aldehydes were also reported (Scheme 6).^[12]



Scheme 6. IDPi-catalyzed [4+2]-cycloaddition reaction of simple dienes with aromatic and aliphatic aldehydes.

Multi-Substrate-Screening Identifies Catalysts for Diels–Alder Reactions of α,β -Unsaturated Aldehydes

Another difficult, but due to its wide synthetic applicability highly desirable substrate class for the Diels–Alder reaction comprises structurally diverse aldehydes. These were reacted with cyclopentadiene using a multi-substrate screening approach (Figure 3) to identify a suitable catalyst. Gratifyingly, highly general IDPi catalysts could be discovered, showing that multi-substrate screenings can aid in identifying broadly useful and highly stereoselective catalysts of challenging carbon–carbon bond forming reactions.^[14]

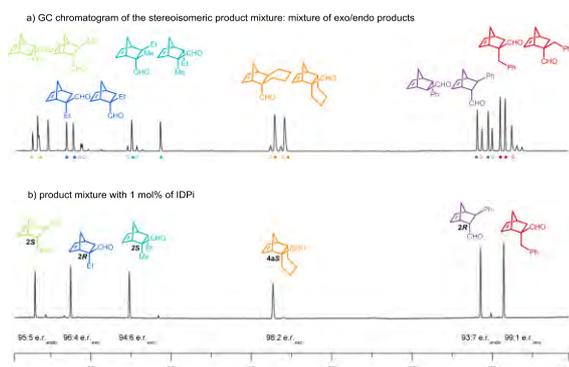
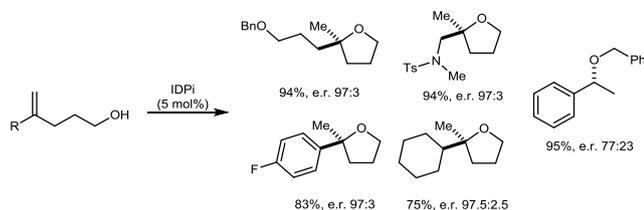


Figure 3. Multi-substrate screening of Diels-Alder reactions of α,β -unsaturated aldehydes and cyclopentadiene.

Hydroalkoxylation of Simple Olefins

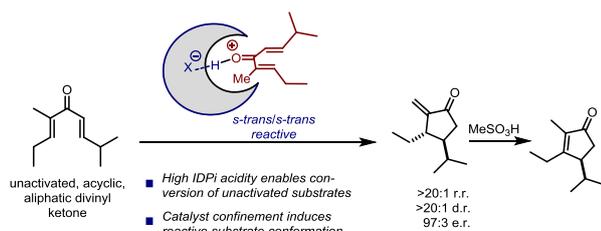
A great challenge in organocatalysis has been the application of simple olefins as electrophiles in hydrofunctionalizations, owed to their inherent low Brønsted basicity. Yet, the intrinsic simplicity, perfect atom economy and the abundant substrate availability renders such hydrofunctionalizations highly desirable. The employment of unactivated olefins as electrophiles in asymmetric hydroalkoxylation, however, has remained elusive in Brønsted acid catalysis. Intriguingly, IDPi catalysts exhibited high catalytic activity toward the desired hydroalkoxylation. A variety of functionalized and unfunctionalized alkenols were successfully converted under the optimized reaction conditions, providing the desired THFs in good yields and excellent enantioselectivities. Diene- and styrene-derived substrates were also well tolerated (Scheme 7).^[9]



Scheme 7. Examples for the IDPi-catalyzed hydroalkoxylation of simple olefins.

Nazarov Cyclization of Simple Divinyl Ketones

Despite being considered one of the most direct and atom-economical transformations for the synthesis of cyclopentenones, the asymmetric Nazarov cyclization is arguably one of the least employed methods toward chiral cyclopentenones.



Scheme 8. IDPi-catalyzed Nazarov cyclization.

The limited application is likely an effect of systematic substrate specificity for given variants and, therefore, a lack of generality. Using IDPi catalysts, a powerful catalytic, asymmetric Nazarov cyclization of simple, acyclic, aliphatic-substituted divinyl ketones could be developed (Scheme 8).^[15]

3. Conclusion

Imidodiphosphorimidates (IDPis) have opened doors to unprecedented reactivities in catalysis, while providing outstanding stereocontrol in a series of challenging inter- and intramolecular C–C and C–O bond-forming reactions.^[11] Small organic molecules such as proline are capable of catalyzing transformations with high enantioselectivities through the presence of covalent and strong non-covalent (H-bonding) interactions with the reacting substrates.^[16] In contrast, IDPis, mimicking enzymes, effect excellent enantiofacial discrimination through the confined chiral microenvironment of their substrate binding sites. The immense potential of IDPi catalysts has been amply illustrated in only a short period of time, and various further applications and mechanistic insights can be expected in the future.

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2.3 Mechanochemistry in Catalysis

Department of Heterogeneous Catalysis by Ferdi Schüth

ABSTRACT: The use of mechanical energy is an emergent research direction in many sub-disciplines of chemistry. Mechanochemistry in heterogeneous catalysis is only little explored, with the exception of pretreating solid catalysts before they are used in reactions. Over the last years, the department has followed several different approaches for the application of mechanical forces in the context of heterogeneous catalysis. These efforts originated in the work of the group on hydrogen storage materials, where light metal hydrides are milled with catalyst precursors to accelerate hydrogen uptake and release. This experience later initiated highly successful efforts to mechanochemically depolymerize cellulose and lignocellulose. Heterogeneously catalyzed gas-phase reactions were then studied in a specially designed flow-through milling vessel, and strong increase in reactivity was observed in CO-oxidation and PROX. While these reactions served as proof-of-concept systems, the mechanocatalytic chlorination of methane to chloromethane with very high selectivity, and the conversion of carbon-containing solids to hydrocarbons in hydrogen atmosphere extended the work towards more practically relevant systems. Incidentally, during the work on mechano-catalytically assisted gas-phase reactions, pathways for the innovative synthesis of interesting solid catalysts were discovered, i.e. the synthesis of supported metal catalysts from oxide supports and metal powders to yield nanometer-sized metal particles on the supports, and the formation of high surface area α -alumina with surface areas around $130 \text{ m}^2/\text{g}$ from boehmite in short milling times.

Milling is one of the oldest dry processing methods, used for millennia for diminution of particles to micrometer size. In addition to simple diminution, milling can also be used to effect chemical transformations. The term “mechanochemistry” had already been coined for this more than 100 years ago by W. Ostwald. In ancient times, the synthesis of mercury from cinnabar by grinding was known. In catalysis as well, milling is used frequently. Oxide catalysts are, for instance, activated by milling, producing defects or an amorphous surface layer, which result in higher activity.

As milling constitutes one of the key research expertise of the department since the early work on catalyzed hydrogen storage materials,^{1,2} a program was initiated to explore the potential of mechanochemistry in heterogeneous catalysis. The available milling systems include (i) different types of shaker ball mills (Retsch), also suitable for work at low temperature down to -196°C and elevated temperature up to approximately 200°C , (ii) planetary ball mills (Pulverisette P6 and P7 from Fritsch), and (iii) E_{max} (Retsch) combining milling principles of shaker and planetary mills. Milling in some of the systems is possible also at high pressures up to 300 bar. In order to test the influence of different milling media, milling vessels and balls made from stainless steel, zirconia, tungsten carbide and corundum are available. This broad range of equipment allows in-depth exploration of milling processes over a wide range of conditions.

The first success of the extension of mechanochemical approaches beyond hydrogen storage materials was achieved in the mechanocatalytic depolymerization of cellulose and lignocellulose,^{3,5} which provided a novel entrypoint into biorefinery schemes. This discovery led to a series of publications on the downstream chemistry of initially obtained cellooligomers. As this was covered in previous reports, the following sections will focus on mechanocatalytic

gas-phase reactions and the synthesis of highly interesting catalytic materials by ball milling.

One problem of mechanochemical processing is relevant for all different systems: abrasion from the milling jars and milling media can be substantial and always has to be considered. If the fundamentals of gas-phase reactions under milling are studied, typically different milling media were used in order to assess their influence. If materials are produced, such as supported catalysts or nano-corundum, one should use inert milling media, so that the properties of the produced solid are not substantially affected by the contamination due to abrasion. For the synthesis of nano-corundum, milling jar and media made of corundum are ideal. Alternatively, one can employ milling media, which can be selectively leached out, i.e. tungsten carbide in the synthesis of nano-corundum.

For mechanocatalytic gas-phase processes it was soon realized that batch operation was unsuitable, since it is almost impossible to follow the course of reaction properly in batch operation, and also sampling and analysis is more difficult than in continuous mode. Thus, a flow-through milling vial was constructed, which essentially operates as a continuously stirred tank reactor (Fig. 1). The flow-through vial has the same dimensions as a regular milling vessel, but it is equipped with two fittings for gas in- and outlet. At the outlet, a funnel is added, which acts to some extent like a cyclone filter, allowing the powder to slip back into the milling vial, which would otherwise be carried out with the gas stream. Here, also a thermocouple can be brought into the vial in order to monitor the temperature on-line. The milling vial can also be fitted to the cryo-mill for experiments at low temperatures; elevated temperatures are achieved by a heating jacket. Product gases are analyzed on-line, either by non-dispersive IR-spectroscopy (URAS), GC, or mass-spectrometry.

First CO oxidation was investigated,⁶ since this reaction is simple and very well studied, also in the group. It thus appeared to be an ideal model system to explore the effects of mechanical energy during a catalytic reaction.

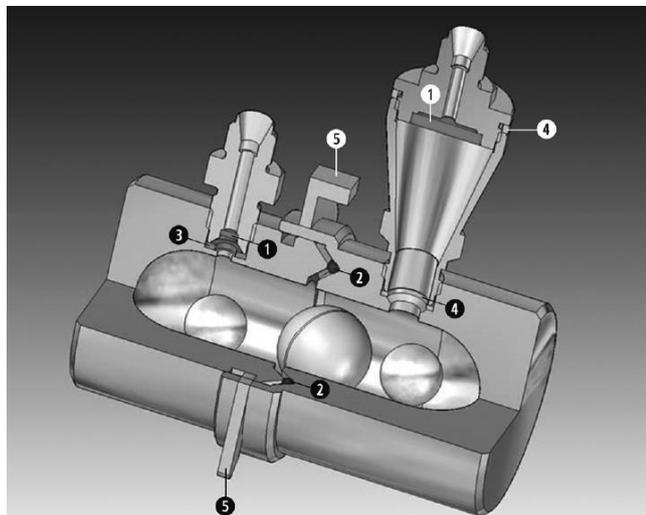


Figure 1. Schematic drawing of flow-through milling vial. 1 frit, 2 rubber sealing, 3 brass sealing, 4 plastic sealing, 5 clamp holding vial together.

Surprisingly, milling has a very pronounced influence on the conversion observed over different solids. Catalysts that are normally not active at room temperature, showed appreciable conversion, when milling was started. Conversion stopped, after the mill had been switched off (Fig. 2). The relatively rapid decay of conversion immediately after stopping the mill might be related to the vanishing of possible hot-spots, which could be present during milling. However, this would not explain the slower decrease of conversion over the course of several ten minutes. The enhanced activity of the catalysts was tentatively attributed to transient defects with higher intrinsic activity, which heal on time-scales of minutes.

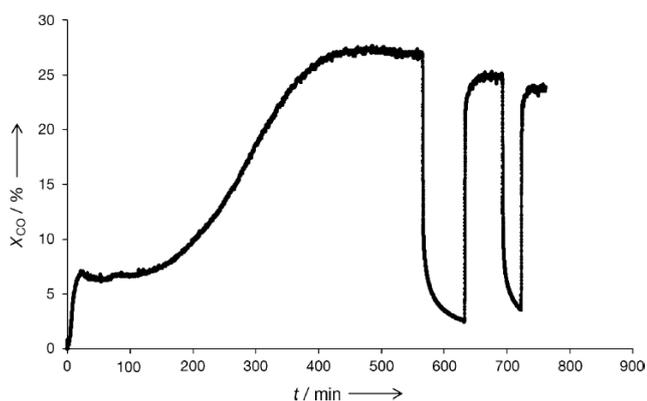


Figure 2. Typical CO conversion curve for an in-situ milling experiment. Catalyst 1 g Cr₂O₃, 50 ml/min 1% CO in air, $f = 25$ Hz, two balls $d = 10$ mm, one ball $d = 15$ mm, balls and vial made of stainless steel.

The conversion was strongly dependent on the conditions of the milling, such as milling frequency, size of balls, or ball-to-powder ratio. A higher mechanical energy input typically led to an increased

conversion – as would be expected, if the mechanical energy is affecting the catalyst's activity.

In order to compare the activity during milling with that observed in a conventional plug-flow reactor, the activity of the pre-milled catalyst (surface area increased by a factor of six during milling; thus, in order to exclude surface area effects, the pre-milled catalyst was studied) was studied at different temperatures in a regular plug-flow reactor. At room temperature, no activity for CO-oxidation was observed at the same space velocity as in the milling reactor. Reaction only started at observable rates slightly above 100°C in the plug-flow system. From these experiments, it could be concluded that milling increased reaction rates by up to three orders of magnitude.

Such increased activity was not only observed for chromium oxide as catalyst, but also for a number of other solids, both bulk catalysts and supported systems. Especially interesting were supported gold catalysts. Bulk gold is normally inactive at room temperature in CO oxidation, but if gold powder was milled under a flow of CO in air, full conversion of CO was reached at room temperature. These experiments were also extended to a mixture of support oxides and gold powder, and incidentally, the formation of supported gold nanoparticles was observed under these conditions (see below).

CO oxidation was chosen as the initial example, since it is simple considering that no selectivity issues arise as CO₂ is the only possible product. Next, to study the effect of milling on selectivity in a catalytic gas-phase reaction, the preferential oxidation of CO in hydrogen (PROX) was investigated. Herein, CO can be oxidized to CO₂, hydrogen to water, and even CO might react with hydrogen in syn-gas type reactions (this is improbable in the presence of oxygen, and no corresponding products were observed in our studies). This reaction is also of technological importance, since it is used to remove traces of CO from hydrogen for use in PEM fuel cells.

In initial screening experiments, various different solids were explored under milling conditions as catalyst for this reaction.⁷ Metal oxides alone were only slightly active at room temperature, even under milling. Copper, milled together with metal oxides, was found to be surprisingly active under these conditions, and Cu-Cr₂O₃ was found to give the highest activity system, with a conversion of 45% and a selectivity of 55% in a gas mixture of 1% CO, 1% H₂, 50% O₂, and 48% N₂ at room temperature. In-depth studies of the PROX reaction were thus carried out with Cu-Cr₂O₃ in a ratio of 1:3. Also in this case, the performance of the system was highly dependent on the milling parameters.

Interestingly, the conversion and the selectivity for CO oxidation increases with decreasing temperature. At -40°C the conversion is close to 100% at a selectivity of around 80% for CO oxidation (Fig. 3). In control experiments with pre-milled catalyst in the plug-flow reactor, a temperature of 100°C was required to achieve such high conversion, and the high selectivities observed in the ball mill were never reached in the plug flow reactor. This supports the notion that it is not just high local temperatures which are responsible for the catalytic performance during milling, because then the behaviour observed in the milling reactor should be observed in the plug-flow reactor at sufficiently high temperatures. Also in the case of PROX, the high activity and selectivity for CO oxidation is attributed to short-lived defects. The slightly negative apparent activation energy

would then be due to almost similar activation energies for the surface reaction itself and the healing of defects, which cancel each other.

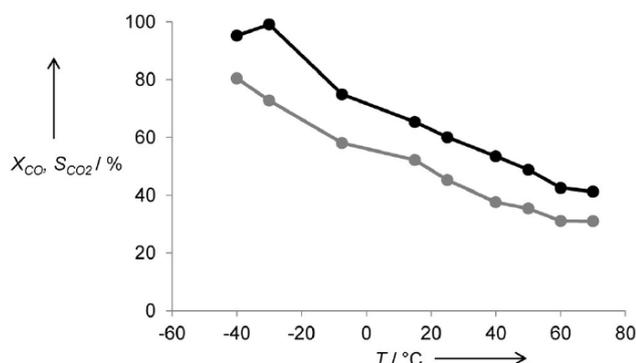


Figure 3. Comparison of conversion (black) and selectivity (grey) for CO-PROX under milling at different temperature. 500 mg Cu, 1500 mg Cr₂O₃, CO/H₂/O₂/N₂ (1:1:50:48) 50 ml/min, six balls 10 mm made from WC, $f = 25$ Hz.

With respect to applications, the most interesting mechanocatalytic reaction studied is the chlorination of methane with trichloroisocyanuric acid (TCCA) over Lewis acidic catalysts, like alumina or ceria.⁸ Various solid Lewis acids were tested, and ceria was found to be the most active catalyst. Under optimized, relatively mild conditions (seven 5 mm \varnothing WC balls, $f = 10$ Hz), a gravimetric productivity of 150 g CH₃Cl kg_{catalyst}⁻¹ h⁻¹ could be achieved, which is in the range of large scale technical processes. Experiments to elucidate the mechanism suggest a radical process (Fig. 4), in which TCCA is activated by homolytic N-C bond cleavage, the N \cdot radical abstracts hydrogen from methane to yield methyl radicals, and the Cl \cdot radical combines with the methyl species to chloromethane. During the laboratory experiments, only about one third of the chlorine in the TCCA is used for the chlorination of methane, the rest of the TCCA is decomposed to cyanuric acid and gas phase chlorine. For a technical process, it will probably be possible to suppress this decomposition by adjusting the rate of radical generation and the residence time of methane in the reactor. Alternatively, one could regenerate TCCA from the product cyanuric acid and the chlorine, since these are the starting materials for industrial TCCA synthesis in any case.

During work on these mechanocatalytic gas-phase reactions, several serendipitous observations led to additional lines of work. On the one hand, it was discovered that carbon-containing solids can be hydrogenated under hydrogen pressure during milling to hydrocarbons in the presence of suitable catalysts. This work is still in progress, and will probably be submitted or published at the time of the SAB meeting. Other projects were targeted at the synthesis of catalytically interesting materials, i.e. supported metal catalysts and α -alumina with exceedingly high surface area.

Normally, supported catalysts are synthesized using wet chemical methods, requiring a number of different steps. There are also scattered reports in the literature that for specific cases milling of metal compounds, accompanied or followed by reduction reactions, can be used to produce supported catalysts. In one publication, as one of

three alternative synthetic processes, elemental silver was used as precursor of a high activity Ag/ γ -Al₂O₃ synthesized by ball milling. Also milling oxides with preformed nanoparticles resulted in a supported catalyst. However, mechanochemical synthesis as a general approach to synthesize supported metal catalysts from macroscopic metal powder had not been explored before. In the studies of catalytic reactions during milling, in some cases, when starting from metal powder and oxides, the solid after the reaction did not consist of separated metal and oxide particles, but in nanometer sized metal particles supported on the oxide, exactly as in conventional supported catalysts. In order to explore the potential of this process in detail, this effect was studied systematically.⁹

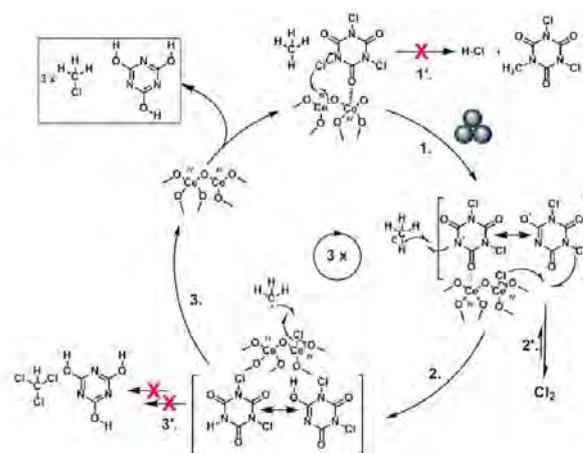


Figure 4. Mechanistic proposal for the selective mechanocatalytic formation of chloromethane from methane and TCCA over solid Lewis acids (in this case CeO₂).

Gold powder consisting of micrometer-sized particles was first milled with different types of titania, and after 3 h of milling, gold particles with sizes of approximately 3 nm supported on titania are obtained (Fig. 5). The method is versatile, since alumina, cobalt oxide as well as iron oxide could be used as supports with similar results. Also the supported metals could be varied: with platinum, silver, copper, and cobalt metal nanoparticles with sizes on the order of 5 nm - with some variation for the different metals - were dispersed on the support oxides. Finally, if two different metal powders were used as starting material, together with a support oxide, bimetallic alloy nanoparticles were synthesized.

As can be seen in the XRD pattern in Fig. 5, the anatase phase of the support transforms via brookite to rutile. A more interesting transformation was observed when starting with γ -alumina: during milling, α -alumina (corundum) with high surface area was obtained. Since corundum is a technologically extremely interesting material, which can hardly be obtained with surface areas exceeding a few m²/g, and since there are several interesting, but partly contradictory studies concerning the stability of high surface area corundum, it was attempted to mechanochemically synthesize high surface area corundum. These attempts were successful. Starting from boehmite, an aluminium oxide hydroxide (γ -AlOOH), corundum with surface areas of up to 140 m²/g was synthesized (Fig. 6).¹⁰ Structural water

in the boehmite precursor was identified to play crucial role: Firstly, it acts as a process control agent to assist the fragmentation of agglomerates formed during milling into corundum nanoparticles, and secondly, it stabilizes the formed corundum nanoparticles *via* hydroxylation. These observations were supported by quantum chemical calculations suggesting that only with hydroxylated surfaces the energetics of the process are favourable for nano-corundum formation. Thus, the water content of the precursors has to be controlled within certain limits for optimum conversion of the boehmite to corundum. The process is rather robust: similar results were obtained with different types of boehmite and also pseudoboehmite as starting materials, and the transformation takes places in different types of milling vessels with different milling materials, although the exact conditions may have to be adapted. The results have been reproduced in an industrial laboratory, and work to scale-up the process to industrial dimensions is under way.

Finally, milling techniques can also be used to modify catalytic materials: The hydrophobicity of oxides can be adjusted by surface modification with, for instance, functional silanes. Carrying out such reactions in ball mills requires only very little energy input and proceeds to a high degree of surface modification in only a few minutes. Also the intercalation of layered materials by milling is easily achieved, as has been demonstrated for several clay types, into which different guest species were intercalated. It is expected, that mechanochemical methods can be extended also further beyond these first examples to result in even further modified catalytic materials.

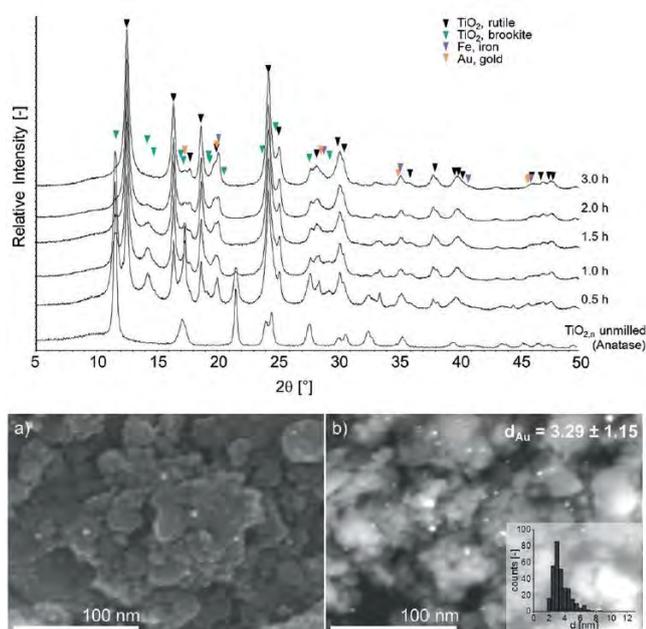


Figure 5. Development of XRD pattern with milling time during milling of gold powder with titania (top). SEM (a) and STEM (b) of microtomed sections of the sample after 3h milling (bottom).

As the previous results and discussion have shown, mechanochemical methods are extremely interesting in heterogeneous catal-

ysis. Yet, the processes are little understood. Thus, mechanochemical approaches in heterogeneous catalysis will be explored in two directions in the future: On the one hand, the potential of these methods for further catalytic reactions of high relevance, such as methane activation and ammonia synthesis, will be elucidated. On the other hand, the scope of the studies will be expanded to obtain a molecular level understanding of the relevant processes. Synchrotron beamtime for in-situ XRD studies during milling has already been granted and a suitable milling vial has been constructed, first tests at BESSY have been carried out. Also microscopic, both electron microscopic methods and probe microscopies, will be employed to lay a sound foundation for the understanding of mechanochemical processes in catalysis.

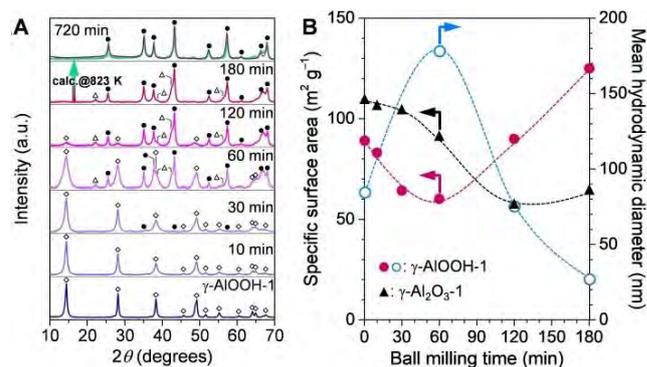


Figure 6. Development of XRD pattern with milling time during milling of boehmite (A) and development of surface area and particle size with milling time for boehmite and γ -alumina as precursor (B). Identified crystalline phases: \diamond : γ -AlOOH, \bullet : α -Al₂O₃, and \triangle : α -AlOOH. Milling conditions: WC jar (25 cm³), 3×12 mm WC balls, 1 g powder charge, $\omega_{\text{mill}} = 25$ Hz, $t = 10$ -720 min.

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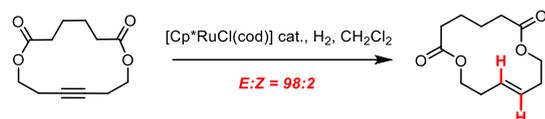
2.4 Advances in Metal-Carbene Chemistry

Department of Organometallic Chemistry by Alois Fürstner

ABSTRACT: The major lines of research in this Department continue to be: (i) alkyne metathesis, (ii) iron catalyzed C-C-bond formation, (iii) π -acid catalysis using platinum, gold and rhodium complexes, and (iv) unorthodox catalytic addition reactions. All areas are prospering, including the application of the in-house methodology to target-oriented synthesis; yet, it was the field of ruthenium-catalyzed addition chemistry which led to the most perplexing and (hopefully) significant results. For the unexpected intervention of discrete metal carbenes as reactive intermediates, the major findings in this area are discussed together with our recent contributions to the related field of rhodium carbene chemistry.

Ruthenium. *cis*-Delivery of H₂ to a π -system of an unsaturated substrate is the canonical course of metal catalyzed hydrogenation reactions. This stereochemical paradigm remained basically unchallenged since the pioneering work of Sabatier until our group reported the semi-reduction of internal alkynes with the aid of [Cp*Ru]-based catalysts. The reaction clearly violates this fundamental rule and affords *E*-alkenes by direct *trans*-hydrogenation (Scheme 1). Answering the question as to how this unorthodox transformation might proceed and whether it is a singularity or the manifestation of a more general reactivity mode became a top priority in our laboratory.¹

Scheme 1. Prototypical *trans*-Hydrogenation Reaction

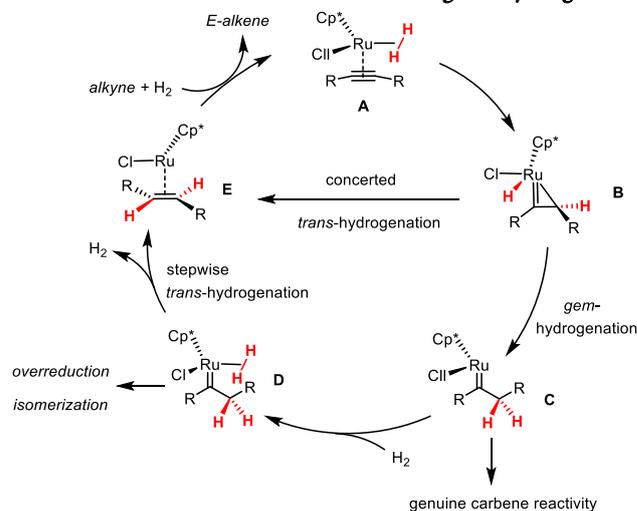


A combined experimental and theoretical approach provided compelling evidence that *trans*-hydrogenation can actually be reached by *two* distinctly different yet interconnected pathways (Scheme 2).² A σ -complex of type **A** is initially formed, which evolves via the rate-determining H-delivery to the activated triple bond into a metallacyclopropene **B**. It is at this stage that the reaction pathway bifurcates: thus, **B** can transform in a concerted process into the desired *E*-alkene **E** by passing through a low-lying stereo-determining transition state; this product-forming step is strongly exergonic and therefore almost certainly irreversible. The computed barrier for the formation of the *Z*-alkene is notably higher, which explains the experimentally observed excellent *E/Z* ratios.

Reagents other than H₂ able to form σ -complexes similar to **A** should undergo analogous *trans*-addition to alkynes. In fact, we were able to accomplish closely related *trans*-hydroboration, *trans*-hydrosilylation (previously described by the Trost laboratory), *trans*-hydrogermylation and *trans*-hydrostannation reactions, which are equally paradigm-changing processes.¹ The stereochemi-

cal outcome is astounding, if one considers that conventional *trans*-hydroboration is *the* textbook example for a *cis*-addition process via a four-membered transition state under frontier-orbital control. All newly discovered *trans*-hydrometalation reactions break this fundamental stereochemical rule; importantly, they are robust, distinguished by excellent functional group compatibility, and have already stood the test of natural product synthesis in a number of demanding cases (see below).¹

Scheme 2. Mechanism of *trans*- and *gem*-Hydrogenation



Only in the case of the *trans*-hydrogenation can the metallacyclopropene **B** evolve by a second pathway, in which both H-atoms of H₂ are transferred to one and the same C-atom of the substrate (Scheme 2). This geminal delivery, which entails formation of a discrete metal carbene **C**, is without precedent in the literature. Computational studies at the DFT and the CCSD(T) level suggest that the *trans*- and the *gem*-pathway have similar barriers, but polar substituents in vicinity to the reacting triple bond foster carbene formation and allow regioselectivity to be imposed on this remarkable transformation (Figure 1). Moreover, it has been unambiguously shown by spectroscopic means (PHIP NMR) that the

resulting carbenes are kinetically competent intermediates rather than thermodynamic sinks off the catalytic cycle; they evolve via associative H₂-dependent processes into the desired *E*-alkene (and possible by-products). The spectroscopic evidence is in excellent accord with the computational results.²

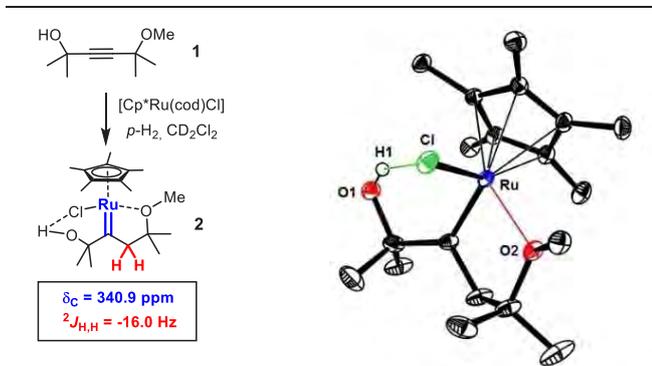
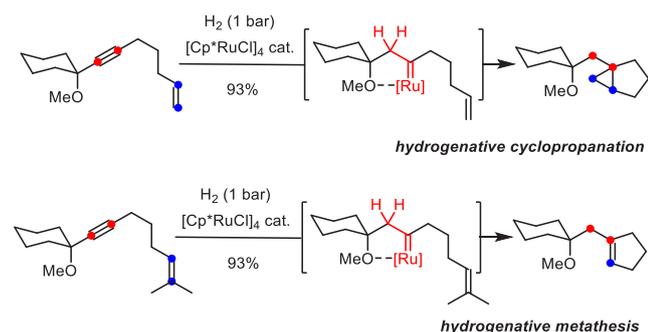


Figure 1. Formation of a Pianostool Ru-Carbene by *gem*-Hydrogenation; Structure of the Complex in the Solid State

Scheme 3. Hydrogenative Cyclopropanation and Hydrogenative Metathesis



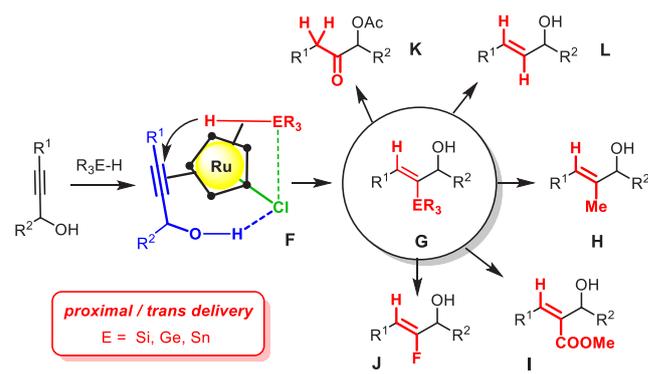
From a conceptual viewpoint, the formation of discrete metal carbenes by hydrogenation of an alkyne is arguably of the highest significance. In a formal sense, the triple bond behaves as a 1,2-dicarbene synthon: one “carbene” intercepts the [Cp*Ru] fragment, whereas the vicinal “carbene” site inserts into the H–H bond (Figure 1). To the best of our knowledge, the *geminal* hydrogenation of a stable carbogenic compound is a new reactivity mode.^{1,2}

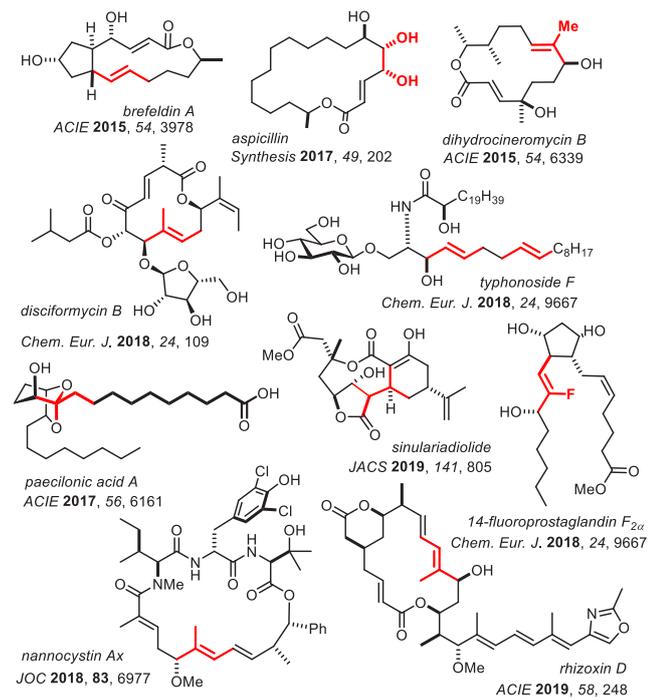
This counterintuitive entry into ruthenium carbenes raises new questions and opens exciting chemical opportunities. Even though we were able to isolate and even crystallize numerous examples, it is not intuitive whether such pianostool ruthenium complexes exhibit Fischer-carbene or Schrock-alkylidene character. For two representative complexes, however, has it been possible to record the solid-state ¹³C NMR spectra and to analyze the chemical shift tensors of the carbene signals.³ Details apart, this advanced spectroscopic technique drew the portrait of a family of metal carbenes that amalgamates purely electrophilic behavior with characteristics more befitting metathesis-active Grubbs catalysts. Moreover, we were able to show that less electron-rich Cp^R ligands facilitate carbene formation by *gem*-hydrogenation.³

Several attempts at harnessing genuine carbene reactivity by alkyne *gem*-hydrogenation have already been successful.² Most notably, it is possible to intercept the carbene primarily formed with tethered olefins (Scheme 3); this allows either cyclopropanes or cyclic olefins to be formed; it is the substitution pattern of the substrate that determines the course of the reaction.⁴ In any case, the new “hydrogenative cyclopropanation” stands in striking contrast to the hydrogenolytic cleavage of cyclopropanes commonly used in organic synthesis. Likewise, the “hydrogenative metathesis” is an entirely new manifold to be distinguished from classical enyne metathesis, because it delivers cyclic olefins rather than 1,3-dienes as the product. The available data allow a fairly detailed mechanistic picture to be drawn, especially with regard to the fate of the secondary carbene formed during the actual metathetic C–C bond cleavage.⁴

***trans*-Hydrometalation.** As mentioned above, the concerted pathway of *trans*-hydrogenation (**A** → **B** → **E**) finds correspondence in ruthenium catalyzed *trans*-additions of pinacolborane (pinBH) or R₃EH (E = Si, Ge, Sn) to internal alkynes.¹ During the report period, these reactions were subject to extensive scrutiny. They are distinguished by excellent stereo- as well as regioselectivity, especially when working with propargylic substrates:⁵ spectroscopic, crystallographic and computational evidence suggests that a nascent hydrogen bond between the protic substituent and the polarized [Ru–Cl] unit of the catalyst locks the substrate in place; at the same time, the –Cl ligand steers the incoming reagent via a hypervalent interaction with the R₃E– group (Scheme 4). These synergistic effects impose directionality on the ligand sphere of the loaded catalyst **F**, which ultimately translates into excellent levels of selectivity.⁵

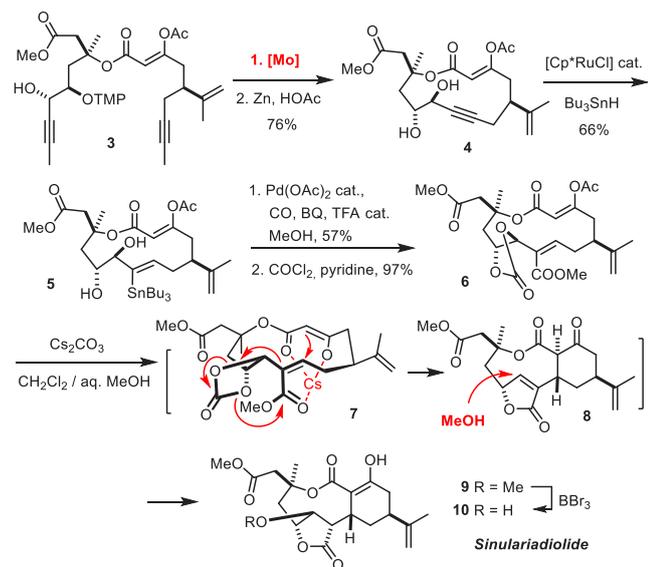
Scheme 4. Directed *trans*-Hydrometalation and Novel Downstream Chemistry





The resulting products **G** provide ample opportunity for downstream functionalization. In addition to the known repertoire of organoboron, -silicon and -tin chemistry, we developed new methods that allow such substrates to be converted into the polyketide motifs **H** and **I** by C-methylation or methoxycarbonylation, respectively. Likewise, stereodefined fluoroalkenes **J** as well as acyloins **K** came into reach (Scheme 4). Each of these transformations has already served as a key step in natural product synthesis.

Scheme 5. Total Synthesis of Sinulariadiolide



The arguably most involved case concerns the *nor*-cembranoid sinulariadiolide (**10**) (Scheme 5).⁶ Specifically, a transannular approach was conceived, which allowed the tricyclic scaffold comprising a central nine-membered ring to be forged. Key to success

was the formation of the macrocyclic precursor **4** by alkyne metathesis (this laboratory) followed by hydroxy-directed *trans*-hydrostannation (this laboratory) and subsequent methoxycarbonylation of the resulting stannane **5** (this laboratory). Treatment of compound **6** thus formed with Cs_2CO_3 in MeOH triggered a cascade comprised of (i) deacetylation, (ii) stereoselective transannular Michael addition with formation of the challenging medium-sized ring, (iii) β -elimination with concomitant cleavage of the carbonate, (iv) attack of the released alkoxide onto the proximal ester with formation of a butenolide ring **8**, and (iv) front-side attack of MeOH from the medium onto this Michael acceptor, which is rendered particularly reactive by the bridgehead alkene moiety. Final ether cleavage then furnished the target compound in excellent overall yield.⁶

Rhodium. Controlled decomposition of diazo compounds with (chiral) dirhodium tetracarboxylate complexes has gained tremendous importance in (asymmetric) catalysis. The transient rhodium carbenes, however, had basically defied direct experimental observation until our group was able in 2016 to present crystal structures of several prototypical members of this elusive series (cf. last progress report). NMR data showed that the structures in solution are very similar to those in the solid state.

The crystal structure of the donor-acceptor carbene **11** derived from $[Rh_2((S)\text{-PTTL})_4]$ (**12**), a chiral catalyst with an excellent track record, is deemed particularly relevant (Figure 2).⁷ Although crystallographic and spectroscopic data can only draw the portrait of the ground state, it is likely that the forces which impose the peculiar and – at first sight – unexpected “all-up” conformation onto the chiral ligand sphere are also operative in the selectivity-determining transition state.

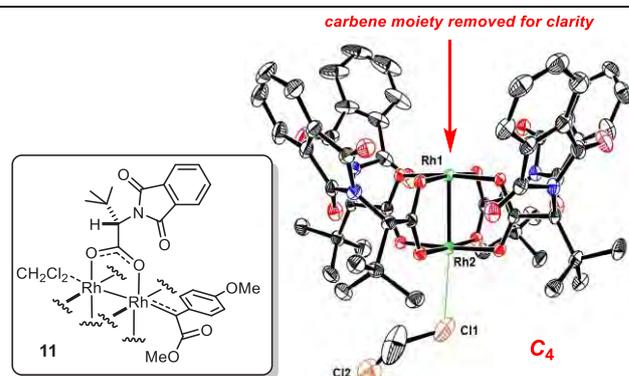
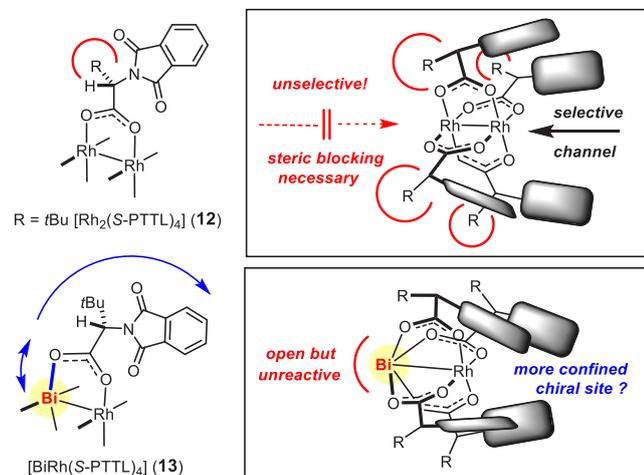


Figure 2. X-ray structure of a chiral dirhodium carbene

Under this premise, it was possible to rationalize the stereochemical course of a cyclopropanation reaction effected by this famous catalyst.⁷ Our model predicted the correct isomer; therefore, it also seemed legitimate to analyze why the level of induction is only modest (78% ee). An essentially C_2 symmetric “all up” array entails two notably different rhodium faces (Scheme 6): although the crystallographic data show that the “achiral” pore between the *tert*-butyl groups is narrower than the aperture of the “chiral” calyx, it remains large enough that CH_2Cl_2 can enter and coordinate to Rh2. If a diazo derivative reaches Rh2 and gets decomposed to the corre-

sponding metal carbene, a racemic background reaction will ensue and the *ee* of the resulting product necessarily drops.⁷

Scheme 6. Concept for an Improved Catalyst Design



Replacement of the *tert*-butyl groups by even bulkier substituents should improve the outcome; earlier empirical catalyst optimization has shown that this is indeed the case. We pursued a less conventional approach to catalyst optimization, which builds upon recent insights into structure and bonding in heterobimetallic paddlewheel carbene complexes.⁸ In a collaboration with the Neese group, we had shown that formal replacement of one Rh^{II} center of the bimetallic core for Bi^{III} enhances the electrophilic character of the resulting carbenes to a significant extent, although the rate of metal-carbene formation is manifestly slower.⁹ More important in the present context is the fact that the Bi site lacks any notable Lewis acidity and proved incapable of decomposing ethyl diazoacetate. Even though the ionic radius of Bi is larger than that of Rh and the Bi center hence certainly more exposed, any deleterious background reaction should cease (Scheme 6). Furthermore, the different radii impart a conical shape on the heterobimetallic core, which likely translates into a narrower chiral pocket and hence potentially improves the level of asymmetric induction. As these factors might synergize, it seemed worthwhile to pursue this design concept.⁸

In line with our expectations, the structure of the heterobimetallic analogue [BiRh((*S*)-PTTL)₄]·EtOAc (**13**·EtOAc) in the solid state shows that the co-crystallized EtOAc is bound to rhodium, whereas the bismuth center is unligated (Figure 3). Once again, the ligand sphere adopts the $\alpha,\alpha,\alpha,\alpha$ -conformation, presumably because this arrangement places the *tert*-butyl groups as the most bulky substituents at maximum distance from each other; their orientation toward the Bi center follows from the larger radius of

this ion, which provides more space. The long Bi–O bonds render the chiral pocket about the rhodium center in **13** more confined than that of its homobimetallic analogue **12**.

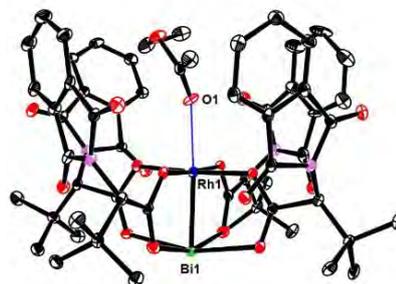


Figure 3. X-ray Structure of [BiRh((*S*)-PTTL)₄]·EtOAc

Scheme 7. Superior Performance of the Heterobimetallic Precatalyst **13**



Importantly, the new precatalyst **13** leads to cyclopropanes with notably higher optical purity than those obtained with the traditional dirhodium congener **12** (Scheme 7).⁸ This lead finding is the basis for ongoing work in our laboratory which intends to explore the new design and its synthetic implications in more detail.

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2.5 In Dialogue with Nature: An integrated experimental and theoretical approach leading from algorithm design to chemical concepts

Department of Molecular Theory and Spectroscopy by Frank Neese

ABSTRACT The department of molecular theory and spectroscopy (DMTS) is involved in three main activities: (1) Theoretical method development with emphasis on efficient algorithms for wavefunctions based calculations on realistic chemical systems (this includes the development of the ORCA program package), (2) Computational chemistry studies in the fields of bioinorganic chemistry, homo- and heterogeneous catalysis as well as molecular magnetism and (3) advanced spectroscopic methods to experimentally study the electronic structure of transition metal complexes with relevance to any of the mentioned fields. The report summarizes the progress that has been made in these areas between March 2017 (date of the previous evaluation at; then at the MPI-CEC) and October 2019.

1. Structure of the department

The DMTS was founded in January 2018 in succession of the theory department of Prof. Thiel. The department had previously existed in similar form at the MPI for Chemical Energy Conversion (MPI-CEC, 2011-2017). In the process of moving, the Joint Workspace (JWS) was established between the institutes, which allows the DMTS to host their experimental facilities at the MPI-CEC.

The work done in the DMTS falls into three main areas. There are currently seven group leaders working in the department who have their main focus within one of the three categories. However, we all work closely together, supervise students jointly and drive projects together thus leading to synergies and frequent exchange between the sub-disciplines covered. The three main areas are:

(1) **Theoretical Method Development** in quantum chemistry. Here we focus on the development of single- as well as multi-reference wavefunction based approaches that are applicable to large systems (molecules, cluster models). The emphasis is not only on total energies, but on molecular properties and theoretical spectroscopy and magnetism. (PIs: Auer, Bistoni, Izsak, Manganas)

(2) **Computational chemistry applications** (mostly) on transition metal containing systems (enzymes, catalysts, solids and surfaces). The emphasis are mechanistic studies in all areas of catalysis as well as the establishment of structure-property relationships (such as in molecular magnetism). (PIs: Atanasov, Auer, Bistoni, Pantazis, Manganas, van Gastel, Ye)

(3) **Spectroscopic studies** aiming at experimentally defining the electronic structure of transition metal species like catalysts or reaction intermediates. A wide variety of techniques is used here including electron paramagnetic resonance (EPR), SQUID magne-

tometry, Mössbauer spectroscopy (MB), absorption (ABS), circular dichroism (CD), magnetic CD (MCD) and resonance Raman (rR) spectroscopy. (PIs: van Gastel, Manganas in cooperation with Eckhard Bill at the MPI-CEC) A wider variety of X-ray absorption and emission techniques are pursued in collaboration with the department DeBeer at the MPI-CEC.

Two recent perspective articles summarize the philosophy that underlies our approach to science.^{1a,b} In essence, we look for an intimate interconnection between theory and experiment using spectroscopy as the main meeting point between the disciplines rather than total energies. In order to develop the full information content of a wide variety of spectroscopic properties, increasingly accurate and versatile tools are being developed for the calculation of spectroscopic properties while on the other hand, methods are also developed to translate the results of elaborate calculations into chemical language (“Interpretation aids”).

2. Quantum Chemical method Development

The ORCA program suite is a general-purpose electronic structure package that has been developed in the department since the late 1990s. Being free for academic researchers, it has found a rapidly growing user community of more than 25000 users world-wide.^{1c} Commercial users can obtain a license via the company FAccTs. The technical aspects of the ORCA development efforts are described elsewhere in this report (PI: Wennmohs).

2.1. Linear scaling single reference correlation methods.

Our development efforts in this area are based on the concept of domain-based pair natural orbitals (DLPNOs). These efforts have ongoing for more than a decade in the DMTS and are based on resurrecting ideas that have been put forward in the late 1960s. The work in the DMTS has greatly pushed these ideas forward leading to a host of new methods that allow for correlated wavefunction

calculations of unprecedented size and accuracy. The DLPNO methods have been embraced by the computational chemistry community and are now widely used world-wide. It has been our main focus of the past several years to make these methods as versatile as possible in order to allow for computational chemistry applications at correlated levels in a black-box fashion in much the same way that DFT is being used. Noticeable recent developments include the development of an open-shell DLPNO-CCSD(T) method,² closed- and open-shell CCSD densities³ (and hence properties), multireference methods (DLPNO-NEVPT2), explicitly correlated variants⁴ of closed- and open-shell approaches (DLPNO-CCSD(T)-F12) and analytic DLPNO-MP2 gradients⁵ (closed-shell) (PI: Neese).

Major development efforts were directed towards the formulation and implementation of a DLPNO based excited state methodology (PI: Izsak).⁶ This is a vastly difficult problem since electronic rearrangements in electronically excited states lead to completely different local orbital structures compared to the electronic ground states. Hence, PNOs for the ground state are not suitable for excited states. This problem was tackled with the similarity transformed equation of motion (STEOM) approach by Nooijen and Bartlett. In this approach one only need to determine ground state coupled cluster amplitudes and solve an excited state eigenvalue problem of the same size as CI-singles (CIS) in order to arrive at a correlated result. This is achieved, by solving the corresponding non-particle conserving EOM-CCSD equations for ionization potentials (IP) and electron affinities (EA) that are then used together with the ground state CC amplitudes to “dress” the CIS matrix. The advantage of having only to solve a CIS size problem allows for calculations of dozens of states on systems with about 200 atoms.

The recent accomplishment of DLPNO-IP-EOM-CCSD, DLPNO-EA-EOM-CCSD and finally DLPNO-STEOM-CCSD leads to method of unprecedented accuracy and efficiency.⁷ The method was subsequently used in a number of application studies with excellent success.⁸

2.2. Multireference methods.

In the field of multi-reference wavefunction methods, we have made significant progress in terms of the performance and convergence of the underlying CASSCF program for large molecules.⁹ In addition, we have implemented quasi-degenerate versions of the NEVPT2 correction and have provided a CASPT2 implementation in ORCA (PI: Neese).

The iterative configuration expansion (ICE-CI) is an approximate Full-CI method that has been developed in order to treat large active space. Calculations with up to 40 active electrons and over 100 active orbitals have been done. The achievable accuracy is on the order of 1 mEh relative to FCI. The method is particularly powerful for antiferromagnetically coupled magnetic systems since our implementation can work on individual configuration state functions (CSFs), which allows for the efficient refinement of any branching diagram state. We currently investigate solutions to the size-consistency problem as well as how to incorporate dynamic correlation on top of these enormous active space (PI: Neese).

The new method DCD-CAS(2) is based on the idea to treat static correlation, dynamic correlation and relativity on equal footing.

In this method, the CASCI matrix is “dressed” to second order in perturbation theory with dynamic correlation contributions and the extension to treat spin-orbit coupling and magnetic fields at the same time was also implemented. The method offers well-defined advantages of NEVPT2 and CASPT2, but suffers from the fact that it is state universal and a single 0th order Hamiltonian carries the burden of describing multiple states.¹⁰ Solutions to the problem are under investigation (PI: Neese).

Significant efforts are directed towards finding a practical multi-reference method that goes beyond second-order in perturbation theory. Since such methods are extremely complex, automatic code generation tools need to be employed. We have developed a powerful framework (ORCA-AGE) that allows for arbitrary single- and multireference wavefunction methods to be implemented. It produces code that is almost as efficient as hand-optimized code. So far, we have implemented full internally contract MRCI (FIC-MRCI), its CEPA-0 variant (FIC-CEPA0) as well a rigorous internally contract multireference coupled cluster method (FIC-MRCC).¹¹ We are currently investigating their properties, computational efficiency and how to simplify these methods to the point that they can become practical computational tools for large-scale use (PI: Izsak, Neese).

2.3. Chemical Analysis tools.

In order to translate the results of elaborate wavefunction based correlation calculations into chemical language, we have developed two particular powerful tools that have found widespread use in our applied studies.

Given a fragmentation scheme of the supersystem (now automated), the local energy decomposition (LED) is able to decompose the DLPNO-CCSD(T) energy into intra- and inter-molecular components. In particular, it is able to extract intermolecular dispersion- and electrostatic- as well as exchange- interaction energies. This has been found to be extremely fruitful in a number of studies. In the evaluation period, open shell- and multi-level variants of the LED were developed as well as an extremely cost-effective scheme that provides near DLPNO-CCSD(T) accuracy at Hartree-Fock cost (HFLD; PI: Bistoni, see below).¹²

The ab initio ligand field theory (AILFT) is tailored towards d- and f-elements. It allows to uniquely extract ligand field parameters (Racah parameters, one-electron ligand field matrices and the one-electron spin-orbit coupling constant) from the the results of CASSCF, NEVPT2 or DCD-CAS(2) calculations. This has found widespread use in our studies in molecular magnetism (PI: Atanasov, see below).¹³

2.4. Methods for Theoretical Spectroscopy.

In the field of theoretical spectroscopy, a traditional mainstay of the group, three main developments have taken place:

(1) Methods for the prediction of NMR parameters. We have developed accelerated versions of the well-known methods to calculate chemical shifts and spin-spin coupling constants based on DFT. In addition, we have developed and efficient implementation of RI-MP2 and double hybrid DFT chemical shieldings that allow for much more accurate calculations than previously feasible with DFT. We currently extend these methods towards the DLPNO variants (PI's: Auer, Neese).¹⁴

(2) Methods for the calculation of X-ray spectra. These developments have been ongoing for about a decade and constitute a major collaborative project between the DMTS and the experimental group of Prof. Dr. DeBeer at the MPI-CEC. In the evaluation period, we have developed wavefunction based methods for the calculation of RIXS and XMCD spectra as well as photoelectron spectra on the basis of the ROCIS protocol (PI: Maganas, Neese).¹⁵

(3) A new module, *orca_esd*, has been developed that works together with TD-DFT as well as DLPNO-STEOM-CCSD. It allows for the calculation of vibronic band shapes of absorption and emission (fluorescence and phosphorescence) spectra as well as resonance Raman spectra and excited state lifetimes (PI: Izsak).¹⁶

3. Computational Chemistry applications

3.1. Enzyme modelling.

The DMTS traditionally has a major focus on theoretical studies in bio-inorganic chemistry. Among many other enzymes, the studies on the oxygen evolving complex (OEC) (PI: Pantazis) particularly fruitful has been. In the evaluation period, we have contributed to clarifying the geometric and electronic structure of the oxygen-evolving complex of photosystem II in the last observable step of its catalytic cycle (the S3 state) by critically analyzing conflicting experimental and theoretical data to eventually propose alternative rationalizations for the structural models presented in recent XFEL crystallographic studies and to elaborate the concept of structural heterogeneity that we proposed a few years ago. A central tenet of this concept is that water binding at the active site can be decoupled from the oxidation of the inorganic cofactor. In a 2019 publication we showed that this idea can lead to a novel formulation for the active oxygen-evolving intermediate of the catalytic cycle, specifically a species that contains a genuine Mn(V)-oxo unit where Mn(V) adopts a five-coordinate trigonal-bipyramidal geometry.¹⁷

In a number of QM/MM studies, the DLPNO-CCSD(T) method allowed us to compute extremely accurate energies for very large systems. As an example, we have recently performed quantum mechanical/molecular mechanical (QM/MM) calculations using a QM region of more than 300 atoms and nearly 7000 basis functions to quantify a series of enzymatic reaction barriers accurately.¹⁸

3.2. Weak intermolecular interactions.

The LED has been proven instrumental in obtaining insight into a wide variety of intermolecular interactions (PI: Bistoni). These include transition metal (TM)-ligand interactions in organometallic chemistry and catalyst-substrate interactions in organocatalytic transformations. For instance, agostic and alkane- σ complexes of TMs are key intermediates in CH activation reactions. An in-depth study of the CH...TM interaction in these systems allowed us to propose a series of design principles for new complexes, highlighting for the first time the importance of London dispersion for their structural stability.^{19a}

The DLPNO-CCSD(T)/LED methodology has also been fruitfully used in collaboration with the department of Prof. List for the case of enantioselective Diels-Alder reactions involving α,β -unsaturated methyl esters.^{19c}

Many of our studies are performed in the framework of the SPP 1807 (“Control of London dispersion in Molecular chemistry”) in which Alexander Auer^{19d,e} and Giovanni Bistoni^{19a-c} are involved as PIs.

3.3. Heterogeneous systems.

The DMTS has been involved in modelling surfaces and solids together with their spectroscopic and reactive properties for a number of years (PI: Manganas). Our approach consists of studying ECP capped and electrostatically embedded cluster models of increasing size. The clusters are considered converged once the results of DFT calculations agree with truly periodic DFT calculations on the same system using the same functional. However, we are then able to apply powerful single- and multireference wavefunction based correlation methods to the problem for which no periodic counterparts exist. In a recent example it has been demonstrated that for both organic and inorganic semiconductors the back-transformed Pair Natural Orbital Similarity Transformed Equation of Motion Coupled-Cluster (bt-PNO-STEOM-CCSD) method provides the best agreement with the available experimental values resulting in errors that are on average lower than 0.2 eV.^{8b}

3.4. Molecular Magnetism.

Molecular magnetism is another mainstay of the DMTS (PI: Atanasov). These studies have been particularly successful in the evaluation period resulting in a number of high-profile publications.²⁰ Particularly noteworthy is a study that, for the first time, experimentally as well as theoretically analyzed and rationalized the all-important spin-phonon coupling that is instrumental for the relaxation mechanisms that spoil the hysteresis that underlies the desired construction of molecular switches.^{20a}

Another important study has found a mononuclear Co(II) transition metal complex with a record unquenched orbital angular momentum of $L=3$. This molecule was theoretical predicted by us in 2015 and finally synthesized. It showed the spectacular world record magnetic moment anticipated together with the extremely unusual situation of featuring an electronic ground state that does not obey the Aufbau principle.^{20b} In all these studies a crucial element was to be able to perform large-scale CASSCF/NEVPT2 calculations with inclusion of spin-orbit coupling and coupled to AILFT.

4. Spectroscopic Studies

Our spectroscopic studies are typically done in collaboration with synthetic groups. A noteworthy collaboration with the department of Alois Fürstner has investigated di-rhodium paddlewheel complexes and bismuth-rhodium analogs that are indispensable tools in modern organometallic catalysis for the controlled decomposition of diazo-compounds. (PI: van Gestel) Here, we have used absorption and rR spectroscopy coupled to calculations in order to establish the underlying electronic structure reasons for

the enhanced reactivity of $\text{BiRh}(\text{esp})_2\text{C}(\text{p-MeOPh})_2$ over $\text{Rh}_2(\text{esp})_2\text{C}(\text{p-MeOPh})_2$.²¹

High-valent iron centers and their reactivity has been a long-standing research interest of the DMTS. In the evaluation period, we investigated the electronic structure and reactivity of low spin tetragonal FeV-nitrido and oxo-complexes using a wide variety of spectroscopic techniques (MCD, EPR, MB, UV/vis). (PI:Ye)^{22a} On the basis of that, we proposed a EPR signal for such species.^{22b} Very recently, we investigated oxygenation of a fleeting FeV-nitrido intermediate to furnish the corresponding Fe-nitrosyl complex using in situ EPR and MB spectroscopy.^{22c}

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2.6 Getting meaningful results fast: Semiempirical methods with orthogonalization corrections

Theoretical Chemistry Emeritus Group by Walter Thiel

Prof. Thiel passed away on August 23rd, 2019. His activities were reviewed by Axel Koslowski and Frank Neese

ABSTRACT The activities of the Thiel Emeritus group are centered around the development and application of semiempirical methods, especially those with orthogonalization corrections. These methods are computationally cheap and yet they provide a realistic and well-balanced description of the potential energy surfaces in the ground state as well as in the low-lying excited states that are dominated by valence transitions. This makes these models ideally suited for the large number of energy and gradient evaluations that occur in non-adiabatic molecular dynamics simulations. Combination with molecular mechanics methods allows studies of chromophores in condensed phases (solvent, protein matrices etc.). Other quantum mechanical methods like density functional and *ab initio* methods are also applied, especially for studies in organometallic catalysis.

1. Method development and evaluation

1.1 Semiempirical models

The advancement of semiempirical methods is one of the central topics of the Theoretical Chemistry Emeritus group. The corresponding work has been funded by the European Research Council with an ERC Advanced Grant till the end of 2018. The focus is on models including orthogonalization corrections, which in the past have proven to be instrumental for obtained more accurate energies and geometries. This strategy has led to the ODM2 and ODM3 models,¹ which are based on the older models OM2 and OM3 methods. The principal improvement is the incorporation of Grimme-type D3 orthogonalization corrections.

Other yet unpublished work concerns the integration of *d* orbitals for the parameterization of biochemically important second-row elements (sulfur, phosphorus), of heavier halogenes and of first-row transition metals. To further develop the model Hamiltonian beyond the established neglect of diatomic differential overlap (NDO) approximation, the multi-center integrals that appear in *ab initio* calculations have been subjected to a statistical analysis and a new model has been proposed in which the largest terms neglected so far are considered.²

The uniform quality of the potential energy surfaces in the ground state and in excited states is a strength of semiempirical methods with orthogonalization corrections. In order to be able to apply these to larger systems and to improve the potential energy surfaces in case of mixing between active and inactive orbitals, configuration interaction (CI) methods based on single excitations have been implemented to complement the existing GUGA-based multi-reference CI module.^{3,4}

1.2 Other methods

The new semiempirical models have been combined with molecular mechanics (MM) methods that take into account the polarization of the MM atoms by the QM region.^{5,6} Unfortunately, it has been found that in order to be able to compete with pure MM methods, the QM and MM components need to be very well adjusted to each other. MM polarization improves the results only marginally.

In order to speed up the computation of potential energy surfaces for MD simulations and rotation-vibration spectra, machine learning methods have been employed to reduce the number of points needed for training these methods to a fraction of the usual number required for interpolation.^{7,8}

Finally, two methods for obtaining the free energy from MD simulations have been comparatively evaluated.⁹

2. Applications

2.1 Photochemical and photophysical processes

A major focus has been the study of non-adiabatic MD on the basis of the new semi-empirical models. Examples are the photoisomerization of urocanic acid¹⁰ which is a natural UV filter found in human skin, and of tetraphenylethylene.¹¹ To determine the quantum yield, 6000 and 1000 trajectories have been computed, respectively.

Combined with a MM method, chromophores in a condensed-matter environment may also be studied. Examples are the photoisomerization of a green fluorescent protein mutant¹² and of azobenzene attached to a DNA duplex replacing one of the bases.¹³

A number of different methods (DFT or *ab initio*) have also been used in applications.¹⁴⁻¹⁸

2.2 Elucidation of mechanisms of catalytic reactions

Chemical catalysis in all variants (homogeneous, heterogeneous and biocatalysis) has been pursued in close collaboration with experimental departments at the institute. For the description of the biological activity of enzymes again combined QM/MM procedures are employed.¹⁹⁻²⁵

The description of processes in homogeneous catalysis is done mainly with DFT methods and occasionally employing wavefunction based *ab initio* procedures. All work in this field is the result of in-house cooperations, namely with Alois Fürstner^{26,27} and with the junior group leaders Manuel Alcarazo²⁸⁻³⁰ and Bill Morandi.^{31,32}

Applications in heterogeneous catalysis include the photocatalytic reduction of nitrogen to ammonia on a rutile surface that was modelled using periodic DFT calculations.³³

Interactions of a solute with the solvent have been examined in two papers.^{34,35}

2.3 Highly accurate calculations on small molecules

Highly accurate equilibrium structures for nitrogen aromates³⁶ and phosphorous halogenes³⁷ have been computed using coupled cluster (CC) methods. By employing an incremental procedure, the following contributions have been taken into account such that results very close to the complete basis set limit (CBS) have been obtained: explicit electron correlation, iterative single, double and triple and perturbative quadruple excitations, core-valence correlations and scalar relativistic effects. Vibrational frequencies have been anharmonically corrected using analytical second and numerical fourth derivatives.

Nine-dimensional potential and dipole surfaces of methyl fluoride have been computed at a similarly high CC level for the variational calculation of the rotation-vibration spectrum.³⁸ The six fundamental frequencies have been obtained with a root mean square error of only 0.69 cm⁻¹ which represents the most precise computation of a rotation-vibration spectrum of this molecule to date.

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2.7.1 Research Highlights for the period 2017-2019

Homogeneous Catalysis and Reaction Design by Bill Morandi

ABSTRACT: During the period 2017-2019, the homogeneous catalysis and reaction design group has produced many research milestones in the area of amination, deoxygenation and catalytic reversible reactions. The short report below concisely describes some of these recent highlights.

The period from 2017 to 2019 has seen many exciting developments in the homogeneous catalysis and reaction design group. These results have culminated in an offer for a tenured Professorship for Bill Morandi at the ETH Zurich (Successor of Prof. Diederich). Two former group members (Zhong Lian and Xianjie Fang) have also secured prestigious independent professorships in China as a result of their work in the group.

Scientifically, the first area where the group has made considerable progress is the area of shuttle catalysis.¹ This concept was introduced previously by our group, and was significantly expanded through the development of a transfer hydrochlorocarbonylation reaction.² This previously unknown reaction allows for the direct synthesis of acid chlorides from simple alkynes and alkenes without using carbon monoxide. Importantly, this reaction was not possible using traditional carbonylation reactions, clearly highlighting the possibility to use the concept of shuttle catalysis to unlock new reactivity in organic synthesis.

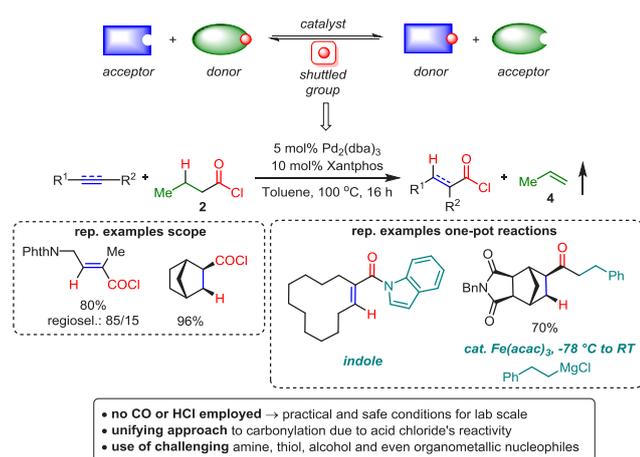


Figure 1: Catalytic transfer hydrochlorocarbonylation of alkynes and alkenes under Pd-catalysis.

Following up on our concept of shuttle catalysis, our group has moved towards the development of group exchange reactions which can be considered as single bond metathesis reactions. We have been able to develop a functional group metathesis reaction wherein two different

functional groups are exchanged between two substrates.³ In this process, a Pd catalyst mediates the exchange between an acid chloride and an iodide group. This metathesis reaction was used in the rapid preparation of acid chlorides and aryl iodides. Interestingly, mechanistic studies revealed that the Xantphos ligand acts as an aryl group shuttle that mediates the group transfer between the two substrates.

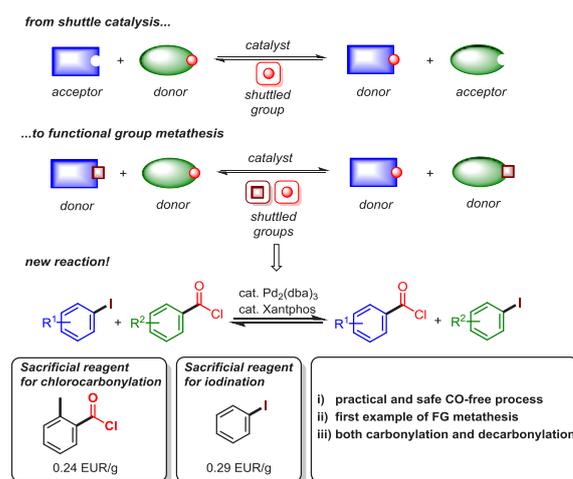


Figure 2: Catalytic functional group metathesis under Pd-catalysis.

A C–S bond metathesis has also been developed using a reversible transfer arylation strategy.⁴ This reaction represents a new, complementary approach to traditional, kinetically controlled cross-coupling reactions. Using this reaction, libraries of bioactive compounds can readily be accessed and a commercial polymer (polyphenylene sulfide) could be depolymerized efficiently. More recently, the development of a Ni-based system allowed us to extend this reactivity to challenging macrocyclizations taking advantage of the self-correcting ability of this metathesis reaction. Overall, this reaction provides a new entry into the manipulation of aromatic thioethers which are key components of bioactive molecules and materials.

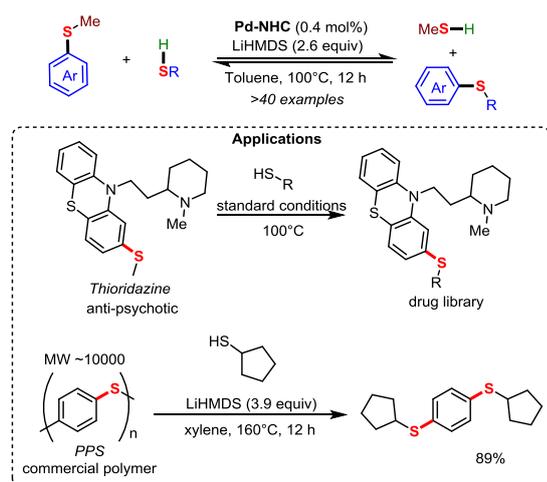


Figure 3: Catalytic C-S bond metathesis and synthetic applications.

This strategy could also be used to perform C-P bond metathesis for the synthesis of complex phosphorous containing heterocycles.⁴ Using this strategy, a commonly encountered side reaction in catalytic cross-coupling, aryl group scrambling, could be turned into a new powerful method for the rapid discovery of novel phosphorous heterocycles for applications in catalysis or materials science.

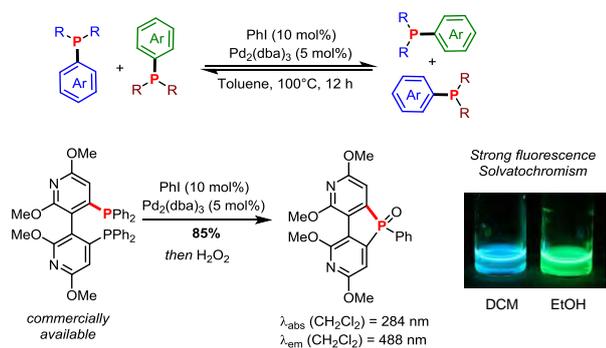


Figure 4: Catalytic C-P bond metathesis and synthetic applications.

The group has further been active in the catalytic amination of alkenes. One of the highlights was the discovery of an alkene aminochlorination reaction which exhibits an extremely broad substrate scope.⁵ This reaction utilizes an inexpensive Fe catalyst and NaCl as the chloride source. Using this new transformation, many unprotected bioactive substrates could be aminated, boding well for the application of this reaction in medicinal and agrochemistry.

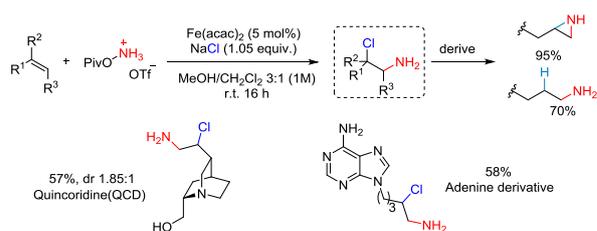


Figure 5: Fe-catalyzed aminochlorination of alkenes using an hydroxylamine-derived reagent and NaCl.

Finally, the group further explored the possibility of selectively defunctionalizing polyol derivatives. One of the highlights was a collaborative project with the Thiel group (MPI) where we developed an unusual example of reductive pinacol type rearrangement.⁶ A salient feature of this work was the possibility to use completely unactivated diols which are traditionally unreactive in pinacol rearrangement. Experimental and theoretical studies have shed light on the underlying effects controlling this intriguing reactivity.

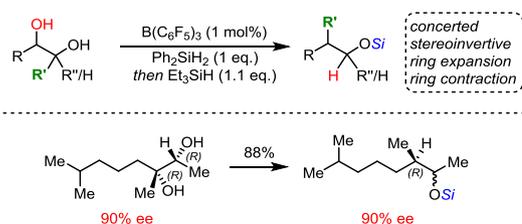


Figure 6: Boron-catalyzed reductive Pinacol-type rearrangement.

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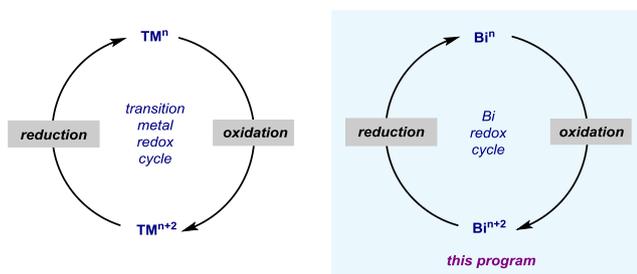
2.7.2 Bismuth Redox Catalysis

Sustainable Catalysis for Organic Synthesis by Josep Cornella

ABSTRACT: Our laboratory focuses in the development of efficient strategies for organic synthesis. Specifically, interests can be divided in four major research lines, namely (i) the catalytic decoration of heterocycles; (ii) the activation of C-N bonds *via* newly designed pyrylium reagents; (iii) the exploration of new reactivity modes for low-valent Ni complexes, and (iv) bismuth redox catalysis. Herein, we summarize our results in the latter program, since the ability of bismuth to maneuver between different oxidation states in a catalytic redox cycle, is an elusive and unprecedented approach in the field of homogeneous catalysis. The main goal of this research program is to translate the unique properties, traditionally associated to transition metals, to bismuth; an earth abundant, non-toxic and inexpensive main group element. In this report, we provide an overview on our efforts to unlock the elusive two-electron redox cycles $\text{Bi(III)} \rightleftharpoons \text{Bi(V)}$ and $\text{Bi(I)} \rightleftharpoons \text{Bi(III)}$ in the context of different organic transformations.

Introduction. The great success of transition metals in homogeneous catalysis is mainly owing to their orchestrated maneuvering between different oxidation states, operating in synchrony for productive catalysis. These features placed transition metals in a privileged situation to serve as workhorse catalysts in a plethora of relevant chemical processes.

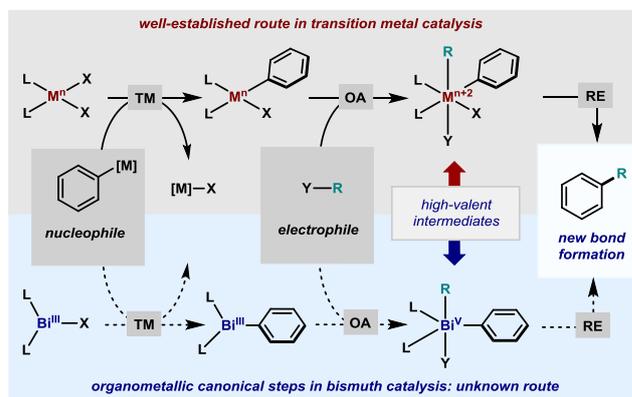
Figure 1. Schematic representation of catalytic redox cycles: transition metals *versus* bismuth.



However in recent years, chemists have questioned the possibility of conferring transition-metal like properties to elements beyond the *d*-block.¹ Indeed, strategies based on FLP (Frustrated Lewis-Pairs), alkali, alkaline, and group 13-17 elements are recently emerging as competent alternatives in certain domains of catalysis.² However, the quest for developing methodologies based on the *redox properties of a main-group element* that surpass the reactivity of transition metals still remains a challenge in organometallic. Herein we describe our recent findings on the catalytic redox properties of bismuth (Bi); an Earth-abundant, non-toxic and inexpensive main-group element, whose redox properties have been largely underexplored (Figure 1).

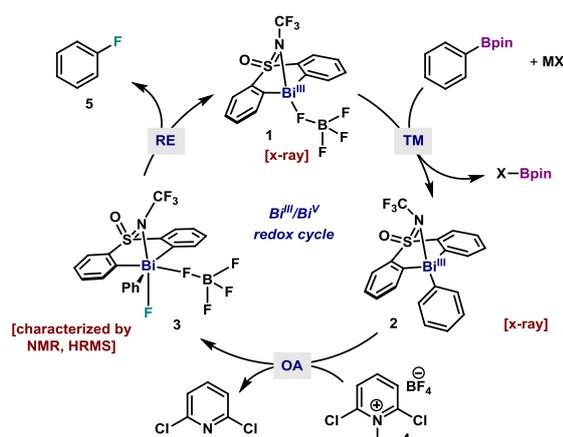
Bi(III) \rightleftharpoons Bi(V) Catalysis. We hypothesized that the provocative idea of exploiting the redox properties of Bi(III) compounds could successfully be realized if a suitable complex was capable of mimicking the canonical fundamental steps in a transition-metal catalytic cycle: transmetalation (TM), oxidative addition (OA) and reductive elimination (RE) (Scheme 1). To explore this hy-

pothesis, we focused on the transition-metal-mediated oxidative fluorination of aromatic boronic acids, a transformation currently restricted to the use of stoichiometric amounts of transition metals (Cu, Pd and Ag).³

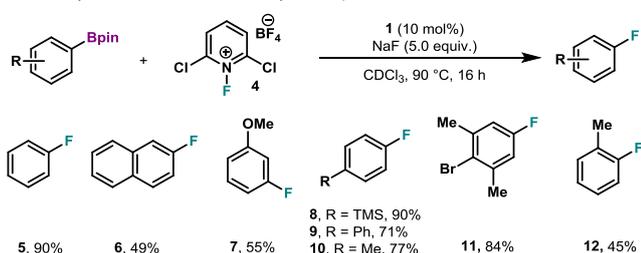


Scheme 1. Organometallic steps in a catalytic redox cycle: transition metal (M) and bismuth (Bi).

To this end, we designed a bismine complex (**1**) featuring a bis-aryl tethered ligand bearing a sulfonimine, and a BF_4 moiety as a weakly coordinating anion (Scheme 2A).⁴ The presence of the sulfonimine ligand permits hypervalent coordination of the N atom to the Bi center which proved crucial in the three ‘organometallic’ steps. The rational design of the ligand permitted a catalytic cycle for the fluorination of arylboronic esters with a fluoropyridinium salt (**4**). A detailed investigation of each individual step resulted in the characterization of the intermediates from a putative mechanism shown in Scheme 2A, where the Bi circulates between oxidation states (III) and (V). A summary of the scope and the substitution patterns in the aryl group is shown in Scheme 2B.

A. Bi^{III}/Bi^V catalytic cycle

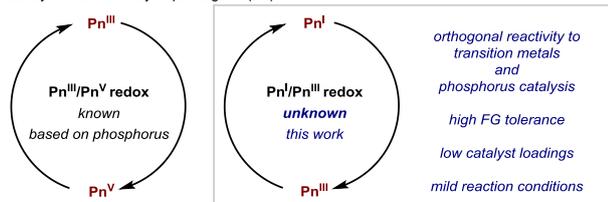
B. Bi-catalyzed oxidative fluorination of arylboronic pinacol esters

**Scheme 2.** (A) Mechanism of the Bi-catalyzed fluorination of arylboronic esters; (B) Scope of the fluorination reaction.

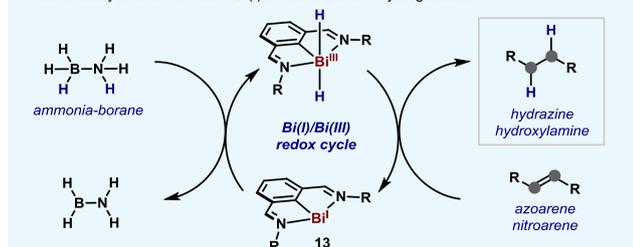
Bi(I)⇌Bi(III) Catalysis. While Bi(III) and Bi(V) compounds are largely known in the literature, the low-valent Bi(I) counterparts are really rare, mainly due to the instability and sensitivity towards oxidation of the $6p^2$ orbital.

Figure 2. (A) Pnictogens in redox-catalysis. (B) Bi-catalyzed transfer hydrogenation.

A. Catalytic redox-activity of pnictogens (Pn)

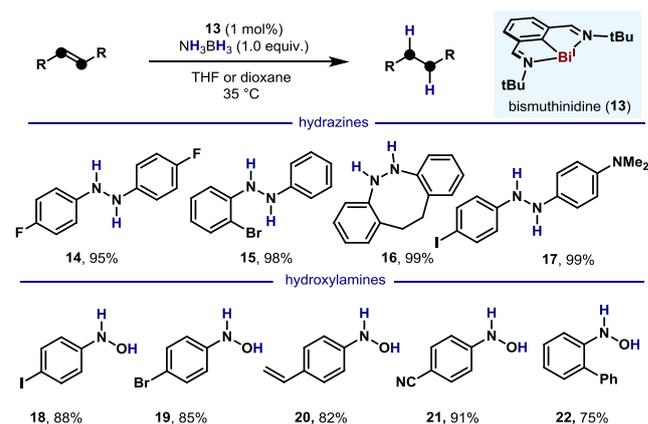


B. Redox catalysis at a low-valent Bi(I) center in transfer hydrogenation



Although P(III)/P(V) catalysis has been demonstrated in the context of transfer hydrogenation,⁵ redox catalysis of pnictogens at the Pn(I) oxidation state was still elusive (Scheme 3A). To this end, we capitalized on Dostál's bismuthinidine **13**⁶ featuring a NCN pincer ligand and demonstrated its catalytic activity in a transfer hydrogenation reaction (Scheme 3B).⁷ Capitalizing on the

high reactivity of Bi hydrides, we speculated that the transfer of the hydrogen atoms to an acceptor would be within reach. Indeed, when **13** was utilized as catalyst in the reduction of azoarenes and nitroarenes with ammonia-borane, excellent yields of the reduced products were obtained under mild conditions. Kinetic analysis of the reaction indicated that **13** is the resting state and the formation of Bi(III) hydrides is rate-determining. Although the nature of the intermediates still remains elusive, high-resolution mass-spectrometry identified putative Bi(III)-H intermediates during catalysis.

**Scheme 4.** Bi(I)-catalyzed transfer hydrogenation.

Conclusions. We have established the feasibility of performing redox transformations based on bismuth catalysis. Initially, we developed a fluorination of boronic acids proceeding via an unprecedented Bi(III)/Bi(V) redox cycle. Exploring complexes in lower oxidation states, enabled the disclosure of the catalytic activity of Bi(I) compounds in transfer hydrogenation reactions. These suggest that Bi holds great potential in the discovery of new reactivity.

Funding Sources

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2.7.3 Electronic Spectroscopy of Open-Shell Molecules and Relativistic Effects in Quantum Chemistry and Spectroscopy

Computational Electronic Spectroscopy and Theory Development by Benjamin Helmich-Paris

ABSTRACT: My research focuses on the development and application of electronic structure theory methods for electronic spectroscopy of open-shell molecules. For open-shell molecules in low-spin states only multi-reference (MR) methods can provide at least a qualitatively correct description of the electronic structure. In a recent benchmark study on singlet excitation energies and UV/Vis absorption intensities with the simplest MR method, i.e. CASSCF, I could show that the linear response (LR) approach is most accurate and generally applicable. Nevertheless, the accuracy of all CASSCF methods is fairly poor and dynamic correlation should be included by either MR second-order perturbation theory or a hybrid CASSCF density functional theory (DFT) approach. Furthermore, I have proposed an efficient implementation of LR-CASSCF which is based on modern integral decomposition techniques and is applicable to large open-shell molecules with hundreds of atoms. Improvements of the accuracy by a hybrid CASSCF – DFT approach are currently investigated. In other research projects, I have introduced spin-orbit coupling to describe (circularly polarized) phosphorescence lifetimes of closed-shell molecules with an approximate coupled cluster method (CC2) and inter-molecular interactions of large heavy-element containing molecules with the Dirac Møller-Plesset second-order perturbation theory method. Future research will be devoted to the development of more accurate MR LR electronic structure methods that are based on second-order perturbation theory. I am confident that these approaches will become standard tools for simulating electronic spectra of open-shell low-spin molecules with 100 atoms and more.

The focal point of my research, since I have joined the *Max-Planck-Institut für Kohlenforschung* in 2018, is the development and application of state-of-the-art electronic structure methods for computing electronic spectra of open-shell molecules. Open-shell molecules frequently occur in many fields of chemistry and physics. In organic synthesis and material science, stable radicals are well-known and serve for many purposes, e.g. radical markers and reagents or organic conductors and even superconductors at low temperatures. Most prominent are open-shell transition metal complexes that are used in homogeneous catalysis or form the active center in many enzymes. Despite a vast progress of molecular electronic structure theory (*quantum chemistry* (QC)) in the last decades, state-of-the-art QC methods are still very limited in providing accurate predictions for open-shell molecules of decent size, in particular if they are in a low-spin state.

To describe molecules in an open-shell low-spin state, a linear combination of spin-adapted determinants is inevitable. The most established and most reliable approaches are based on a linear combination of all combinatorially possible determinants (configuration interaction (CI)) generated from a small subset of active orbitals - the so-called active space. The conceptually and also computationally simplest method is the complete active space self-consistent field (CASSCF) method that minimizes the energy with respect to the molecular orbital and CI coefficients. The CASSCF ansatz is not meant for high accuracy but can rather describe the electronic structure of the open-shell complexes qualitatively correct. With CASSCF there several approaches one can pursue to compute excitation energies and transition moments that are required to simulate the UV/Vis absorption and electronic circular

dichroism spectra. The most practical and efficient variants for computing many electronic states are state averaging (SA) and linear response (LR) theory that are from a conceptual point of view very different. To explore the accuracy of SA- and LR-CASSCF for singlet excitation energies and oscillator strengths (UV/Vis intensities), I have recently performed a benchmark study^[1] with a well-established test set originally designed by the former Max-Planck director Prof. Walter Thiel, which contains more than 150 valence transition in prototypical organic chromophores. I could show that LR-CASSCF is more accurate than SA-CASSCF. Furthermore, the study revealed that all CASSCF variants showed the poorest performance of all ab initio QC methods as dynamic electron correlation is not accounted for. A good compromise between accuracy and efficiency can be obtained when combining CASSCF with density functional theory (DFT), i.e. in particular the long-range LR-CASSCF short-range DFT method (srDFT) proved to be fairly accurate (Fig. 1).

The recent findings of the benchmark study were the motivation to work on an efficient computer implementation of the LR-CASSCF method that can be easily applied when simulating many electronic transitions in large open-shell molecules with hundreds of atoms^[2]. The newly developed LR-CASSCF implementation is integrated into the QC package ORCA of the Max-Planck director Prof. Frank Neese and benefits from a well-established infrastructure and efficient algorithms for computing and processing two-electron integrals, which is the major computational bottleneck of CASSCF calculations with decent active space sizes. I have also revised some of the time-critical integral transformations and, therefore, could also contribute to improving the performance of

the conventional CASSCF energy minimization algorithm^[3]. Within the LR-CASSCF project, I have also found a simple and very convenient way to visualize the electronic transitions by employing so-called natural transition orbitals, which are well known and frequently used for simpler excited methods as time-dependent (TD) DFT, but were so far not proposed for the more elaborate LR-CASSCF method.

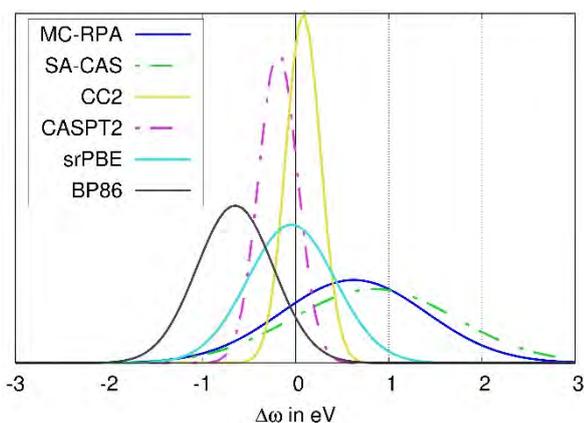


Figure 1. Normal distribution of deviation from the CC3 reference singlet excitation energies computed with various methods.

Based on experience gained from the previous benchmark study and several other applications it is clear that the LR-CASSCF absorption spectra can only be sufficiently accurate (even almost as accurate as second-order multi-reference perturbation theory) if all spectroscopically relevant orbitals can be included in the active space. This is not feasible for most chromophores and a more effective way of including dynamic electron into LR-CASSCF is the addition of a DFT exchange-correlation functional, e.g. as done by the range separation-based srDFT variant. I am currently pursuing an efficient LR-srDFT implementation in ORCA together with an external collaboration, Prof. Hans Jørgen Aa. Jensen (SDU Odense, DK).

In a side project, I have also contributed to the computation of circularly polarized phosphorescence (CPP) rates with the approximate coupled cluster method CC2^[4]. CPP can only be described by the theory of relativity, in particular, spin-orbit coupling, as it involves an electronic transition from a triplet excited state back to the singlet ground state, which is spin-forbidden (zero probability) in non-relativistic quantum mechanics. Moreover, CPP can be detected only for chiral molecules that absorb linearly polarized light, which might be exploited to distinguish between different enantiomers. In that work, we reported for the first time calculations of CPP at the coupled cluster level with different levels of sophistication when treating relativistic effects.

In another project, me and my collaborators have explored how to make Dirac wave function (second-order Møller-Plesset perturbation theory (MP2)) calculations feasible for large molecules^[5]. This is particularly relevant when computing inter-molecular interaction energies of molecules with heavy elements that cannot be described properly by standard DFT methods as the dispersion interaction is either missing or accounted for by an additional empirical correction term. In this work, we have generalized a low-scaling non-relativistic MP2 approach for the Dirac two-

component formalism, which employs the Laplace transformation (LT) of the orbital-energy denominator and sparse-matrix operations. With our efficient implementation we were able to perform the largest Dirac two-component wave function calculation that has been ever performed (nearly 10'000 orbital basis functions). Unfortunately, screening of negligible intermediates only worked effectively for nearly linear molecules. A re-design of the algorithm together with a new implementation in ORCA is currently pursued which will facilitate large calculations with so-called second-order wave function methods. This is a collaboration with Dr. Róbert Izsák and Dr. Bernardo de Souza (Universidade Federal de Santa Catarina, BRA).

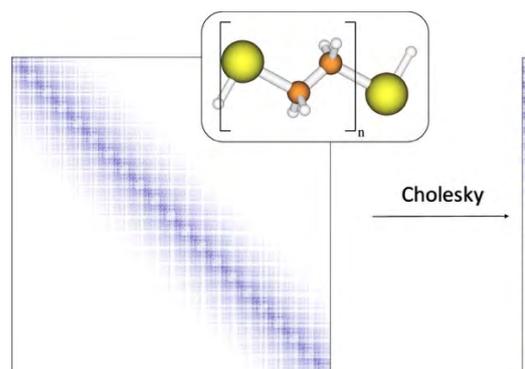


Figure 2. Sparse intermediates of LT-based MP2 implementation.

Future research will be devoted primarily to develop more accurate LR MR methods that have at least the same accuracy and scope of application as standard MR second-order perturbation theory methods, but are also capable of providing many electronic states without exceedingly large active spaces. Also, extending the applicability of the LR-srDFT method for fluorescence and resonance Raman spectra will be of high priority.

Funding Sources

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2.7.4 Methodology Developments in the Directed Evolution of Selective Enzymes as Catalysts in Organic Chemistry and Biotechnology

Biocatalysis by Manfred T. Reetz

ABSTRACT: At the MPI für Kohlenforschung more than 20 years ago, the Reetz group pioneered the concept of directed evolution of stereoselective enzymes, the goals being the generation of useful biocatalysts, and learning lessons concerning the intricacies of enzyme mechanisms. Today the Darwinian methods and strategies that were developed for probing protein sequence space efficiently are used by essentially all academic and industrial groups in the field. During the last three years the focus was on establishing maximal speed and reliability of directed evolution. Highlights include the use of machine learning (artificial intelligence), utility of solid-phase chemical synthesis of designed saturation mutagenesis mutant libraries on Si-chips, evolving high activity of hyperthermally stable enzymes at room temperature, producing enzymes for promiscuous and/or difficult organic transformations, and QM/MM-based mechanistic advances.

Introduction

The Reetz lab in Marburg was closed in November 2017, but the initiated projects were continued in the labs of former Chinese postdocs, now full professors, e.g., Zhoutong Sun at the Tianjin Institute of Industrial Biotechnology (Chinese Academy of Sciences), all efforts leading to >35 publications in the reporting 3-year period with emphasis on methodology development (Figure 1).¹ Recently, Manfred Reetz returned to Mülheim, and is also Adjunct Professor in Tianjin/China. A few highlights published during the research period are listed below:

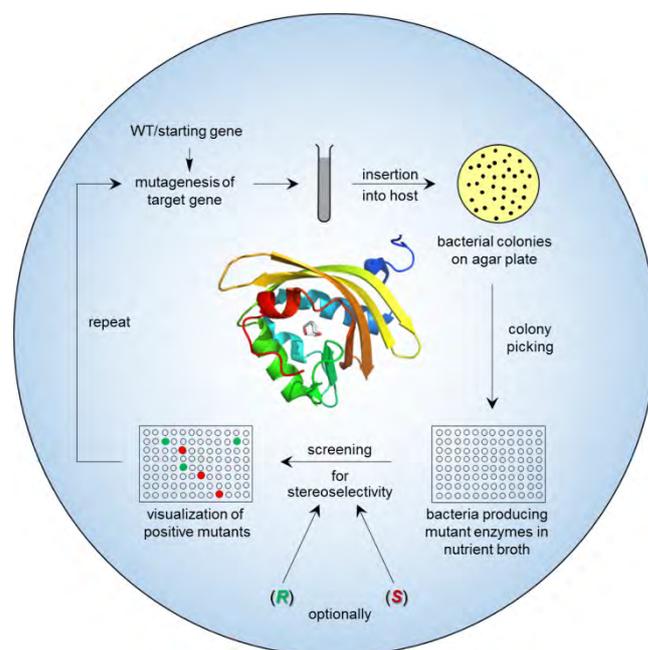
Artificial intelligence in directed evolution

In collaboration with Frederic Cadet (France), the predictive power of the machine learning algorithm Innov'SAR was successfully tested in directed evolution based on **Combinatorial Active-site Saturation Test (CAST)** and **Iterative Saturation Mutagenesis (ISM)**.² Highly stereoselective epoxide hydrolase mutants were obtained, superior to those previously evolved by first-generation CAST/ISM.

Designed chemical solid phase synthesis of saturation mutagenesis libraries

The inherent limitations of saturation mutagenesis in general, including amino acid bias, were eliminated by exploiting the commercial TWIST technique of chemical gene synthesis on Si-chips. Experimentally, 97% of the designed library members appeared in screening, in contrast to only 50% using traditional molecular biology-based mutagenesis.¹ This advance means an enormous increase in library quality as measured by the frequency of hits, their activity and stereoselectivity, and dramatically less screening effort! If the prices continue to go down, this could well constitute the future of directed evolution.

Figure 1. General concept of directed evolution of stereoselective enzymes;¹ activity and regioselectivity can be handled similarly by this Darwinian approach.



Evolution of high activity of hyperthermally stable enzymes at room temperature

Extremophilic enzymes generally require high operating temperatures. For the first time, extremely high activity of such an enzyme at room temperature was obtained by directed evolution!¹

Promiscuous and/or difficult to achieve chemical transformations

The chemo- and regioselective dihydroxylation of benzene with no overoxidation (!) flanked by the cascade synthesis of arbutin was achieved by directed evolution.³ In other work, an artificial metalloenzyme⁴ was evolved that catalyzes the Kemp elimination, not by the traditional acid/base mechanism, but by single electron transfer.⁵ A giant step in solving the challenging problem of P450-based targeted hydroxylation of steroids at any desired position was taken by means of mutability landscaping and mutational scanning,⁶ planned oxidation at the C16-position with α - and optionally β -diastereoselectivity being achieved for half a dozen steroids, while C7- and C11-selectivity was also evolved, likewise for pharmaceutical applications. Overriding electronic effects of Baeyer-Villiger reactions for inverting regioselectivity was also successful by again using second generation CAST/ISM.⁷

QM/MM studies

A 60-year old open mechanistic question was unambiguously settled by directed evolution, enzyme kinetics and QM/MM computations.⁸ Another QM/MM study, flanked by X-ray data of mutants, provided mechanistic details of an epoxide hydrolases, which led to surprising insights.⁹

Fusing directed evolution and rational design

Second-generation CAST/ISM^{10,11} suggested the fusion of directed evolution and rational design as perhaps the ultimate form of protein engineering: First example of a new strategy dubbed **F**ocused **R**ational **I**terative **S**ite-specific **M**utagenesis (FRISM) may prove to be a logical step in the right direction.^{1,12}

Funding Sources

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CHAPTER 3

Scientific Service Units

3 Scientific Service Units

Several service units are supporting the research at the Institute. The policy is generally to keep and expand on core competences in analytical techniques and instrumentation that benefit from long-term, knowledgeable employees. Whenever possible, the directorate supports the service units with senior scientist position that go beyond machine maintenance and standard measurements, but enable high-profile scientific collaborations. The service units are led by scientists who are encouraged to also perform original research. The service units are generally regarded as an extremely beneficial resource for the Institute. All research groups at the Institute have access to all service units.

The service units are comprised of those for analytical methods (Chromatography, Mass Spectrometry, Nuclear Magnetic Resonance, Crystallography, Electron Microscopy), and information or data handling systems (Library, IT). A maximum standard of safety, reliability, and flexibility is essential for these units to respond to the needs of modern basic research in catalysis and related areas of chemistry.

In addition to providing the appropriate infrastructure and know-how, several service facilities are actively involved in specific projects, generally in cooperation with the scientific groups of the five Departments. For example, new techniques have been developed over the years in the fields of high-throughput screening, microfluidics, and chip-electrophoresis, to name just a few representative cases.

In order to make this approach truly successful, a long term strategy is essential for maintaining and developing the know-how and expertise of the staff. This includes the active role of the scientific service units in specific research projects, participation in conferences, and the hosting of postdoctoral fellows with the aim of introducing new techniques.

In line with the rules stipulated by the MPG, all data recorded in the analytical departments or directly in one of the experimental groups are securely archived in electronic and/or hardcopy format for a minimum of ten years (usually much longer). A user-friendly electronic laboratory notebook (ELNA) has been developed and further extended during the reporting period, which ensures secure data storage and retrieval.

At the same time, ELNA provides a constantly growing searchable in-house database.

3.1 Technical Laboratories and Central Occupational Safety (N. Theyssen – 6.3 FTE)

The **technical laboratories** (3.5 FTE) provide the necessary infrastructure for performing high pressure experiments up to 1.000 bar in stainless steel or Hastelloy reactors in milliliter to liter scale. Particular effort is made to ensure safe operation by providing both constructive measures of explosion protection in 27 high pressure boxes (testing grounds) of different sizes and continuous technical support of highly experienced staff members. The information content of the experiments is maximized by routine recording of pressure/temperature curves with a resolution of four value pairs per second. In 2019, the compressors of the gas ring lines for hydrogen, carbon monoxide and ethylene were fundamentally rebuilt by the manufacturer and now fulfill the ATEX directive of the European Union.

In addition, the technical laboratories house appropriate distillation equipment for solvent purification and drying (turnover between 16.000 and 18.000 L per year), thereby allowing a cost-effective purchase of technical quality solvents which are then upgraded to meet the Institute's needs. Very recently, a second rectification plant for the distillation of hexane isomers on a scale of 200 L was installed, as continuous operation (almost 24/7) as the first unit turned out to be insufficient in peak periods of consumption. In 2018, the steel-based central solvent drying plants for diethyl ether, n-pentane, THF and toluene were equipped with radar sensors, thus allowing level control and refilling processes to be undertaken safely without the staff members being exposed to solvent vapors.

Worth mentioning is also the centrally provided service for the disposal of chemical waste. The current amount of 32 t per year accounts for more than one third of the overall chemical waste of the Max Planck Society. In 2019, an extensive ergonomic improvement was implemented in the solvent disposal by the installation of high-quality guide systems for the suction lanes. These units were designed and built in-house.

The central **occupational safety** department (2.8 FTE) develops, coordinates, and supports legal requirements in terms of occupational safety, emergency management, and security. Together with the board of directors, department leaders, their safety officers, and appointees for the electronic safety and health management system (ASi) as well as other delegated / qualified persons delegated for more specific entrepreneurial duties, work safety at the Kohlenforschung is organized and carried out with high standards striving for excellence. The same holds for numerous employees engaged as emergency personnel: two paramedics, more than 150 first aiders, 17 members in the Institute's fire brigade and approximately 40 emergency evacuation assistants represent a respectable commitment for a research Institute of its size. Close and continuous cooperation with professional local rescue services as well as significant improvement in coping capacities of possible crisis situations during the last two years complete our activities. Not surprisingly, inspection of both governmental regulatory agencies and our employers' liability insurance association resulted in very positive feedback in the reporting period. In this way, we are pleased to report that we had no serious incidents.

3.2 Chromatography and Electrophoresis (P. Schulze – 10 FTE)

The department is divided into three subgroups: the gas chromatography, the analytical high pressure liquid chromatography, and the preparative HPLC team. Each team provides analytical services for in-house scientists, such as qualitative and quantitative determinations, chiral analysis, and preparative purifications.

The gas chromatography service is executed by five employees using about 25 GC systems, e.g. split/splitless injection, (dynamic) headspace GC, high/low temperature GC, GC-MS, cooled injection systems with and without the combination of a thermal desorption unit. To gain superior chromatographic performance, mostly capillary columns and hydrogen carrier gas are used combined with different detectors like flame ionization or thermal conductivity detection. Unknown substances are identified using quadrupole mass spectrometric detection. About 10.000 GC runs are measured per year.

In the analytical HPLC laboratory a variety of instrumental liquid phase separation techniques is applied by three employees. We provide one- and two-dimensional HPLC (heart-cutting or comprehensive) and supercritical fluid chromatography with different detectors like UV diode arrays, refractive index detection, evaporative light scattering, electrochemical detection or the hyphenation to TOF- or qMS. Achiral and chiral separation columns for reversed-phase, normal-phase and ion exchange modes are available in particle sizes from sub 2 μm to 3 μm . During the reporting period, low temperature HPLC down to -20°C was introduced to increase the chromatographic efficiency and to analyze temperature-sensitive compounds. The team also provides micro-preparative HPLC purifications of small substance amounts for spectroscopic characterization. About 5800 runs are performed per year.

Three employees of the preparative liquid chromatography purify mainly reaction batches with separation columns of 10 to 50 mm inner diameter. A variety of stationary phases for reversed-phase, normal-phase or enantioselective separations are available as well as instrumentation for heart-cut HPLC and peak recycling HPLC. Semi-automatic fraction work-up is performed in rotary evaporators and a high vacuum pump. Roughly, 80 samples with a maximum substance amount between 5 and 4000 mg are processed per year. Additionally, a walk-on service is provided for scientists who would like to process urgent samples on their own.

During the reporting period the group collaborated with the University of Erlangen-Nürnberg and the University of Pavia. A third party funded ZIM-AiF project (BMW i) about online HPLC-Raman detection was conducted in cooperation with the IUTA, the University of Düsseldorf, and the companies PSS GmbH and CS-Chromatographie Service GmbH.

3.3 Mass Spectrometry (W. Schrader – 7.2 FTE)

The mass spectrometry laboratory is providing a mass spectrometric service for both Institutes on campus in analyzing all emerging problems. Currently, the group operates eleven different mass spectrometers utilizing all available ionization methods. While the majority of work can be served using both standard electron ionization (EI) and electrospray ionization (ESI) additional atmospheric ionization methods such as atmospheric pressure laser ionization (APLI) and atmospheric pressure photo ionization (APPI) have been made available for routine operations.

During the last years, the development in MS was staggering, making instruments available that have increased mass resolution while being much more sensitive than older instruments. Therefore, an emphasis has been placed on advancing the group towards these high-resolution instruments. We have started to replace older instruments with newer ones. During the reporting period, a new high-resolution GC/MS Orbitrap instrument has replaced an older sector field mass spectrometer. This instrument now allows high-resolution studies of volatile compounds and mixtures.

A similar Orbitrap instrument with an ESI source was purchased in the previous reporting period but for low volatile compounds. Therefore, we now have two comparable high-resolution instruments for the two major compound workflows in the laboratory. In addition, we are working to upgrade the software for the ultrahigh resolution FT-ICR MS systems but this will continue during the next year. Here, new software developments can double the resolving power of the instruments providing both sensitivity and analyzing power.

During the last years, the group has developed a number of different applications to investigate chemical mechanisms and established two new direct coupling systems for both size-exclusion-chromatography and ion-mobility spectrometry to high-resolution MS.

The generational exchange has continued during the reporting period as the last members of the older generation have retired. The positions have been filled by new young co-workers, which are eager and good technicians but need training to gain more experience. All members of the group are being trained in operating and maintaining all instruments and in interpretation of MS data. Here, a mixture of physical and chemical technicians is providing a good complementary mixture. Training of young co-workers takes at least five years in all of these techniques and this has been an important part of the development of the group.

The group is headed by Prof. Schrader. His work is supported by Dr. Vetere, who is a new scientific member, to assist the work of the group. N. Haupt, D. Kampen, F. Kohler, S. Marcus, D. Margold plus an apprentice are the additional members of the team. Their duty is to evaluate of how to best solve the problem on hand, measurement of incoming samples, interpret the results, provide expertise to the scientific groups and maintain the instruments. During the reporting period, each year between 12,000 and 14,000 measured and interpreted chemical compounds have passed through the group.

3.4 Nuclear Magnetic Resonance (NMR) (C. Farès – 9.1 FTE)

The NMR department provides a broad range of specialized NMR techniques and analytical service. During the reporting period, approximately 74,000 NMR spectra have been recorded on a wide range of samples, from natural products, active enzymes and metal complexes in solution to porous silicas and zeolites in solids. To meet demands, the department is equipped with six NMR spectrometers with field strengths corresponding to ^1H frequencies of 300, 400, 500 and 600 MHz for analyses in solution and of 300 and 500 MHz for analyses in solid state. The department is organised in three broad areas of service.

(1) Open-Access and Routine NMR: Scientific employees can carry out basic NMR measurements in liquid state in high-throughput mode on a dedicated “open access” 300-MHz NMR spectrometer. The selection of available experiments is limited to those with high sensitivity, high information content, and rapid execution with predefined parameters. Liquid samples requiring special set-up or treatment can be submitted for measurement to our operators on available spectrometers. The most common requests are: (a) special nuclei, (b) high or low temperature NMR, (c) optimized experiments (eg. NOESYs), and (d) kinetic NMR chemical reactions. These services cover nearly 90% of all experiments run in our department.

(2) Advanced NMR: Particularly challenging NMR studies of solution compounds are accepted for advanced analysis. For these samples, our experienced staff members provide full measurement, analysis and interpretation assistance in close collaboration with the chemical research groups. The advanced techniques are carried out on dedicated spectrometer: (a) a high-sensitivity 600-MHz system, equipped with a cryogenically-cooled probehead, which is ideally suited for sub-milligram quantities of 50+ carbon organic molecules; (b) a more versatile modern 500-MHz instrument which provides the possibility to measure at high and low temperature, to cover a broad range of NMR-active isotopes, and to run advanced triple-resonance experiments. A large part of the analytical work is dedicated to determine or confirm structures, stereochemistry, conformations and dynamics.

(3) Solid-State NMR: Solid-state NMR spectroscopy remains one of the most important techniques for the characterisation of solid catalysts, functional materials, and potential hydrogen storage materials synthesized in the institute (Schüth group). In continuation of work performed in previous years, solid-state NMR spectroscopy has particularly been applied for the characterisation of the following solids: (a) Catalysts and functional materials from mesoporous silicas or zeolites (^{29}Si , ^{13}C and ^{27}Al); (b) Complex aluminium hydrides (mainly ^{27}Al NMR); (c) Adducts of alane (AlH_3) with tertiary amines (^{13}C and ^{27}Al NMR); (d) Materials obtained by ball milling.

3.5 Chemical Crystallography and Electron Microscopy (C. W. Lehmann – 10.5 FTE)

The EmRay-Group combines all electron microscopy activities of the Institute and selected areas of crystallography, namely crystal structure determination from single crystals and polycrystalline organic materials. In addition to operating in-house facilities the group is part of a team building the dedicated chemical crystallography beamline P24 at PETRA III in Hamburg.

For single crystal structure analysis, state-of-the-art technology is employed, comprising three area detector systems. A Cu-rotating anode equipped with a four circle goniometer and a large surface area CCD-detector is used for the determination of the absolute configuration of enantiopure light atom compounds. Inorganic and organometallic compounds are investigated using either a Mo-rotating anode or a molybdenum micro focus X-ray source, both equipped with four circle goniometers. All diffractometer systems employ graded multilayer optics to maximise X-ray intensities and are equipped with liquid nitrogen low temperature devices for sample cooling and stabilisation. A total of approximately 500 data sets are collected annually, however an increasing number of samples yield only very small crystals with dimensions less than 20 μm . Samples containing such small crystals are collected for data collection at the synchrotron. About every six to eight weeks a small team from this group measures these crystals at PETRA III in Hamburg employing the macromolecular beamline P11 as well as the chemical crystallography beamline P24.

At the end of 2018, a new large area cadmium telluride hybrid pixel detector was acquired through central funds of the Max-Planck-Society to improve the chemical crystallography beamline P24. In return, a total of 400 hours per annum are available for all Max-Planck researchers.

For electron microscopy, a total of seven electron microscopes are operated. A 200 kV cold field emission gun dedicated STEM with aberration corrector and two EDS detectors covering approximately 2 steradian of solid angle permits sub-nanometre spatial resolution for elemental analysis and 72 pm resolution in HAADF micrographs. This microscope is complemented by one further cold FEG 200 kV TEM and two additional 120 kV transmission electron microscopes. Scanning electron microscopy is spearheaded by a combined 30 kV SEM/STEM also equipped with a cold FEG offering 3.4 Å lattice fringe resolution. For routine scanning electron microscopy, two additional microscopes, one including EDS analysis are operated.

Two of the electron microscopes are available for self-service. PhD students and Post-Docs are trained by experienced technicians and engineers to operate these microscopes. The hands-on training is complemented by a series of lectures on electron microscopy, given by the group leader.

At the end of 2017, beginning of 2018 a focused-ion-beam (FIB) system for sample preparation was acquired and installed. Sample preparation methods available in the group now cover mechanical microtomes as well as argon milling and gallium atom bombardment for obtaining thin samples suitable for TEM investigations. For SEM studies, cross sections can be prepared using both mechanical methods as well as argon milling / polishing. The set-up is completed by several coating and sputtering devices.

3.6 Library and Information Management (C. Baumert – 1.5 FTE)

Our one Person library is responsible for providing all library-services for the Institute. It serves the five chemical departments by buying, collecting, and archiving books and journals. The focus of the collection is organic, organometallic, theoretical, polymer, and materials science. More than 17.000 books and monographs and over 700 Theses cover all aspects of catalysis. All media are electronically catalogued and searchable by the ALEPH program. The library also contains a large collection of recent and historic print-journals. The 75+ subscribed journals and book series are electronically catalogued and most of them can be accessed as digital media.

Our library participates in the “Max Planck Digital Library (MPDL)” which covers the digital activities of the Max Planck Society.

The MPDL basic service also allows the Institute to get print journals for discount prices.

Additionally, we subscribe to 70 print journals that are not included in the MPDL basic service.

Scientific papers not available in our or any other MPG library; can be ordered and accessed via SUBITO, Fernleihe, IFLA, etc.

Library projects:

- More digitalization
- Reorganization

3.7 IT - Group (C. Baumert – 10.5 FTE)

The IT group is responsible for the entire IT infrastructure of the Institute. The central requirements are performance, service orientation, security and standardization. The IT group is divided into four different areas with different foci.

- 1.) High Performance Computing and Linux-based Systems
- 2.) Network infrastructure and Security
- 3.) Application development
- 4.) Microsoft-based Systems

1.) **High performance computing and Linux-based systems**

The High-Performance-Computing division provides approx. 400 computer servers for theoretical chemistry (Neese group). The two IT staff members maintained and monitored the systems by using a monitoring system. Additional services such as DNS, Radius, LDAP, etc. are also provided and supported. Fifty-five additional servers are deployed on a VMware basis.

2.) **Network infrastructure and security systems**

The network division is responsible for IT infrastructure. The approx. 3.600 switch ports (76 switches) and 80 WLAN access points form the basic framework for the network infrastructure of the Institute. Four firewall systems protect the network against external attacks. In addition, further security measures protect the network (for example 802.1x authentication, virus scanner, etc.).

VPN dial-in realized the external dial-in for authorized users.

3.) **Application development**

The area of application development has developed the electronic laboratory notebook (ELNA). ELNA is an in-house developed software. The user support, technical support and further development will be done by the development division. The IT employees analyzed and implemented new requirements in new applications.

4.) **Windows-based systems**

A large proportion of client PCs are based on Microsoft operating systems (approx. 640 clients). These clients are managed and operated via a Windows domain. Five domain controllers that will run on a Hyper-V server cluster manage the user rights.

Different software products and services provided on a Microsoft Hyper-V-Cluster (31 servers).

The three IT staff members support the Microsoft infrastructure. Data will be stored on two Netapp SAN systems with a capacity of 28 TByte. The Backup Storage has a capacity of 74 TByte.

3.8 ORCA (F. Wennmohs – 5.9 FTE)

The quantum chemistry program package ORCA has been developed since the late 90s first by Frank Neese alone, and later as part of a group effort. By now, the ORCA package has more than 25.000 users world-wide and is one of the most highly used and cited quantum chemistry packages world-wide. The ORCA development group has been founded in order to support the development efforts concomitant with the establishment of the Department of Molecular Theory and Spectroscopy at the MPI for Chemical Energy Conversion in 2011.

The development group has moved together with Prof. Neese to the MPI für Kohlenforschung in 2018 in order to fulfill the same role. It is the central unit that takes care of all ORCA related questions and code management issues. In 2019, Dr. Axel Koslowski, a former group member of Prof. Thiel, joined the team.

The ORCA software has advanced to a state where it is one of the most cited quantum chemistry packages in the scientific community, second only to the Gaussian program. The success of the software has been made possible to a large extent by the continuous and high-level efforts of the ORCA Development Team. As of today, the ORCA program is made up of more than 80 million lines of source code, with several international groups actively contributing to it, which makes it one of the largest scientific programs available. A scientific program as large as ORCA requires an expert team in order to maintain its infrastructure, support the academic developers at programming in the ORCA program framework, as well as teach the practical use of ORCA to chemists at the MPI für Kohlenforschung at large.

At the Institute, the ORCA Development Team set up and maintains an up-to-date software infrastructure including revision control systems, automatic build systems accompanied by regression tests, providing instant access to ORCA updates on all compute clusters.

As part of the development effort, there were three major releases of ORCA in the past few years, namely ORCA 4.0.0 in 2017, ORCA 4.1.0 in 2018, and ORCA 4.2.0 in 2019. Besides being responsible for the release process, that is, building, quality testing, and producing distribution ready software packages, the ORCA Development Team also contributed to the scientific enhancement of the ORCA suite of programs (cf. publications).

In order to establish ORCA at the MPI für Kohlenforschung as a general tool for chemistry, an introductory workshop was organized on 08.03.2018. This led to an increased use of ORCA on the institute's computer clusters by all groups of the Institute.

Introductions to ORCA were also held at the Summer Schools 'Spectroscopy and Electronic Structure of Transition Metal Complexes' in September 2017 and September 2019, in which ORCA plays an important role to examine the electronic structure of molecules.

To provide a platform for more advanced ORCA users, an ORCA User Meeting was established and held in September 2017 and September 2018. The audience was made up of international participants, ranging from enthusiastic students to professors of chemistry.

The ORCA Development Team works closely with the FAccT's GmbH, which is the distributor of the ORCA software to commercial users. This cooperation provides detailed feedback about the use of ORCA in commercial environments.

CHAPTER 4

The Training of Young Scientists

4 The Training of Young Scientists

The Institute puts an emphasis on the training of young scientists (bachelor, master, and doctoral students as well as postdocs). Their number has been relatively constant over the past five years (Figure 4.1.). Roughly half are financed through external research grants; the other half is supported by internal grants originating with the Max-Planck Society.

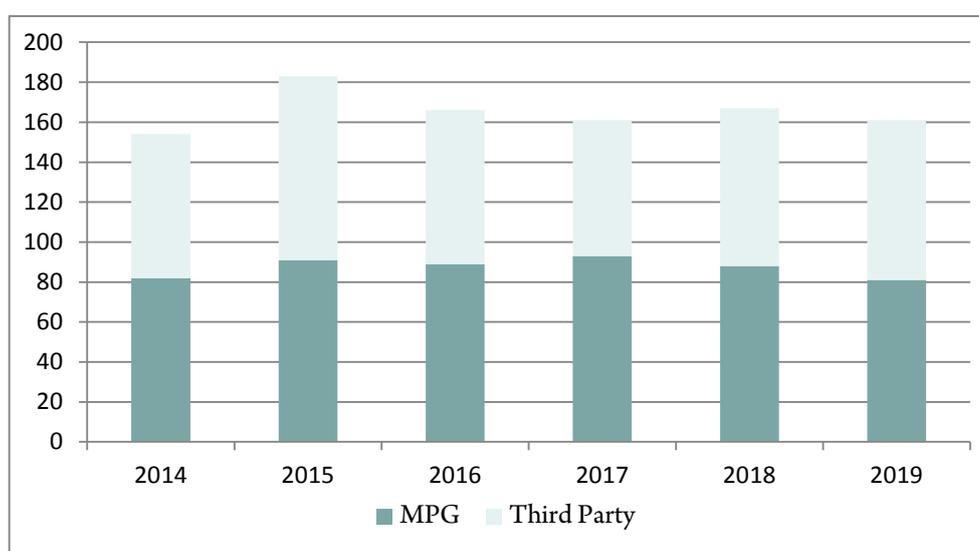


Figure 4.1. Financial Sources of Support for Young Scientists (reporting date: 09/30/2019).

The financial resources of the Institute allow to support about 80 – 90 junior researchers, whereas costs to support postdocs is roughly double that of graduate students. In addition, the independent junior research groups have secured a separate budget for such positions from central funds of the Max-Planck Society.

The majority of our undergraduate students (bachelor/master) are domestic, while the majority of the PhD students come from Asia, closely followed by Europe (Table 4.1.). Similarly, the postdocs of the Institute are mostly from Asia and Europe (Table 4.2.).

Status	Total	MPG and Found. Funds.	Third-Party Funds	Male	Female	Domestic	Intern.
Dec 31, 2017							
Undergr. St.	15	3	12	9	6	13	2
PhD students	76	40	36	60	16	35	41
Post-docs	70	50	20	51	19	5	65
	161	93	68	120	41	53	108
Status							
Dec 31, 2018							
Undergr. St.	8	2	6	6	2	7	1
PhD students	84	43	41	64	20	41	43
Post-docs	75	43	32	56	19	5	70
	167	88	79	126	41	53	114
Status							
Sept 30, 2019							
Undergr. St.	12	3	9	12	0	8	4
PhD students	88	45	43	64	24	47	41
Post-docs	61	33	28	45	16	3	58
	161	81	80	121	40	58	103

Table 4.1. Demographics of Young Scientists.

Postdocs (country of origin)	2014	2015	2016	2017	2018	Sept. 30th, 2019
Europe	38	41	39	28	28	22
USA / Canada	5	7	5	2	3	1
Latin & South America	5	7	5	2	2	3
Asia	38	47	44	37	41	34
Africa / Australia	0	1	0	1	1	1
Total	86*	103*	93*	70*	75*	61*

Table 4.2. Postdocs / Country of Origin.

* (Since 2014, including staff members who have had a scholarship before.)

The training of our junior scientists is complemented with an excellent lecture series (see “Chemistry Frontiers at the Kohlenforschung”), workshops, and lectures at the Institute. For example, a selection of our scientists participates in workshops on catalysis organized by the chemical industry such as the Catalysis Research Laboratories (BASF together with the University of Heidelberg) and the Bayer PhD Student Course from the Institute participate every year. In total, 39 PhD students finished their dissertation in the last reporting period, and our postdocs regularly secure top positions around the globe.

The summer school „Transition Metal Electronic Structure and Spectroscopy“ organized jointly by the Department of Molecular Theory and Spectroscopy and the Department of Inorganic Spectroscopy at the MPI-CEC has been running regularly since 2009, most recently in a biannual mode in odd years (in the other years, there is an analogous school on heterogeneous catalysis organized by the Department of Robert Schlögl at the neighboring CEC). The school, which takes place at the Wissenschaftspark in Gelsenkirchen, has acquired a world-wide reputation and typically is attended by 80 - 100 students. Due to the high demand, future editions will have to select students based on a recommendation letter or entrance exam. While students working at German institutions are in a majority, participants from the USA, China, Japan, and India regularly attended. The school runs for one week with lectures in the morning and practical exercises in the afternoon with poster sessions or clinics in the evenings. The teaching staff as well as the tutors are all coming from the two MPIs with the exception of Prof. Glaser from the University of Bielefeld, who has kindly agreed to provide the lecture on magnetic susceptibility measurements. A comprehensive textbook summarizing the lecture material is near completion and will be published by the Royal Society of Chemistry.

A second summer school focused on theoretical chemistry with special emphasis on wave function based electron correlation methods (“Modern wave function methods in electronic structure theory”) has been established by the Department of Molecular Theory and Spectroscopy jointly with Prof. Jürgen Gauss from the University of Mainz, Germany. The school, which runs in even years, also takes place at the Wissenschaftspark but will likely move to a different location for future editions. The school is limited to 64 participants, which are selected based on recommendation letters for each individual student. The format of the school consists of lectures in the morning followed by problem set solving in small groups in the afternoons. There is a poster session and a clinic as well. The teaching staff consists of world-wide renowned colleagues from all over Europe. The school replaces the very popular school that took place in Aarhus/Denmark which was discontinued due to the retirement of Prof. Paul Jörgensen.

The MWM school alternates with the European Summer School in Quantum Chemistry (ESQC), which takes place in odd years at the Terre Norman on Sicily. Prof. Neese has been a regular lecturer there since 2010.

In addition to the three summer schools mentioned, the DMTS hosts a yearly ORCA Users meeting (3 day event), where new features of ORCA as well as tips and tricks are discussed. One-off events like a full day of ORCA tutorials for the members of the MPI Kofo have also been organized.

The Institute has been very successful in the past to support young research group leaders. A total of 19 scientific group leaders perform research within their own research groups at the Institute, two of which are led by independent research group leaders. In the past few years, six junior scientists have received and accepted calls from universities as shown in table 4.3.

Name	Year	University
Alcarazo	2015	Georg-August-University Göttingen
Barbatti	2015	Aix-Marseille Université
Rinaldi	2015	Imperial College London
Prieto	2017	ITQ Spanish Research Council
Morandi	2018	ETH Zurich
Tredwell	2019	Cardiff University

Table 4.3. Calls from Universities.

Dissertations 2017 - 2019

2017

- January 12th Gabriele Pupo (Universität zu Köln)
Non-classical Carbocations and Enols in Asymmetric Catalysis
- March 6th Jo-Chi Tseng (Ruhr-Universität Bochum)
Microstructure Analysis of Nano-sized Materials Based on X-Ray Diffraction Study: A Practical Protocol
- March 10th Lilla Molnárné Guricza (Universität Duisburg-Essen)
Comprehensive characterization of chemical structures in heavy crude oil asphaltenes by using liquid chromatography and ultrahigh-resolution mass spectrometry
- March 17th Marina Kristina Ilg (TU Dortmund)
Enantioinversion in der Gold(I)-katalysierten Hydroalkoxylierung von Allenen & Studien zur Totalsynthese von Chagosensine
- March 31st Rene Eckert (Ruhr-Universität Bochum)
Mechanokatalytische CO-PROX
- March 31st Jorge Augusto Mendes Burak (Ruhr-Universität Bochum)
Raney Ni stability and characterization upon different systems and solvents

- March 31st Valentina Nese (Ruhr-Universität Bochum)
Solid Catalysts for the Production of 5-Hydroxymethylfurfural and 2,5-Furandicarboxylic Acid
- May 5th Sumit Mittal (Ruhr-Universität Bochum)
Small Molecule Modulation of Protein-Protein Interactions: A Computational Study
- May 24th Ann-Christin Swertz (Bergische Universität Wuppertal)
Elektronenmikroskopische Untersuchungen an mehrschichtigen Nanopartikeln
- August 1st Nesrine Said (RWTH Aachen)
Selective Transformation of Biomass through Dehydration and Reduction
- August 23rd Andreas Ahlers (TU Dortmund)
Concise Total Synthesis of Enigmazole A & Studies towards the Total Synthesis of Rhizoxin D.
- September 29th Nicolas Duyckaerts (Ruhr-Universität Bochum)
In-situ Hydrocracking of Fischer-Tropsch Hydrocarbons: How α -Olefins Influence the Final Product Distribution
- October 6th Georgios Dodekatos (Ruhr-Universität Bochum)
Copper-Cobalt-Based Catalysts and Gold/Titania Nanostructures for Thermocatalytic and Surface Plasmon-Assisted Glycerol Oxidation
- October 6th Yan Xiong (Ruhr-Universität Bochum)
Nano-sized BaTiO₃ and TiO₂ in Photochemical Energy Conversion Systems
- October 11th Luping Liu (Universität zu Köln)
Catalytic Asymmetric Reactions between Alkenes and Aldehydes
- October 23rd Johannes Knossalla (Ruhr-Universität Bochum)
Utilizing Confined Space to Attain High Performance Catalysts and Support Materials
- December 18th Michael Dierks (Ruhr-Universität Bochum)
Hydrophobic Ni₂P/SiO₂ catalysts with improved stability for bio-oil hydrodeoxygenation
- December 18th Jan Engelhardt (Ruhr-Universität Bochum)
Nanostructured Catalysts for Biomass Conversion

2018

- March 2nd Hannah Schreyer (Ruhr-Universität Bochum)
Mechanochemical Activation in Heterogeneous Catalysis
- March 6th Viren Pattni (Ruhr-Universität Bochum)
Understanding Hydration via Solvent Thermodynamics and Vibrational Signatures
- March 21st Christian Marco Pichler (TU Graz, AUT)
Surface casted metal oxides as catalysts for the conversion of renewable resources and Synthesis of dumbbell shaped fullerene assemblies
- April 10th Seyma Ortatagli (Ruhr-Universität Bochum)
Monitoring the Structures of Inorganic Materials by ex situ/in situ X-Ray Powder Diffraction and Pair Distribution Function Analysis
- April 27th Gabriele Prina Cerai (Ruhr-Universität Bochum)
First Row Transition Metal Catalyzed Radical Transformations
- June 22nd Daniel J. Tindall (TU Dortmund)
Fe-Catalyzed Cross-Coupling of 1-Substituted Cyclopropyl Tosylates & Rh(III) Complexes in Carbene Transfer Reactions: Development of an Azo Metathesis
- June 29th Nikolaos Drosos (Ruhr-Universität Bochum)
Boron-catalyzed, reductive deoxygenation of aliphatic diols
- June 29th Luca Legnani (Ruhr-Universität Bochum)
Iron-catalyzed Synthesis of Unprotected Primary Amines
- July 19th Denis Höfler (Universität zu Köln)
Highly Active C-H Acids for Catalysis – Design and Application
- July 20th Grigory André Shevchenko (Universität zu Köln)
Enol Catalysis – Enantioselective Transformations via Bifunctional Brønsted Acid Promoted Enolization
- September 3rd Lucas, Schreyer (Universität zu Köln)
IDPi Catalysis: The Hosomi-Sakurai Allylation and a Mukaiyama Aldol Reaction with Enolsilanes of Acetaldehyde
- September 3rd Nobuya Tsuji (Universität zu Köln)
Activating Olefins via Asymmetric Brønsted Acid Catalysis

- September 4th Tim Gatzenmeier (Universität zu Köln)
Asymmetric Counteranion-Directed Lewis Acid Catalysis with α,β -Unsaturated Esters
- September 14th Schünemann, Stefan (Ruhr-Universität Bochum)
Novel Nanostructured Materials for Optoelectronic, Photocatalytic and Thermocatalytic Applications
- September 17th Bastien Cacherat (Ruhr-Universität Bochum)
From Transition Metal to Brønsted Acid Catalysis: New Strategies in Organic Synthesis
- October 24th Sylvester Größl (TU Dortmund)
Total Synthesis of Belizentrin Methyl Ester: The Polyhydroxylated Sidechain
- December 5th Daniel Dariusch Jalalpoor (Ruhr-Universität Bochum)
Morphology Controlled High-Surface Area Support Materials for Electrochemical Applications
- December 18th Bibhab Bandhu Majumdar (Ruhr-Universität Bochum)
Macromolecular Crowding Effects in Crowded Biomolecular Environments

2019

- February 26th Felix Anderl (TU Dortmund)
Totalsynthese von Belizentrin Methylester & Ein enantiodivergender Zugang zu chiralen Allenen
- August 6th Jonas Börgel (RWTH Aachen)
Late-Stage Functionalization of Arenes: from C-H Amination to C-H Oxygenation and Deoxyfluorination
- September 13th H. Jens Rickmeier (RWTH Aachen)
¹⁸F-Labeling of Small Molecules and Peptides
- November 28th Anna Grünert (Ruhr-Universität Bochum)
Synthesis of Oxymethylene Ethers
- November 28th Edward Nürenberg (Ruhr-Universität Bochum)
Cellulose to 2,5-Dimethylfuran Process
- November 29th Bernhard Wölfl (TU Dortmund)
Totalsynthese von Callyspongiolid
- December 4th Adrián Hery Barranco (Ruhr-Universität Bochum)
Reduction Reactions with Complex Hydrides

- December 4th Jonglack Kim (Ruhr-Universität Bochum)
Oxide Promotion Effects in Copper-Catalyzed Hydrogenation of CO₂ and Organic Carbonate Derivatives
- December 18th Rene Albert (Ruhr-Universität Bochum)
Thermal Conductivity Measurements of Metal Hydrides as High Temperature Heat Storage Materials under Operating Conditions

Chemistry Frontiers at the Kohlenforschung

Chemistry Frontiers at the Kohlenforschung represents a unified seminar program for scientific talks carried out at the Max-Planck-Institut für Kohlenforschung. This initiative started in the academic year of 2018 - 2019 and targeted the broad interest of all the members of the different departments of the Institute. Currently, in its second edition, this seminar series was created with the aim of providing full involvement of the body of students and postdocs, thus actively participating in designing the program and choosing the speakers.

The seminar program is coordinated by Dr. Josep Cornella together with one representative of the students from each department of the Institute.

Chemistry Frontiers at the Kohlenforschung 2018 - 2019

September 3 rd , 2018	Prof. Frank Glorius (<i>GDCh-JCF</i> , University of Münster)
October 9 th , 2018	Prof. Dean Toste (University of California, Berkeley)
October 10 th , 2018	Prof. Naoya Kumagai (<i>Merck-Banyu Lectureship</i> , Institute of Microbial Chemistry, Tokyo)
October 16 th , 2018	Prof. Brad Carrow (Princeton University)
October 29 th – 31 st , 2018	Prof. Kyoko Nozaki (<i>Ziegler Lecture</i> , The University of Tokyo)
November 12 st , 2018	Prof. Ralf Tonner (University of Marburg)
December 5 th , 2018	Prof. Thomas Magauer (University of Innsbruck)
December 7 th , 2018	Prof. Susannah Scott (University of California, Santa Barbara)
December 16 th , 2018	Institut Seminar (<i>Turck Preis Lecture</i>)
January 24 th , 2019	Prof. Erik Meggers (University of Marburg)
February 7 th , 2019	Prof. Cristina Nevado (University of Zürich)
March 7 th , 2019	Prof. Bettina Lotsch (MPI Festkörperforschung)
March 14 th , 2019	Prof. Paul Chirik (Princeton University)
March 25 th , 2019	Prof. Paolo Melchiorre (ICIQ)
April 10 th , 2019	Prof. Hosea Nelson (University of California, Los Angeles)
May 15 th , 2019	Prof. Jean Tremblay (Freie Universität Berlin)
June 6 th , 2019	Prof. Varinder Aggarwal (University of Bristol)
June 18 th , 2019	Institut Seminar

Chemistry Frontiers at the Kohlenforschung 2019 - 2020

October 10 th , 2019	Dr. Marcos Suero (ICIQ)
October 28 th – 30 th , 2019	Prof. Bert Weckhuysen (Ziegler Lecture, University of Utrecht)
November 11 th , 2019	Prof. Dirk Trauner (New York University)
November 14 th , 2019	Prof. Armido Studer (University of Münster)
November 27 th , 2019	Prof. Aiko Fukazawa (Merck-Banyu Lectureship, University of Kyoto)
December 17 th , 2019	Institut Seminar
January 21 st , 2020	Prof. Johannes Lercher (Technische Universität München)
January 23 rd , 2020	Prof. Konrad Tiefenbacher (University of Basel)
February 13 th , 2020	Prof. Sandra Luber (University of Zürich)
February 19 th – 20 th , 2020	Prof. Douglas Stephan (University of Toronto)
April 6 th , 2020	Prof. Antonio Togni (ETH Zürich)
May 11 th , 2020	Prof. Javier Perez-Ramirez (ETH Zürich)
May 20 th , 2020	Prof. Xing Yi Ling (NTU Singapore)
June 4 th , 2020	Prof. Ursula Rothlisberger (EPFL Lausanne)
June 19 th , 2020	Institut Seminar
June 22 nd – 24 th , 2020	Prof. David Milstein (Ziegler Lecture, Weizman Institute of Sciences, Rehovot)

CHAPTER 5

Equal Opportunities

5 Equal Opportunities

The Institute is committed to guarantee equal opportunities and specifically to increase the number of female scientists at all levels but especially at advanced career stages. Both, the percentage of female PhD and female postdoc scientists have been low over the years. The number of more senior female scientists is even lower, best exemplified by the all-male Directorium.

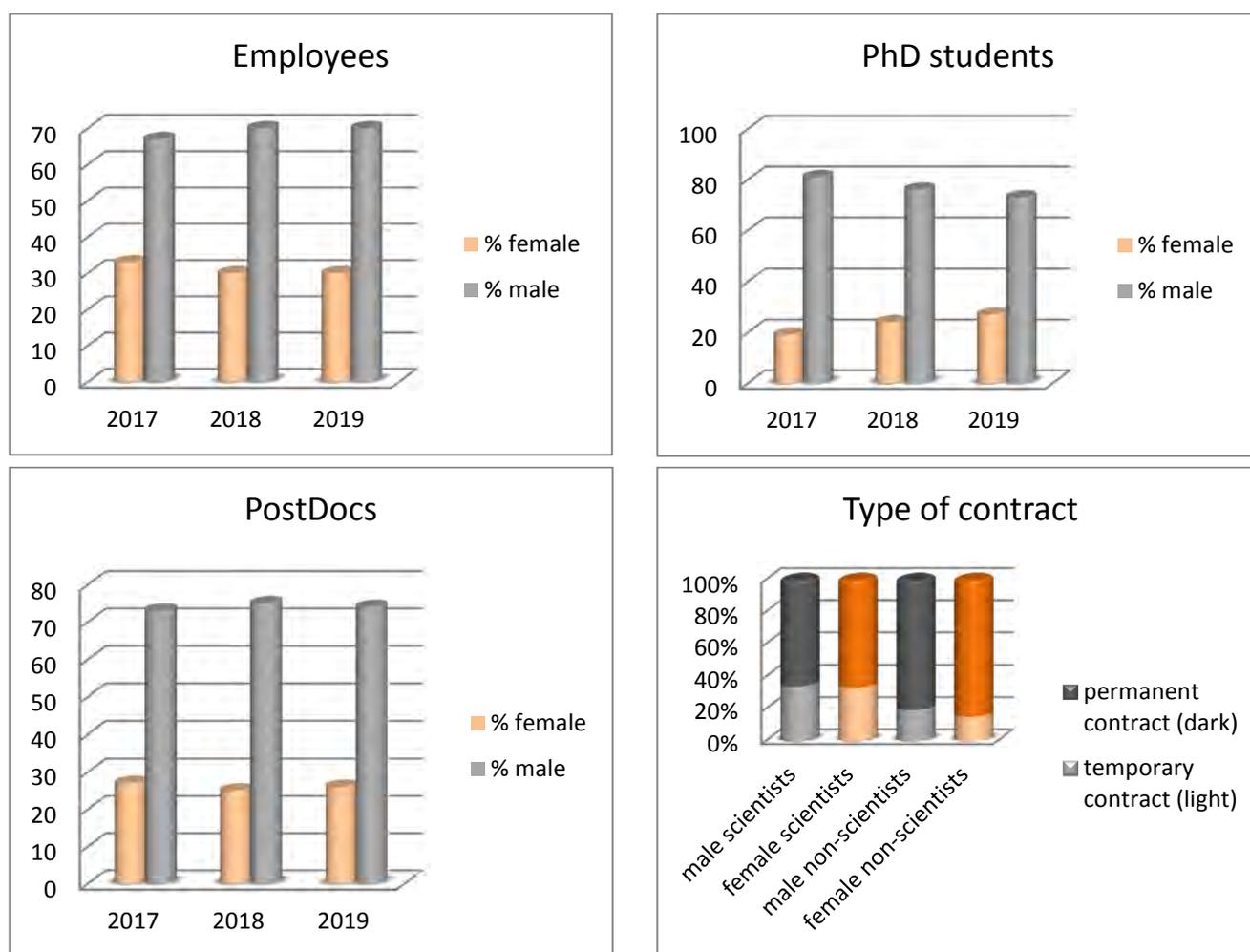


Figure 5.1. Gender Balance.

Currently, the Kohlenforschung has only two senior female scientists, namely Priv.-Doz. Dr. Claudia Weidenthaler (group leader of Powder Diffraction and Surface Spectroscopy in the Department of Heterogeneous Catalysis) and Dr. Monika Lindner (Department of Homogeneous Catalysis). In addition, Kateryna Peinecke works in the group of Hydrogen Storage (Department of Heterogeneous Catalysis), but her position is not

permanent. A gender-balanced composition is currently only realized in the sectors of technical and non-technical staff.

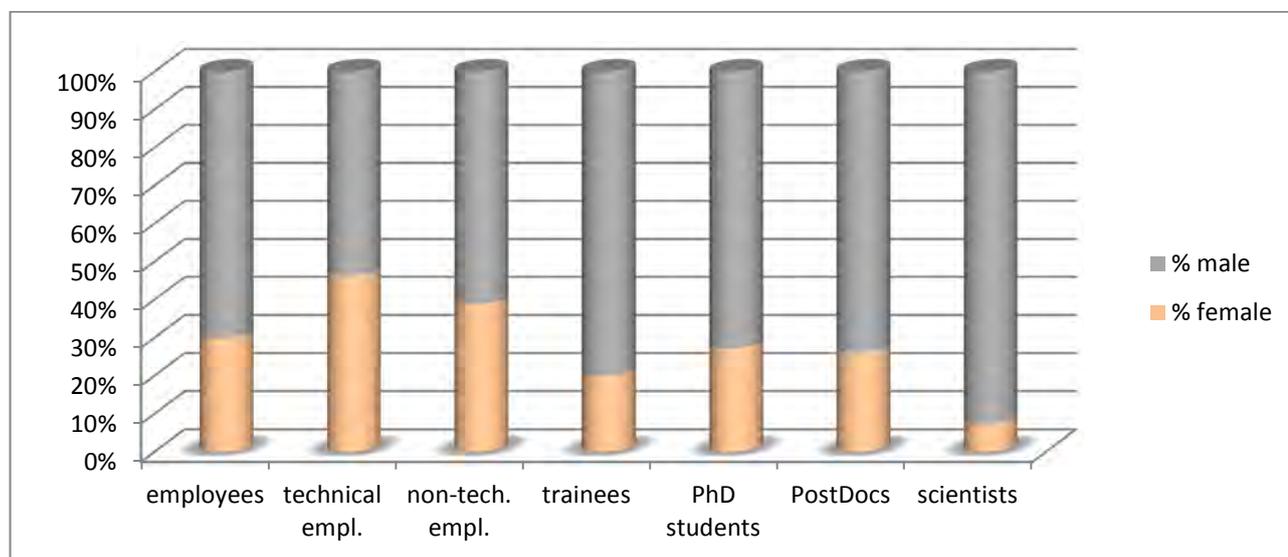


Figure 5.2. Gender Balance by Career Groups.

To counteract our previous and still current situation with respect to gender balance, we have initiated two substantial programs: First, we have established a strategic analysis, with yearly meetings of all directors, and frequent efforts throughout the year to identify the best female scientists in all fields of chemistry that may be appropriate for the Kohlenforschung. Goal of this effort is to identify, evaluate, and ultimately recruit the top female talent within the next ten years. The program was established in 2018 and resulted in a list of promising female candidates for independent positions. Within 2019, several of the candidates have been invited to present their research. Our best outcome so far is an offer to Dr. Constanze Neumann, MIT, who successfully competed in the Max-Planck-wide competition for a Lise-Meitner research group, which only six candidates received this year across all disciplines.

The second program is a detailed gender equality plan, which was first created for the period of 2019 – 2021 by the equal opportunities officer. Here, the Institut für Kohlenforschung formulates goals to increase the number of female co-workers in all areas in which they are currently underrepresented at the Institute. The plan, amongst other goals, aims to provide a more appropriate internet page to provide an overview of the support by the MPG for female scientists and define the family-friendly employment policy of our Institute. We try to identify female role models to support our efforts, for example with a phenomenal Karl Ziegler Guest Lecture by Prof. Kyoko Nozaki from University of Tokyo in 2018.

We have instituted a physical equal opportunity office for face-to-face conversations with our equal opportunity officer and expanded the Girls' Day event to provide support to young female high-school students. A landmark achievement in 2019 was the introduction of a day-care on the ground of the Institute with priority for young children of Max-Planck-employed parents.

CHAPTER 7

Technology Transfer

7 Technology Transfer - Studiengesellschaft Kohle mbH (SGK)

The Max-Planck-Institut für Kohlenforschung has a long tradition in transferring the results of basic research in chemistry into industrial applications:

In the 1920's the Fischer-Tropsch process for the synthesis of gasoline from coal was developed and is still in use today. The economical impact of the Ziegler catalysts for the production of polyethylene and polypropylene, discovered in 1953/54, as well as of the process for the decaffeination of coffee beans by extracting the caffeine with supercritical carbon dioxide resulted in almost four decades of economical independence for the Institute.

In order to exploit the research results of the Institute, a company acting as its trustee was founded decades ago (Studiengesellschaft Kohle mbH, SGK).

The purposes of Studiengesellschaft Kohle are

- patenting of inventions based on the research results
- licensing of the technology to industrial partners
- enforcing intellectual property rights
- negotiating research co-operations with industrial partners.

Six new patent applications in 2017, two in 2018 and four in 2019 were filed (see list of patent applications). For 41 applications from earlier years, patents were issued in 2017 to 2019 in Australia, Canada, China, Eurasia, Europe, India, Israel, Japan and USA.

License agreements exist in the reporting period for: Method for decarboxylating C-C bond formation of carboxylic acids with carbon electrophiles; Chiral Disulfonimides, Catalysts for the alkyne metathesis; Molybdenum and Tungsten Metal Complexes and use thereof as precatalysts for olefin metathesis; The Development and Exploitation of the ChemShell Software; Direct Palladium Catalyzed Aryl Fluorination; Direct ¹⁸F- Labelling of native Peptides for PET Imaging; Reagents and Process for direct C-H functionalization; and The Use of Quantum chemical software-suite „Orca“.

Over the period 2017 to 2019, 12 direct co-operations with industrial partners were in operation. Such cooperative projects are partially financed by the partner, who in return is granted an option to a license for patents resulting from the project.

The Studiengesellschaft also assists researchers of the Institute who want to start up companies based on results and know-how from the Institute. The Heidelberg-based hte AG was co-founded by Professor Dr. F. Schüth several years ago but has now been sold to BASF SE.

General Manager (“Geschäftsführer”) of the Studiengesellschaft is Professor Dr. Ferdi Schüth. Operational functions are performed by Dr. Matthias Nobbe, a patent lawyer, who works for the Institute for about 6 days/month on a freelance contract, and who has a power of attorney for SGK. To foster the licensing activities,

the Institute signed a contract in 2009 with Max Planck Innovation, Munich, as the central technology transfer agency of the Max Planck Society. This contract was extended in 2011, whereby it shall automatically be extended for a further year, if none of the parties terminates it at least three months before the end of the year, and this contract is still in place.

Patent Applications 2017

1. Catalytic C-X-Bond Metathesis through Reversible Arylation
(Bill Morandi, Benjamin Bhawal, Zhong Lian, Peng Yu, Tristan Delcaillau)
2. Process for Converting Synthesis gas to liquid Hydrocarbons, device for carrying out the process and catalyst for use therefor
(Ferdinand Schüth, Gonzalo Prieto, Nicolas Duyckaerts)
3. Process for the Preparation of High Surface Area Metal Oxides and their Use
(Ferdinand Schüth, Dong Gu)
4. Process for Hydrocyanation of Terminal Alkynes
(Tobias Ritter, Fei Ye)
5. Process for the Transition Metal Catalyzed Cyanation of Aryl/Vinyl Halides
(Bill Morandi, Peng Yu)
6. Process for Deoxyfluorination of Phenols
(Applicants are Studiengesellschaft Kohle and Harvard University)
(Tobias Ritter, Martin Georg Strebl-Bantillo, Debashis Mandal, Mohammad Hassan Beyzavi, Constanze Neumann)

Patent Applications 2018

1. Reagents and Process for direct C-H functionalization
(Tobias Ritter, Florian Berger)
2. Reagent and Process for the Site-Specific Deoxyfluorination of Peptides
(Tobias Ritter, Henrick Jens Rickmeier)

Patent Applications 2019

1. A Process for the Preparation of high surface area alpha alumina and the use thereof
(Amol Amrute, Hannah Schreyer, Ferdinand Schüth)
2. Process for the Direct Halogenation of an Aliphatic Hydrocarbon to a Halogenated Aliphatic Hydrocarbon
(Ferdinand Schüth, Pit Losch, Olena Vozniuk, Marius Bilke, Alexander Bodach)
3. Air-Stable Ni(0)-Olefin Complex and its Use as Catalyst and precatalyst
(Josep Cornella, Lukas Nattmann)
4. Verfahren zur Entfernung von Kohlenmonoxid und/oder gasförmigen Schwefelverbindungen aus Wasserstoffgas und/oder aliphatischen Kohlenwasserstoffen
(Michael Felderhoff, Kateryna Peinecke, Sun Tai, Bodo Zibrowius)

CHAPTER 8

Special Activities

8.1 Special Events

Karl Ziegler Lectureships

In 1978, the wife and daughter of Karl Ziegler, the noble prize laureate and former Director of the Max-Planck-Institut für Kohlenforschung, initiated the Karl Ziegler Foundation and the Karl Ziegler Lectureship to commemorate Karl Ziegler as an outstanding scientist. The aim of the Foundation is to bring renowned scientists for lectureships to Mulheim. Since 1978, 31 Karl Ziegler guest professors from all over the world have been invited to deliver lectures and workshops as well as interact with the scientists.



2017: Professor Amir H. Hoveyda (Boston College, US)



July 5th: Main Lecture: *Increasing Challenges in Catalytic Chemistry: Implications Regarding the Future*

July 6th: 1st Seminar: *Sulfonate-Containing NHC Ligands for Enantioselective Catalysis*

July 7th: 2nd Seminar: *Small-Molecule Organoboron Catalysts for Enantioselective Synthesis*

2018: Professor Kyoko Nozaki (University of Tokyo, JP)



October 29th: Main Lecture: *Coordination copolymerization of propylene with polar monomers*

October 30th: 1st Seminar: *Homogeneous Catalysis toward Utilization of Renewable Resources*

October 31st: 2nd Seminar: *Sequential Bond Formation Reactions for the Synthesis of Novel π -conjugated Molecules*

2019: Professor Bert M. Weckhuysen (University of Utrecht, NL)



October 28th: Main Lecture: *Catalysts Live and Up Close. Hunting for the Hidden Chemistry in Catalysis*

October 29th: 1st Seminar: *Catalyst Images, Imaging and Imagination: Visualizing Molecules and Atoms in Action on Catalytic Surfaces*

October 30th: 2nd Seminar. *Spectroscopy of Solid Catalysts: A Tutorial Lecture on Catalysts Characterization and Related Challenges & Opportunities*

Ernst Haage Symposium

Established in 2006, the Ernst Haage Prize honors young scientists for outstanding achievements in the field of chemistry and fosters young academics in particular. The award is given in honor of the entrepreneur Ernst Haage (1901-1968) who lived in Mülheim. The prize is endowed with € 7,500. Since 2018, a symposium and an award ceremony are organized together with the MPI for Chemical Energy Conversion.

November 12th- 13th, 2018, Schloss Broich, Mülheim an der Ruhr, DE

Two day symposium with lectures by:

- Prof. Michele Aresta (University of Bari, IT)
- Prof. Marco Mazzotti (ETH Zurich, CH)
- Univ.-Prof. André Bardow (RWTH Aachen University, DE)
- Prof. Bruno Chaudret (University of Toulouse III, FR)
- Prof. Walter Leitner (Max Planck Institute for Chemical Energy Conversion, DE)
- Prof. Frank Neese (Max-Planck-Institut für Kohlenforschung, DE)
- Dr. Elsje Alessandra Quadrelli (CPE Lyon, FR)
- Prof. Helmut Schwarz (TU Berlin, DE)
- Dr. Etsuko Fujita (Brookhaven National Laboratory, US)
- Dr. Ya-Huei Chin (University of Toronto, CD)

Awardees 2018

Ernst Haage-Prize: Dr. Tim-Patrick Feller, TU Munich

Ernst Haage-Prize for PhD's: Dr. Lucas Schreyer, MPI für Kohlenforschung

Apprentice-Prize: Julia Busch (MPI KOFO) and Till Wehner (MPI CEC)



November 11th - 13th, 2019, MPI für Kohlenforschung, Mülheim an der Ruhr, DE

Three-day symposium with lectures by:

- Prof. Robin B. Bedford (University of Bristol, UK)
- Dr. Thibault Cantat (CEA, FR)
- Prof. Clémence Corminboeuf (École Polytechnique Fédérale de Lausanne, CH)
- Prof. Marc Koper (Universiteit Leiden, NL)
- Prof. Kathrin Lang (TU München, DE)
- Prof. Antoni Llobet (ICIQ - Institut Català d'Investigació Química, ES)
- Prof. Markus Reiher (ETH Zürich, CH)
- Prof. Erwin Reisner (University of Cambridge, UK)
- Prof. Corinna Schindler (University of Michigan, US)
- Prof. Dirk Trauner (New York University, US)
- Prof. Atsushi Urakawa (TU Delft, NL)

Awardees 2019

Ernst Haage-Prize: Dr. Thomas-Christian Jagau, Ludwig-Maximilians-Universität München

Ernst Haage-Prize for PhD's: Dr. Casey van Stappen, MPI für Chemische Energiekonversion

Apprentice-Prize: Vanessa Richter (MPI CEC) and Pia Münstermann (MPI KOFO)

March 8th, 2019, Symposium on Perspectives in Theoretical Chemistry, Mülheim an der Ruhr, DE

The Symposium on Perspectives in Theoretical Chemistry in 2019 was held in honor of Walter Thiel who celebrated his 70th birthday in March 2019. The symposium highlighted the status and perspectives of current research in selected areas of theoretical chemistry that were related to the work of Walter Thiel.

Lectures were given by:

- Feliu Maseras (Institute of Chemical Research of Catalonia, Tarragona, ES)
- Qiang Cui (Boston University, US)
- Christian Ochsenfeld (University of Munich, DE)
- Ali Alavi (Max Planck Institute for Solid State Research, Stuttgart, DE)
- Benedetta Menucci (Dept. of Chemistry, University of Pisa, IT)
- Stefan Grimme (Mulliken Center of Theoretical Chemistry, Bonn, DE)
- Leticia González (University of Vienna, AU)
- Peter Schreiner (University of Giessen, DE)



June 30th - July 5th, 2019, Molecular Quantum Mechanics Conference, Heidelberg, DE

The 9th Molecular Quantum Mechanics conference (MQM19), celebrating the German School of Quantum Chemistry, was held in Heidelberg. Scientific Chair of the event was Professor Frank Neese. The event gathered 350 experts of Quantum Chemistry from more than 35 countries in the Heidelberg Convention Center. Almost 70 oral presentations including four historical lectures were delivered and two poster presentations were held. The conference organization was handled by the Public Relations Departments of the MPI for Chemical Energy Conversion and the MPI für Kohlenforschung supported by an external agency. The conference was sponsored by Turbomole, Q-Chem, Faccts, Cosmologic, PCCP, and Molpro.



Summer Schools

The Summer Schools of the MPI für Kohlenforschung were dedicated to master's students, doctoral students and post-docs. According to the thematic focus of the program, the organizing department cooperated with other departments, the MPI for Chemical Energy Conversion, universities or other institutions. The following Summer Schools were offered:

- MPI KOFO/Johannes-Gutenberg-University Mainz, “MWM Summerschool”, Gelsenkirchen, DE, September/October 2018: Organizer: F. Neese
- “ORCA User Meeting”, Mülheim an der Ruhr, DE, September 2018, Organizers: A. Auer, F. Neese, F. Wennmohs
- International Summer School DGK-AK20 “Synthesis and Characterization of Inorganic Functional Materials”, Mülheim an der Ruhr, DE, July 2019: Organizer: C. Weidenthaler
- Summer School “Spectroscopy and Electronic Structure of Transition Metal complexes”, Gelsenkirchen, DE September/October 2019, Organizers: D. Pantazis, F. Neese and S. De Beer



Institute Seminar

The Institute Seminar is a platform for communication and exchange between the researchers of the different laboratories. It is an opportunity to get into touch with the other departments, listen to oral presentations and participate at a poster session. In 2017 and 2018 the Institute Seminar was linked with the awarding of the Turck Prize that went to a young scientist with an outstanding publication.



- 2017**
December 12th
- Dr. Matthew Tredwell, Department of Organic Chemistry
Synthesis of 19F- and 18F-perfluorinated motifs
- Dr. Luping Liu, Department of Homogeneous Catalysis (Turck-Prize)
A general Catalytic Asymmetric [4+2]-Cycloaddition of Dienes with Aldehydes
- 2018**
June 11th
- Dr. Giovanni Bistoni, Department of Molecular Theory and Spectroscopy
Accurate theoretical approaches to homogeneous catalysis. From numbers to chemical insights
- Dr. Chun-Xiang Zhuo, Department of Organometallic Chemistry
Catalysis-Based Total Synthesis of the Anti-Cancer Agent Pateamine A
- December 10th
- Xiang Sun, Department of Organic Synthesis
Catalytic dehydrogenative decarboxyolefination of carboxylic acids
- Georgi L. Stoychev, Department of Molecular Theory and Spectroscopy (Turck-Prize)
Calculation of NMR chemical shifts with double-hybrid DFT
- 2019**
June 18th
- Dr. Dimitrios Pantazis, Department of Molecular Theory and Spectroscopy
Theory-Driven Discovery in Photosynthesis Research
- Dr. Josep Cornellà, Department of Organometallic Chemistry
Bismuth Redox Catalysis
- December 17th
- Dr. Amol Amrute, Department of Heterogeneous Catalysis
Mechanochemical synthesis of nanomaterials
- Dr. Florian Berger, Department of Organic Synthesis
Site-selective aromatic C-H functionalization

Internal Symposia

Another platform for communication and exchange within the scientific staff are the seasonal two-day MPI KOFO/CEC Joint Workspace Symposia of the Neese group, regularly organized at the institute. Group leaders and members give talks and participate in Poster Sessions. Organization: F. Neese

- MPI KOFO/CEC Joint Workspace Winter Symposium, Mülheim, DE, February 2018
- MPI KOFO/CEC Joint Workspace Summer Symposium, Mülheim, DE, June 2018
- MPI KOFO/CEC Joint Workspace Fall Symposium, Mülheim, DE, October 2018
- MPI KOFO/CEC Joint Workspace Winter Symposium, Mülheim, DE, February 2019
- MPI KOFO/CEC Joint Workspace Summer Symposium, Mülheim, DE, June 2019
- MPI KOFO/CEC Joint Workspace Fall Symposium, Mülheim, DE, October 2019

IMPRS-RECHARGE

IMPRS-RECHARGE is a unique postgraduate training program founded 2015 by the Max-Planck-Institut für Chemische Energiekonversion (MPI CEC), Ruhr-Universität Bochum, Universität Duisburg-Essen, Universität Bonn and the Max-Planck-Institut für Kohlenforschung. It focuses on interdisciplinary research between chemistry and physics with an emphasis on catalytic mechanisms, physical-chemical analysis and energy topics.

Neese, F.

- Speaker of IMPRS/ RECHARGE, since 2015

List, B.

- IMPRS-Recharge - Day of Catalysis, Mülheim an der Ruhr, DE, November 2018

Atanasov, M.

- Course “Ligand Field Theory”, IMPRS-RECHARGE, Mülheim an der Ruhr, DE, November 2019

Fares, C.

- Course “NMR in Catalysis”, IMPRS-RECHARGE, Mülheim an der Ruhr, DE, November 2019

IMPRS-SURMAT

IMPRS-SURMAT is a unique postgraduate training program founded in 2004 by the Max-Planck-Institut für Eisenforschung, Max-Planck-Institut für Kohlenforschung, and the Ruhr-Universität Bochum. Now, also the Universität Duisburg-Essen and the Max-Planck-Institut für Chemische Energiekonversion (MPI CEC) are involved in this program. IMPRS-SURMAT focuses on interdisciplinary research in chemistry, physics and engineering with an emphasis on surface and materials topics.

Schüth, F., Marlow, F., Weidenthaler, C., Schmidt, W.

- 2-weeks Course “Solids (T4)”, IMPRS-SURMAT in Mülheim an der Ruhr, DE, October 2018 (together with the University of Duisburg-Essen)

Day of Catalysis

Lectures on aspects of Catalysis for IMPRS Recharge, November 6th, 2018, Mülheim, DE

Conference Organizer: Professor Benjamin List

- Prof. Dr. Benjamin List (Max-Planck-Institut für Kohlenforschung)
Organocatalysis
- Prof. Dr. Ferdi Schüth (Max-Planck-Institut für Kohlenforschung)
Synthetic Approaches for the Production of Solid Catalysts
- Prof. Dr. Tobias Ritter (Max-Planck-Institut für Kohlenforschung)
Late-Stage Functionalizations
- Prof. Dr. Alois Fürstner (Max-Planck-Institut für Kohlenforschung)
Advances in Metal Carbene Chemistry
- Prof. Dr. Walter Thiel (Max-Planck-Institut für Kohlenforschung)
Theoretical Studies of Transition Metal Catalysis and Biocatalysis

Liebig Lecture

November 2017

Prof. Dr. Ruben Martin (ICIQ, Tarragona, ES)

Turning simplicity into complexity via Ni-catalyzed cross-coupling reactions

MBLA Lectureships

October 2018

Dr. Naoya Kumagai (Institute of Microbial Chemistry Tokyo, JP)

Chemistry Empowered by Unique Heterocycles

November 2019

Prof. Aiko Fukazawa (iCeMS, Kyoto University, JP)

Exploring Stable Yet Unusual π -Electron Materials by Making Use of Phosphorus and Sulfur

8.2 Public Relations

The Public Relations Department is responsible for presenting the institute's research activities to the public and other interested parties, such as journalists, research institutions, partners, donors and potential employees, as well as the wider scientific community. The aim is to convey information, bestow trust, and create a positive image of the research undertaken in the institute. Depending on the target group and content, various communication measures, such as press work, news on the institute's website, brochures, events, or social media campaigns are conceived and carried out. In order to open up to the public, the institute offers guided tours and participates in public events such as the biennial WissensNacht Ruhr in 2018 with a participation of some 8000 visitors in the Ruhr Area.

Public relations projects:

- Max Planck Day Celebration, September 14th, 2018 with primary school students
- Experimental Lecture with Professor Ferdi Schüth, August 30th, 2019
- MPI goes Social Media: Set up of a Facebook fanpage for the MPI KOFO in 2018
- Introduction of an employee newsletter “Neues aus der Kohlenforschung” in 2019
- MQM Conference in Heidelberg, Heidelberg, DE, July 2019



Students from elementary schools visiting the MPI on Max Planck Day 2018

Activities for Schools and Families & Girls' Day

In order to promote interest in scientific topics among young people, the institute maintains extensive cooperations with secondary schools in Mülheim and the surrounding area. School coordinator Claudia Weidenthaler carries out about 10-15 activities per year with students of different grades. These events are supported by students from the departments of the institute. The sessions are planned together with the teachers and range from lectures during a science week to group lessons on various topics. About 200-400 students per year are reached in this way.



Participants of Junioruni Ruhr (left) and the team of C. Weidenthaler with teachers from the Karl-Ziegler-Gymnasium

8.3 Local Activities of the Young Chemists Forum (JCF) of the German Chemical Society (GDCh)

List of Talks and Workshops Given by Guests

2017

April 21 st	Workshop	Dr. Philip Gramlich (Natural Science Careers) <i>Goodbye Academia</i>
May 4 th	Industry	Volker Berg and Michael Engels (BCG) <i>Consulting – Career Opportunities for Chemists</i>
May 11 th	Research	Prof. Bernhard Breit (Universität Freiburg, DE) <i>Rhodium-Catalyzed Addition of Pronucleophiles to Alkynes and Allenes: An Atom-Economic Alternative to the Tsuji-Trost Reaction</i>
September 14 th	Popular Sciences	Rolf Breinbauer (TU Graz, AT) <i>Insanity in Science</i>
September 29 th	Industry	Prof. Schrader, Dr. C. Roosen (SABIC Geleen, NL) <i>Introduction to Steam Cracking</i>
December 7 th	Popular Sciences	Dr. Klaus Roth (FU Berlin, DE) <i>Das chemische Geheimnis des Weihnachtsdufts</i>

2018

January 25 th	Industry	Clariant <i>Von Laborleitung zu Sales</i>
June 5 th	Workshop	Dr. Philip Gramlich (Natural Science Careers) <i>Goodbye Academia</i>
July 5 th	Research	Prof. Martin Oestreich (TU Berlin, DE) <i>Wheland Intermediates in Catalysis</i>

July 12 th	Industry	Dr. Johannes Panten (Symrise)
August 28 th	Workshop	Dr. A. Kitzmann <i>Stress Management</i>
September 3 rd	Research	Prof. Frank Glorius (Universität Münster, DE) <i>Discovery in Catalysis</i>
September 20 th	Industry	Dr. Suzanne Tobey (Wiley, Weinheim, DE) <i>The Editorial Office – Demystifying the Black Box</i>
November 29 th	Popular Sciences	Dr. Gerhard Heywang <i>Polymers – simply amazing</i>
2019		
February 22 nd	Workshop	McKinsey (MPI for Chemical Energy Conversion, DE)
April 23 rd	Research	Prof. Regina Palkovits (RWTH Aachen, DE) <i>Design of Solid Catalysts for the (Electro)Catalytic Valorisation of Renewable Carbon Sources</i>
June 6 th	Workshop	Dr. Karin Bodewits (Natural Science Careers) <i>Goodbye Academia</i>
June 11 th	Industry	Dr. Adrian Komainda (Schrödinger Inc.)
July 10 th	Research	Prof. Klaus Kümmerer (Leuphana Universität Lüneburg, DE) <i>Beyond Green Chemistry-Sustainable Chemistry!</i>
September 20 th	Workshop	Katharina Keune, Thomas Müller (Artsbased) <i>Artful Leadership – Successful Communication from a Leader's Perspective</i>
October 23 rd	Workshop	Herr Armbruster (MPG, Berlin, DE) CV-Workshop
December 5 th	Research	Prof. Nicolai Cramer (EPF Lausanne, CH)

Activities Organized by the JCF Mülheim

- March 23rd, 2017 JCF Kegeln (Hotel Thiesmann, Mülheim, DE)
Possibility for new members of the Institute to get to know each other
- May 15th, 2017 Sherlock-Holmes-Projekt (RUB)
- September 14th, 2017 Summer BBQ (MPI für Kohlenforschung, Mülheim)
Social get-together of PhD and PostDocs of both Mülheim-based MPI's
- October 12th, 2017 8th Young Chemists Symposium (JCS) 2017 (MPI für Kohlenforschung, DE)
Chemistry students of the Ruhr area presented and discussed research results of their Bachelor-, Master- and PhD-theses. The symposium was organized by the JCFs of Bochum, Dortmund, Essen and Mülheim.
- May 15th, 2018 After-Work Session (Mülheim Chemistry Campus, DE) with Prof. Schüth and Prof. Leitner
Future of Energy – A Chemical Perspective
An after work get-together with experts/professors, in order to discuss trending topics of the scientific world
- June 25th, 2018 After-Work Session (Mülheim Chemistry Campus, DE) with Prof. Candice Chan, Prof. Petra de Jong, Dr. Pep Cornella
International Research Environments
- September 20th, 2018 After-Work Session (Mülheim Chemistry Campus, DE) with Prof. DeBeer, Suzanne Tobey and Prof. List
Publishing in Science
- October 10th, 2018 9th Young Chemists Symposium (JCS) 2018 (RUB, DE)
- November 29th, 2018 Winter/Christmas BBQ (Mülheim Chemistry Campus, DE)
- September 19th, 2019 10th Young Chemists Symposium (JCS) 2018 (University Duisburg-Essen, DE)
- December 5th, 2019 Winter/Christmas BBQ (Mülheim Chemistry Campus, DE)

CHAPTER 9

Appendices

9.1 Invited Presentations

2017

Farès, C.

- ORCA Summer School, Gelsenkirchen, DE, September 2017
- Treffen der Junganalytiker der GDCh, Mülheim an der Ruhr, DE, November 2017

Felderhoff, M.

- 11th Int. Symposium Hydrogen & Energy, Waikoloa Village, HI, US, March 2017
- Université catholique de Louvain, BE, September 2017
- Meeting of the International Energy Agency, Task 32, Schloß Ringberg, Kreuth, DE, December 2017

Fürstner, A.

- University of Strasbourg, Strasbourg, FR, February 2017
- 82nd ICS Annual Meeting and 6th Angewandte Symposium, Tel Aviv, IL, February 2017
- 22nd ISOM Conference, Zurich, CH, July 2017
- 26th ISHC Congress, Regensburg, DE, September 2017
- 7th Organic Chemistry Day, Madrid, ES, October 2017
- Bohlmann Lecture, TU Berlin, Berlin, DE, November 2017
- Xingda Lecture, Peking University, Peking, CN, November 2017

Gatzenmeier, T.

- 19th Frühjahrssymposium, Mainz, DE, March 2017
- 8th Young Chemists' Symposium Ruhr, Mülheim an der Ruhr, DE, October 2017

Höfler, D.

- Max-Planck Institute for Solid State Research, Stuttgart, DE, May 2017

Klußmann, M.

- Hochschule Darmstadt, DE, June 2017
- 2nd International Conference on Hydrogen Atom Transfer (iCHAT 2017, 02 – 07 July), Frascati, IT, July 2017

Lehmann, C. W.

- Incoatec GmbH, Geesthacht, DE, June 2017
- Pharmaceutical Powder X-ray Diffraction, Hyderabad, IN, August 2017
- Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, DE, October 2017

List, B.

- Förderverein Chemie-Olympiade e.V. (FChO) 25jähriges Bestehen, Festveranstaltung in Frankfurt, DE, January 2017
- Texas A&M University, Texas, US, February 2017
- Institute of Chemistry, Academia Sinica, Taipei, TW, March 2017
- National Tsing Hua University, Hsinchu City, TW, March 2017
- National Taiwan Normal University, Taipei, TW, March 2017
- UCB, Slough, UK, May 2017
- University of Manchester, UK, May 2017
- Münster SFB Symposium, DE, May 2017
- GDCh lecture, University of Leipzig, Leipzig, DE, June 2017
- 16th Annual Symposium on Chemical Synthesis, Boston University, US, June 2017
- Blue Danube Symposium on Heterocyclic Chemistry, Linz, AT, August 2017
- ISHC 2017, Regensburg, DE, September 2017
- 17th Tateshina Conference, JP, November 2017
- Indian Institute of Science (IISC), Bangalore, IN, December 2017
- Indian Association for the Cultivation of Science (IACS), Kolkata, IN, December 2017

Marlow, F.

- Fayoum University, Fayoum, EGY, February 2017
- Pontificia Universidad Católica de Chile, Santiago, CHL, March 2017
- University of Paderborn, Paderborn, DE, October 2017

Morandi, B.

- RWTH Aachen University, Aachen, DE, 2017
- 9th Workshop on Fats and Oils as Renewable Feedstock for the Chemical Industry, Karlsruhe, DE, 2017
- University of Zurich, Zurich, CH, 2017
- Boehringer Ingelheim, Ingelheim, DE, 2017
- UniCat Cluster (TU Berlin), Berlin, DE, 2017
- German-Spanish Symposium, ICIQ, Tarragona, ES, 2017
- Leibniz-Institut für Katalyse e. V. (LIKAT), Rostock, DE, 2017
- Lieseberg-Kolloquium, Heidelberg University, Heidelberg, DE, 2017
- Symposium of de Chemische Binding, Groningen, NL, 2017

- Bayer alumni days, Cafe Moskau, Berlin, DE, 2017
- Givaudan AG, Dübendorf, CH, 2017
- Bayer Chemical Development, Wuppertal, DE, 2017
- Workshop hosted by Syngenta (Hochschule trifft Industrie), Freiburg im Breisgau, DE, 2017
- Cologne University, Cologne, DE, 2017
- University of Manchester, Manchester, UK, 2017
- ETH Zurich, Zurich, CH, 2017
- Liverpool University, Liverpool, UK, 2017

Prieto, G.

- 4th EuChemS Inorganic Chemistry Conference – EICC-4, Copenhagen, DK, July 2017
- Exxon-Mobil Chemical European Science & Engineering Award Symposium, Brussels, BE, July 2017
- JungChemikerForum, GDCh, Berlin, DE, September 2017

Reetz, M. T.

- Technische Universität Hamburg-Harburg, Hamburg, DE, January 2017
- Leibniz-Symposium, Hannover, DE, February 2017
- Tianjin Institute of Industrial Biotechnology, Tianjin, CN, May 2017
- Nankai University Organic Chemistry Department, Tianjin, CN, May 2017
- Shanghai Institute of Organic Chemistry, Shanghai, CN, May 2017
- East China University of Science and Technology, Shanghai, CN, May 2017
- Peking University Organic Chemistry Department, Beijing, CN, May 2017
- Beijing Institute of Microbiology, Beijing, CN, May 2017
- Vazyme Biotech (company), Nanjing, CN, May 2017
- BioTrans Congress, Budapest, HU, July 2017
- Benzon Symposium, Copenhagen, DK, August 2017
- Cytochrome P450 Symposium, Dusseldorf, DE, August 2017
- International Symposium Synthesis & Catalysis, Evora, PT, September 2017
- TWIST Synthetic Biology Symposium, Munich, DE, November 2017
- Biomillenia (company), Paris, FR, November 2017

Rehosek, M.

- M. Rehosek, F. Marlow, Bunsentagung, Berlin, DE, May 2017

Ritter, T.

- 50th annual Sheffield Stereochemistry Meeting, University of Sheffield, Sheffield, UK, January 2017
- Colloquium for Organic Chemistry and Chemical Biology, Phillips-Universität Marburg, Marburg, DE, January 2017
- GDCh Lecture, Universität des Saarlandes, Saarbrücken, DE, February 2017
- International Symposium Imaging agents in Medicine, University Medical Center Groningen, Groningen, NL, February 2017
- University of Cambridge, Cambridge, UK, March 2017
- 253rd ACS National Meeting and Exposition, San Francisco, US, March 2017
- GDCh Lecture, TU Braunschweig, Brunswick, DE, April 2017
- Science Day at CARBOGEN AMCIS AG, Bubendorf, CH, May 2017
- Junior Faculty Professional Development Workshop, Mainz, DE, May 2017
- University of Nankai, Tianjin, CN, June 2017
- University of Tianjin, Tianjin, CN, June 2017
- Tsinghua University, Beijing, CN, June 2017
- OMCOS-19, Jeju Island, KR, June 2017
- Pohang University of Science and Technology, Pohang, KR, June 2017
- EuCOMC-2017, Amsterdam, NL, July 2017
- UCB Super Network Conference 2017, London, UK, July 2017
- Bayer AG, Frankfurt, DE, September 2017
- International Isotope Society Central European Division Workshop, Bad Soden, DE, September 2017
- Annual meeting of the AG Radiochemie, Starnberg, DE, October 2017
- Meeting of the French Chemical Society, Toulouse, FR, November 2017

Schmidt, W.

- Dalian University of Technology, Dalian, CN, 14 April 2017

Schrader, W.

- Thermo Workshop on GC/MS, Gelsenkirchen, DE, February 2017
- Industrial Seminar, SABIC, Geleen, NL, March 2017
- Colloquium, University of Pittsburgh, Pittsburgh, US May 2017
- Workshop ASMS Interest Group Energy Petroleum and Biofuels, Indianapolis, US, June 2017
- Thermo Workshop on LC/MS, Dusseldorf, DE, June 2017
- PEFTEC Conference, Antwerp, NL, November 2017

Schulze, P.

- Treffen der Junganalytiker (GDCh), Mülheim an der Ruhr, DE, November 2017
- Knauer Wissenschaftliche Geräte GmbH, Berlin, DE, March 2017

Schüth, F.

- UCL London, London, UK, 2017
- MPI for Molecular Biomedicine Münster, DE, 2017
- University of Münster, Münster, DE, 2017
- International Conference on Materials Chemistry, Liverpool, UK, July 2017
- University of Dalian, Dalian, CN, 2017
- Merck Advisory Board Meeting, Darmstadt, DE, 2017
- MPIE anniversary colloquium, Dusseldorf, DE, 2017
- 4. Ruhr-Symposium, Duisburg, DE, October 2017
- Carbon2Chem, Dusseldorf, DE, November 2017
- CHAINS 2017, Veldhoven, NL, December 2017

Tredwell, M.

- RIKEN Institute, Wako, JP, February 2017
- Graduate School of Pharmaceutical Sciences, The University of Tokyo, JP, February 2017
- RIKEN CLST, Kobe, JP, February 2017
- Department of Chemistry, Graduate School of Science, Osaka University, JP, February 2017

Tüysüz, H.

- GDCh Scientific Forum Chemistry, Berlin, DE, September 2017
- 7th Slovenian-Serbian-Croatian Symposium on Zeolites, Ljubljana, SL, May 2017
- AMOLF colloquium, Amsterdam, NL, February 2017
- University of Vienna, Vienna, AT, May 2017
- University of Bern, Bern, CH, June 2017
- Max-Planck Institute für Chemische Physik fester Stoffe, Dresden, DE, August 2017
- University of Leipzig, Leipzig, DE, November 2017
- Inaugural lecture RU Bochum, DE, November 2017

Weidenthaler, C.

- Zintl Symposium University Darmstadt, DE, November 2017
- Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences, CN, April 2017
- Dalian University of Technology, State Key Laboratory of Fine Chemicals, CN, April 2017

- Shandong University, Jinan, CN, April 2017
- University Aachen, Aachen, DE, March 2017
- German Zeolite Conference, Frankfurt a.M., DE, February 2017

2018

Atanasov, M.

- 47. Hirscheegg-Seminar Festkörperchemie, Kleinwalsertal, AT, May/June 2018
- The XXIVth International Symposium on the Jahn-Teller Effect, Santander, ES, June 2018
- Theoretical Studies on Magnetic Systems, Methodological Development and Applications, Toulouse, FR, June 2018
- 4th ORCA User Meeting, Mülheim an der Ruhr, DE, September 2018
- IMPRS-RECHARGE School, Ligand Field Theory, Mülheim an der Ruhr, DE, October 2018

Auer, A.

- Theoretisch Chemisches Kolloquium, Ruhr Universität Bochum, Bochum, DE, July 2018
- Statusseminar BMBF InnoEMat, Frankfurt am Main, DE, October 2018

Fares, C.

- 40th Ann. Disc. Meeting FGMR/GDCh, Leipzig, DE, September 2018

Felderhoff, M.

- Universität Osnabrück, DE, January 2018
- 16th International Symposium on Metal-Hydrogen Systems, Guangzhou, CN, October 2018
- Workshop on Hydrogen Storage – Indian Oil Company, Faridabad, IN, December 2018
- International Conference on Hydrogen & Fuel Cell, Jodhpur, IN, December 2018

Fürstner, A.

- GDCh Lecture, Justus-Liebig-University, Gießen, DE, January 2018
- JCF, TU Dortmund, Dortmund, DE, January 2018
- EPFL, Lausanne, CH, March 2018
- University of Zurich, CH, March 2018
- Givaudan, Zurich, CH, March 2018
- Novartis Lecture, University of Illinois, Champaign, US, April 2018
- Ernest E. Campaigne Lecture, Indiana University, Bloomington, US, April 2018
- Georg-Büchi-Lecture, Massachusetts Institute of Technology, Cambridge, US, May 2018

- GDCH Lecture, University of Leipzig, Leipzig, DE, June 2018
- ISRIUM Conference, Ascona, CH, September 2018
- 22nd ICOS Conference, Florence, IT, September 2018

Gatzenmeier, T.

- 21st International Symposium of Homogeneous Catalysis, Amsterdam, NL, July 2018
- 7th EuCheMS Chemistry Congress, Liverpool, UK, August 2018
- Bader Student Chemistry Symposium 2018, Darmstadt, DE, September 2018
- 9th Young Chemists' Symposium Ruhr, Bochum, DE, October 2018

Helmich-Paris, B.

- TU Darmstadt, Darmstadt, DE, March 2018
- Universität Bremen, Bremen, DE, July 2018

Höfler, D.

- MedChem PhD Course, Boehringer Ingelheim (BI), Biberach, DE, July 2018

Izsak, R.

- LUEST Meeting, Telluride, US, June 2018
- CESTC Meeting, Srni, CZ, September 2018

Klußmann, M.

- KU Leuven, Leuven, BE, February 2018
- Summer School "Advanced Organocatalysis" (ADVOCAT) of the Universität zu Köln, Bergisch-Gladbach, DE, August 2018

Lehmann, C. W.

- Symrise AG, Holzminden, DE, October 2018

List, B.

- Xenon Pharmaceuticals, Burnaby, CAN, February 2018
- University of Southern California, Los Angeles, US, February 2018
- Key speaker at 55th edition of the SECO - Semaine d'Etudes en Chimie Organique, Lacanau, FR, May 2018
- Hangzhou Normal University, Hangzhou, CN, May 2018
- Nanjing University, Nanjing, CN, May 2018
- Shanghai Institute of Organic Chemistry, Shanghai, CN, May 2018
- East China Normal University, Shanghai, CN, May 2018

- Second Oxford Synthesis Summer Conference, UK, June 2018
- Merck „Curious2018 – Future InSight”, Darmstadt, DE, July 2018
- Summer School "Advanced Organocatalysis", Cologne, DE, August 2018
- Celebration of Organic Chemistry Symposium, UCB Celltech, Braine-l'Alleud, BE, September 2018
- University of California Santa Barbara, Santa Barbara, US, October 2018
- IKCOC-14, Kyoto, JP, November 2018
- Frontiers in Chemical Sciences, IIT Guwahati, IN, December 2018
- IIT Bombay, Bombay, IN, December 2018
- Organometallic and Catalysis conference, Goa, IN, December 2018

Manganas, D.

- Molecules in Motion (MOLIM) workshop, session 4, Graz, AT, February 2018
- 5th Oxidation Day. Department of Inorganic Chemistry Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE, September 2018

Morandi, B.

- Scripps Research Institute, La Jolla, US, 2018
- California Institute of Technology, Pasadena, US, 2018
- Stanford University, US, 2018
- UC Berkeley, US, 2018
- OM&Cat 2018, Taipei, TW, 2018
- Dozententagung, DE, 2018
- University of Lyon, Lyon, FR, 2018
- TU Graz, Graz, AT, 2018
- Syngenta, UK, 2018
- SECO, Bordeaux, FR, 2018
- University of Mainz, Mainz, DE, 2018
- EMD Serono, Rockland, US, 2018
- Symposium in honor of Barry Trost, Paris, FR, 2018
- UCB Pharma Conference, Brussels, BE, 2018
- Gordon Research Conference on Natural Products & Bioactive Compounds, Andover, US, 2018
- Firmenich, Geneva, CH, 2018
- Genentech, San Francisco, US, 2018
- Berlin, DE, 2018
- University Paris-Sud, Orsay, FR, 2018
- University of Bremen, Bremen, DE, 2018
- University of Edinburgh, Edinburgh, UK, 2018

- 1st European Meeting of Excellence in Chemistry and Molecular Sciences, Vienna, AT, 2018

Neese, F.

- Retreat for IMPRS-ReCharge members, Burg Hülshoff, Nottuln, DE, April 2018
- Universität Bern, Bern, CH, May 2018
- École polytechnique fédérale de Lausanne (EPFL), Lausanne, CH, May 2018
- University of Geneva, Geneva, CH, May, 2018
- University of Zurich, Zurich, CH, May 2018
- Penn State University State College, State College, US, June 2018
- 16th International Congress on Quantum Chemistry (ICQC), Toulouse, FR, June 2018
- Gordon Research Conference on Computation Chemistry, West Dover, US, July 2018
- 7th EuChemMS Chemistry Congress, Arena and Convention Centre, Liverpool, UK, August 2018
- 130. Versammlung der Gesellschaft Deutscher Naturforscher und Ärzte, Saarbrücken, DE, September 2018

Pantazis, D.

- 44th International Conference on Coordination Chemistry (ICCC), Sendai, JP, July/August 2018
- 14th European Biological Inorganic Chemistry Conference (EuroBIC), Birmingham, UK, August 2018
- Quantum Bioinorganic Chemistry Conference IV, Bath, UK, September 2018

Prieto, G.

- International Syngas Convention, Cape Town, ZA, March 2018
- National Young Researchers Meeting of the Spanish Catalysis Society, ES, June 2018

Reetz, M. T.

- Leibniz Institute of Plant Biochemistry, Halle, DE, March 2018
- Tianjin Institute of Industrial Biotechnology, Tianjin, CN, May 2018
- State Key Laboratory of Biocatalysis & Enzyme Engineering, Hubei University, Wuhan, CN, May 2018
- State Key Laboratory of Phytochemistry, Hunan Normal University, Changsha, CN, May 2018
- ALMAC (company), Craigavon, UK, June 2018 (3 lectures)
- BioCat Annual Conference, Oslo, NOR, June 2018
- 9th International Congress on Biocatalysis, Hamburg, DE, August 2018
- Novel Enzymes Conference, Darmstadt, DE, October 2018
- Aachen-Osaka Symposium SeleCa, Aachen, DE, November 2018

Rehosek, M.

- M. Rehosek, A. Jeganathan, and F. Marlow, DPG2018, March 2018

Ritter, T.

- 9th Munster Symposium on Cooperative Effects in Chemistry, Münster, DE, March 2018
- Klinikum rechts der Isar, München, DE, April 2018
- ICBMS, University of Lyon, Lyon, FR, April 2018
- Talk at TUM, TU München, Garching, DE, June 2018
- 22nd International Symposium on Fluorine Chemistry (ISFC), Oxford, UK, July 2018
- Sir Derek Barton Centenary Celebration, Imperial College, London, UK, September 2018
- University College London, London, UK, October 2018
- Institut Català d'Investigació Química (ICIQ), Tarragona, ES, October 2018
- University of Barcelona, Barcelona, ES, October 2018
- Università degli Studi di Milano, Milan, IT, October 2018
- Sapienza University of Rome, Rome, IT, October 2018

Schmidt, W.

- Fraunhofer-Institut Umsicht, Oberhausen, DE, 28 November 2018
- MPI für Eisenforschung, Düsseldorf, DE, 20 November 2018

Schrader, W.

- Analytica Conference, Munich, DE, April 2018

Schulze, P.

- University of Pavia, Pavia, IT, November 2018

Schüth, F.

- Leibniz-Universität, Hannover, DE, 2018
- Universität Darmstadt, Darmstadt, DE, 2018
- Robert-Bosch-Stiftung, Öhningen, DE, 2018
- Shell, Amsterdam, NL, 2018
- Familienunternehmer, Wuppertal, DE, 2018
- University of Cardiff, Cardiff, UK, 2018
- Max-Planck-Förderstiftung, Munich, DE, 2018
- University of Shanghai, CN, 2018

- EFCATS School on Catalysis, Liblice, CR, 2018
- Max-Planck-Gesellschaft, Berlin, DE, 2018
- ExxonMobil, Machelen, BE, 2018
- Beilstein Organic Chemistry Symposium, Ruedesheim, DE, 2018

Tredwell, M.

- Universität Duisburg Essen, Essen, DE, May 2018
- 22nd International Symposium on Fluorine Chemistry, Oxford, UK, July 2018
- Klinikum rechts der Isar der Technischen Universität München, Munich, DE, August 2018

Tüysüz, H.

- University of Fribourg, Fribourg, CH, April 2018
- Workshop “Interfaces and pores in solids, Mülheim an der Ruhr, DE, July 2018
- XXVII International Materials Research Congress, Cancun, MX, August 2018
- 8th NRW Nano Conference, Dortmund, DE, November 2018
- IMPRS-Recharge Symposium, Mülheim an der Ruhr, DE, November 2018

Weidenthaler, C.

- University of Bremen, Bremen, DE, October 2018
- GDCh Fachgruppentagung Chemie und Energie, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, DE, October 2018
- DESY Hamburg, Hamburg, DE, February 2018

2019

Atanasov, M.

- Computation and Understanding in Quantum Molecular Science, JPM80 Meeting, Toulouse, FR, September 2019
- 7th International Conference on Molecular Magnetism, Florence, IT, September 2019
- MQM Conference 2019, Heidelberg, DE, June/July 2019
- Summerschool on Spectroscopy, Gelsenkirchen, DE, September/ October 2019

Auer, A.

- Workshop of the SPP 1807, Erlangen, DE, February 2019
- Lecture series in two parts: Summerschool of the EPS (European Physical Society) and SIF (Societa Italiana di Fisica), Varenna, lake Como, IT, July 2019
- Small molecule NMR conference "SMASH", Porto, PT, September 2019
- "Molecular theory and spectroscopy in catalysis", 1st French - German joint symposium on materials for catalysis and energy applications, Univ. Paris-Sud, Orsay, FR, November 2019
- Seminar "Ausgewählte Kapitel der Theoretischen Chemie" HHU Düsseldorf, Düsseldorf, DE, November 2019

Bistoni, G.

- 3rd Workshop SPP1807, Erlangen, DE, February 2019
- CECAM workshop, Sorbonne, Paris, FR, August 2019
- Summer School "Spectroscopy and Electronic Structure of Transition Metal complexes"; Gelsenkirchen, DE, September 2019
- 1st International conference on Noncovalent Interactions; Lisbon, PT, September 2019
- HBOND2019 conference; Amsterdam, NL, September 2019

Cornella, J.

- Universität Regensburg, Regensburg, DE, January 2019
- University of Geneva, Geneva, CH, April 2019
- Bergische Universität Wuppertal, Wuppertal, DE, April 2019
- Bürgenstock Conference, Brunnen, CH, May 2019
- University of Munster, Munster, DE, May 2019
- University of Basque Country, Leioa, ES, June 2019
- Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, DE, June 2019
- ESOC-Wien, Vienna, AT, July 2019
- Junge Chemiker Forum (JCF)-Ruhr, Essen, DE, September 2019
- ETHZ, Laboratory for Organic Chemistry, Zurich, CH, November 2019

- NOVARTIS Basel, CH, November 2019
- University of Basel, Basel, CH, November 2019
- EPFL. Lausanne, CH, November 2019
- Philipps University Marburg, DE, November 2019
- ICIQ. Tarragona, ES, November 2019
- UCB Pharma. Brussels, BE, November 2019
- Aulin-Erdtman Young Investigator Symposium (AEYIS 2019), Stockholm, SE, December 2019
- Queen Mary University, London, UK, December 2019

Felderhoff, M.

- Energypolis Seminar, EPFL Sion, CH, January 2019
- IHK Würzburg-Schweinfurt, 3. Energiegipfel, Würzburg, DE, July 2019
- Doktorandentagung GSC ESE TU Darmstadt, Schloß Buchenau, DE, September 2019

Fürstner, A.

- GDCh Lecture, University of Tübingen, Tübingen, DE, January 2019
- 2nd Pharmaron Symposium, Hoddesdon, UK, March 2019
- Minafin R&D Seminar, Lille, FR, May 2019
- Wolf-Prize Symposium, Haifa, IL, May 2019
- Heinrich-Heine-University, JungChemikerForum, Dusseldorf, DE, July 2019
- Patai-Pappoport Lecture, ESOC Conference, Vienna, AT, July 2019
- EFMC / ASMC International Symposium, Athens, GR, September 2019
- DSM, Kaiseraugst, CH, October 2019
- University of Geneva, Geneva, CH, November 2019
- 2nd ACES & GDCh Symposium, Taipei, TW, December 2019

Helmich-Paris, B.

- 9th Molecular Quantum Mechanics, Heidelberg, DE, Juli 2019
- Universität Innsbruck, Innsbruck, AT, September 2019
- 55th Symposium on Theoretical Chemistry, Rostock, DE, September 2019

Izsak, R.

- LCAMS Meeting, Regensburg, DE, June 2019
- MQM Meeting, Heidelberg, DE, June 2019
- New Developments in Coupled-Cluster Theory workshop, Telluride, US, July 2019

Klußmann, M.

- Universität Rostock, DE, March 2019
- KU Leuven, BE, May 2019
- Roskilde Midsummer Seminar, Roskilde Universitet, DK, June 2019
- Northwest Institute of Plateau Biology, Chinese Academy of Sciences, Xining, CN, May 2019
- East China Normal University, Shanghai, CN, May 2019
- Shanghai Institute of Organic Sciences, Chinese Academy of Sciences, Shanghai, CN, May 2019
- Universität Tübingen, Tübingen, DE, November 2019

Lehmann, C. W.

- University Duisburg-Essen, Essen, DE, January 2019
- Fraunhofer IMWS, Halle, DE, June 2019
- BASF SE, Ludwigshafen, DE, October 2019

List, B.

- SCI Young Chemists Panel Organocatalysis meeting, London, UK, February 2019
- UC Irvine lecture, University of California, Irvine, US, February 2019
- ICReDD Intern. Symposium Hokkaido University, JP, March 2019
- LIKAT Rostock, Rostock, DE, April 2019
- 36th Annual Herbert C. Brown Lectures, Purdue University, West Lafayette, US, April 2019
- 5th International Scientific Conference: Advances in Synthesis and Complexing, Moscow, RU, April 2019
- Keynote lecture at 5th International Conference Catalysis in the Fine Chemicals Industry, Lucerne, CH, May 2019
- GDCh-Colloquium, Saarbrücken, DE, July 2019
- ICReDD Intern. Symposium Hokkaido University, JP, August 2019
- GDCh-Wissenschaftsforum Chemie 2019, Aachen, DE, September 2019
- 11th Paul Walden Symposium, Riga, LVA, September 2019
- Junior Scientist Symposium (Bio)-organic Chemistry 2019, University Duisburg-Essen, Essen, DE, September 2019
- University of Chicago, Closs Lecture, Chicago, US, September 2019
- TOCUS, Day of Organic Chemistry, University of Stuttgart, Stuttgart, DE, October 2019
- LMU Munich, JCF, Munich, Munich, DE, October 2019
- Plenary Speaker at XXII SINAQO Argentinean Symposium on Organic Chemistry, Mendoza, ARG, October 2019
- Sichuan University, Sichuan, CN, December 2019
- Nankai University, Nankai, CN, December 2019
- Institute for Molecular Science/National Institutes of Natural Sciences, Okazaki, JP, December 2019

Manganas, D.

- 2nd Scientific Symposium of IMPRS-RECHARGE, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, DE, May 2019
- Local electronic structure and coordination probed by X-ray emission spectroscopy EBS X-ray Emission workshop, ESRF, Grenoble, FR, December 2019
- Spanish National Research Council (CSIC), Madrid, ES, December 2019

Marlow, F.

- COORNET's SPP 1928, DFG-Proposal Review Colloquium, Munich, DE, October 2019

Morandi, B.

- University of Basel, Basel, CH, 2019
- Swiss Snow Symposium, Saas-Fee, CH, 2019
- Princeton University, Princeton, US, 2019
- Janssen, BE, 2019
- Covestro, Leverkusen, DE, 2019
- ICSN, Gif-sur-Yvette, FR, 2019
- DCO Journée de printemps, Paris, FR, 2019
- GDCh Lecture, Darmstadt, DE, 2019
- University of Cambridge, Cambridge, UK, 2019
- Young Faculty Meeting, Bern, CH, 2019
- Boehringer Ingelheim, Biberach, DE, 2019
- Novartis, Basel, CH, 2019
- Idorsia, Allschwil, CH, 2019
- Copenhagen University, DK, 2019
- Roche, CH, 2019
- BASF, Ludwigshafen, DE, 2019
- SIOC, Shanghai, HN, 2019
- Jiao Tong University, Shanghai, CN, 2019
- Fudan University, Yangpu, CN, 2019
- University of Ottawa, Ottawa, CAN, 2019
- INEOS-65, Moskow, RU, 2019
- EPFL, Lausanne, CH, 2019

Nattmann, L.

- ISySyCat, Evora, PT, September 2019

Neese, F.

- 19th “Total Energy” international Workshop at ICTP, Trieste, IT, January 2019
- 5th Virtual Winterschool on Computational Chemistry, organized by The Budapest University of Technology and Economics (BME), Budapest, HN, February 2019
- Gordon Research Conference on Inorganic Reaction Mechanisms, Galveston, US, March 2019
- Warwick University, Coventry, UK, Keynote Speaker, March 2019
- DFG SPP Evaluation 1927/2 – Iron Sulfur for Life, Potsdam, DE, April 2019
- Universität Leipzig, Leipzig, DE, May 2019
- QBIC-V – Quantum BioInorganic Chemistry Conference, Plenary Speaker, Marseille, FR, July 2019
- TSRC Workshop on Biological and Bioinspired Redox Catalysis, Telluride Science Research Center, Telluride, US, July 2019
- TSRC Workshop New Development in Coupled-Cluster Theory, Telluride Science Research Center, Telluride, US, July 2019
- 19th International Conference on Biological Inorganic Chemistry (ICBIC-19), Interlaken, CH, August 2019
- Computation and understanding in quantum Molecular Science- in honour of Jean-Paul Malrieu, Toulouse, FR, September 2019
- 7th European Conference on Molecular Magnetism (ECMM2019), Palermo, IT, September 2019
- European Summer School in Quantum Chemistry 2019 (ESQC 2019), Sicily, IT, September 2019
- SPP2102 Workshop “Theoretical Methods for Transition Metal Compounds”, HHU Düsseldorf, Dusseldorf, DE, October 2019
- Johannes-Gutenberg-Universität, Mainz, DE, November 2019
- 8th BRNO EFEPR School, Brno, CZ, November 2019

Pantazis, D.

- 3rd International Solar Fuels Conference (ISF-3) & International Conference on Artificial Photosynthesis (ICARP-2019), Hiroshima, JP, 2019
- 8th Workshop on Current trends in Molecular and Nanoscale Magnetism (CTMNM), Rhodes, GR, 2019
- Max-Planck-Institute Seminar, Mülheim an der Ruhr, DE, 2019
- Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, CZ, 2019
- Catalysis Towards Greener Chemistry (2nd IMPRS RECHARGE Symposium), Mülheim an der Ruhr, DE, 2019
- CEA-Cadarache, Saint-Paul-lez-Durance, FR, 2019
- Freiburg Inorganic Days Symposium, Freiburg, DE, 2019
- 9th Asian Biological Inorganic Chemistry Conference (AsBIC), Singapore, SG, 2019

Prieto, G.

- 12th Natural Gas Conversion Symposium NGCS-AIChE, San Antonio, US, July 2019
- ASC5. 5th Anatolian School of Catalysis, Izmir, TR, September 2019

Reetz, M. T.

- Schinzer Natural Products Symposium, Magdeburg, DE, March 2019
- Tianjin Institute of Industrial Biotechnology, Tianjin, CN, May 2019
- State Key Laboratory for Biology of Plant Diseases, Beijing, CN, May 2019
- Institute of Chemistry, Graz University, Graz, AT, November 2019
- Protein Engineering Congress EU, Frankfurt, DE, November 2019
- Tianjin Institute of Industrial Biotechnology, Tianjin, CN, November 2019
- Workshop Enzyme Directed Evolution for Advanced Biotechnology, State Key Laboratory of Microbial Metabolism, Jiao Tong University, Shanghai, CN, November 2019

Ritter, T.

- GDCh Colloquium, Hannover, DE, January 2019
- Bristol-Myers Squibb, New Brunswick, US, March 2019
- Princeton Student Invited Lecture Series, Princeton University, Princeton, US, March 2019
- GlaxoSmithKline, Collegeville, US, March 2019
- Merck, Kenilworth, US, March 2019
- 8th Grubbs Symposium, Southern University of Science and Technology, Shenzhen, CN, March 2019
- Organic Chemistry Colloquium, ETH Zürich, Zürich, CH, April 2019
- Roche, Basel, CH, April 2019
- 17th Rencontres de Chimie Organique (RCO), Gif-sur-Yvette, FR, April 2019
- 54th SCS Conference on Stereochemistry, Bürgenstock Conference, Brunnen, CH, May 2019
- Chem East Organic Symposium, University of East Anglia, Norwich, UK, May 2019
- GDCh Lecture, TU Dortmund, Dortmund, DE, May 2019
- 26th International Symposium on Synthesis in Organic Chemistry, University of Cambridge, Cambridge, UK, July 2019
- Organic Chemistry seminar series, California Institute of Technology, Pasadena, US, August 2019
- 27th International Society of Heterocyclic Chemistry Congress, Kyoto, JP, September 2019
- The Dr. Paul Janssen Invited Lecture series, Janssen Pharmaceutica N.V., Beerse, BE, September 2019
- Novartis Institutes for BioMedical Research, Cambridge, US, October 2019
- Mamma Forum, Klinik für Senologie & Evangelische Kliniken Gelsenkirchen, DE, November 2019
- Centre for Synthesis and Chemical Biology (CSCB) Annual Symposium on Recent Advances in Synthesis and Chemical Biology XVIII, Trinity College Dublin, Dublin, IE, December 2019

Schmidt, W.

- Dalian University of Technology, Dalian, CN, 26 April 2019
- DGK-AK20 Summer School, Mülheim, DE, 22 July 2019
- Dalian University of Technology, Dalian, CN, 23 April 2019
- Dalian University of Technology, Dalian, CN, 22 April 2019
- University of Vienna, AT, 11 April 2019

Schrader, W.

- CERN MS Workshop, University of Wuppertal, Wuppertal, DE, March 2019
- Symposium Chemical Engineering, GDCh Chemietage, Linz, AT, September 2019
- DGMK Symposium Analytic Group, Hamburg, DE, November 2019

Schüth, F.

- Lüscher Symposium, Klosters, CH, February 2019
- CBI Symposium at the University of Erlangen, Erlangen, DE, February 2019
- Spring Conference of the DPG, Rostock, DE, March 2019
- ACS Spring Conference, Orlando, US, March/April 2019
- Evonik, Marl, DE, 2019
- Lecture at Secondary School, Mülheim an der Ruhr, DE, 2019
- RWTH, Aachen, DE, 2019
- HTE Conference, Heidelberg, DE, 2019
- International Zeolite Conference, Perth, AU, July 2019
- University of Prague, Prague, CZ, 2019
- SfF Conference, Beijing, PRC, August 2019

Tüysüz, H.

- 31st German Zeolith Conference, Dresden, DE, March 2019
- Materials Chemistry Symposium, UC Berkeley, Berkeley, US, June 2019
- DGK-AK20 Summer School, Mülheim an der Ruhr, DE, July 2019
- Utrecht University, Utrecht, NL, January 2019
- GDCh Lecture University of Paderborn, Paderborn, DE, April 2019
- RWTH, Aachen, DE, May 2019
- TU Kaiserslautern, Kaiserslautern, DE, July 2019

Weidenthaler, C.

- Young Crystallographers Meeting University Cologne, Cologne, DE, September 2019
- European Crystallographic Meeting Vienna, Vienna, AT, August 2019
- Gordon conference on hydrogen metal systems, Castelldefels, ES, July 2019
- University Vienna, Vienne, AT, April 2019
- MATRAC School “Application of Neutrons and Synchrotron Radiation in Materials Science”, Herrsching (Ammersee), Ammersee, DE, April 2019
- European Young Chemists’ Meeting (JCF Bremen) University of Bremen, Bremen, DE, March 2019
- DESY Hamburg, Hamburg, DE, January 2019

9.2 Scientific Honors, Name Lectureships, Awards

Anderl, F., Biberger, T., Caló F., Heinrich, M., Herlé, B., Hillenbrand, J., Löffler, L., Peil, S.

- Merck 350 Compound Challenge Winner

Bistoni, G.

- Habilitation (associate professor) from Italy, since 2018

Börgel, J.

- Reaxys PhD Prize Finalist, 2019

Cornella, J.

- Thieme Chemistry Journals Award, 2018
- ERC Starting Grant (European Research Council), 2019
- MS-CEC Young Researcher Award, 2019
- Junior Scientist Program Fellowship (JSP - Bürgenstock), 2019

Fang, X.

- Thousand Talents Program, 2017

Fürstner, A.

- Bohlmann Lecture, Berlin, DE, 2017
- Xingda Lecture, Peking, CN, 2017
- Givaudan-Karrer Lecture, Zurich, CH, 2018
- Ernest E. Campaigne Lecture, Bloomington, IL, US, 2018
- Georg Büchi Lecture, Cambridge, US, 2018
- Novartis Lecture, Urbana, US, 2018
- Patai-Rappoport Lecture, Vienna, AT, 2019
- Prix Mondial Nessim Habif, Geneva, CH, 2019

Gatzenmeier, T.

- Selected Participant of the 134th BASF International Summer Course, DE, 2017
- European Young Chemist Award Gold Medal on PhD level (EuChemS, SCI), Liverpool, UK, 2018

- Alfred Bader Award for Student Innovation 1st Prize (MilliporeSigma), DE, 2018
- Lecture Award JCS Ruhr (Evonik), DE, 2018

Klußmann, M.

- Award by Angewandte Chemie for frequent and competent reviews in 2016, 2017
- Award by Angewandte Chemie for frequent and competent reviews in 2017, 2018
- Award by Angewandte Chemie for frequent and competent reviews in 2018, 2019

Lee, Y.-H.

- Reaxys Prize Finalist, 2019

Lian, Z.

- Thousand Talents Program, 2018

List, B.

- Ta-shue Chou Lectureship, TW, 2017
- Prof. U. R. Ghatak Endowment Lecture, Kolkata, IN, 2017
- Member of the German National Academy of Science Leopoldina, DE, 2018
- Herbert C. Brown Lecture, Purdue University, Indiana, US, 2019
- Closs Lecture, University of Chicago, Chicago, US, 2019
- Nankai Organic Lectureship, Nankai University, Nankai, CN, 2019

Liu, L.

- CGCA Young Researchers Award (First Class), DE, 2017
- Turck-Prize, DE, 2017

Morandi, B.

- ADUC Prize from the German Chemical Society, DE, 2017
- Hoechst Dozentenpreis der Aventis Foundation from the Fonds der chemischen Industrie, DE, 2017
- ERC Starting Grant, 2017
- Phamaron Lecturer, University of Toronto, US, 2017
- Akademiepreis für Chemie from the Akademie der Wissenschaften zu Göttingen, Göttingen, DE, 2017
- Novartis Early Career Award in Organic Chemistry, 2017
- Carl-Duisberg-Gedächtnispreis from the German Chemical Society, DE, 2018
- Harlan L. and Margaret L. Goering Visiting Professorship from the University of Wisconsin Madison, Madison, US, 2018 (*declined*)

Neese, F.

- Ceremonial Lecturer on the Occasion of “The 2017 Golden Symposium of the Lise-Meitner-Center for Computational Quantum Chemistry”, Jerusalem, ISR, 2017
- Award Lecturer, William B. Tolman Award Symposium, 253rd ACS National Meeting and Exposition, San Francisco, US, 2017
- Ceremonial Lecturer on the Occasion of the 150th Anniversary of the Gesellschaft Deutscher Chemiker (GDCh) and the 125th Anniversary of the Journal, DE, 2017
- Löwdin Lectureship, Quantum Theory Project, University of Florida, Gainesville, US, 2017
- Johnston Lectureship in Honor of Harold Johnston, Emory University, Atlanta, US, 2017
- The 27th Rudolf Brdička Memorial Lecturer at the J. Heyrovsky Institute of Physical Chemistry, Prague, CZ, 2017
- Ceremonial Lecturer on the Occasion of the 10th Anniversary of UniCat and BIG-NSE, Berlin, DE, 2017
- The Harry Emmett Gunning Lecture Series, University of Alberta, Edmonton, CA, 2018
- Admission into the Academia Europaea, Chemistry Section, 2018
- The Harry Emmett Gunning Lecture Series, University of Alberta, Edmonton, CA, 2018

O’Neill, M. J.

- Fulbright Scholarship, 2017

Peil, S.

- Wiley Poster Award, 20th OMCOS Symposium, Heidelberg, DE, 2019

Planas, O.

- Alexander von Humboldt Postdoctoral Fellowship, 2018
- Ramon Areces Postdoctoral Fellowship, 2018 (declined)
- Marie Skłodowska Curie Postdoctoral Fellowship, 2019
- Runner-up Poster Prize MS-CEC Symposium, University of Münster, Münster, DE, 2019

LeVaillant, F.

- Swiss National Foundation-Early Postdoc Mobility, CH, 2019

Pang, Y.

- China Scholarship Council PhD Fellowship, CN, 2018

Properzi, R.

- Springer Chemistry Poster Prize, OMCOS 20 (20th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis), Heidelberg, DE, 2019

Reetz, M. T.

- BioTrans Senior Award, 2017
- BioCat Award for Lifetime Achievements in Biocatalysis, 2018
- Distinguished Scientist of the Chinese Academy of Sciences, CN, 2018
- Honorary Director of Protein Engineering Department of the Tianjin Institute of Industrial Biotechnology, CN, 2019

Ritter, T.

- The 75th Yangtze Academic Forum, Wuhan University, Wuhan, CN, 2018
- Chinese Chemical Society Award in Fluorine Chemistry, Shanghai, CN, 2018
- Susan P. & Barry M. Trost Lectureship, University of Pennsylvania, Philadelphia, US, 2018

Schmidt, W.

- Hai Tian Lecturer, Dalian University of Technology, CN, 2019

Schrader, W.

- Chairman GDCh Division „Chemistry and Energy“, since 2018

Schreyer, L.

- Ernst Haage-Prize, DE, 2018
- Otto-Hahn-Medal, DE, 2019

Stoychev, G.

- Turck-Prize, DE, 2018

Thiel, W.

- Kolos Medaille, Polnische Chemische Gesellschaft, PL, 2017
- Almlöf-Gropen Lectures, NO, 2018

Tredwell, M.

- Thieme Chemistry Journals Award, 2018

Tüysüz, H.

- Chemistry of Materials Reviewer Award, 2017
- Volkswagen Foundation Award for Funding Initiative "Life?", 2019
- Dechema Prize, 2019

Turberg, M.

- Thieme Chemistry Poster Prize, OMCOS 20 (20th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis), Heidelberg, DE, 2019

Vetere, A.

- Wolfgang-Paul-Prize of the Deutsche Gesellschaft für Massenspektrometrie, Saarbrücken, DE, 2018

9.3 Further Activities of Members of the Institute

Auer, A.

- Scientific Coordination of the MAXNET Energy Initiative of the Max-Planck-Society, since 2013
- Financial Auditor of the Arbeitsgemeinschaft Theoretische Chemie (AGTC), DE, since 2018
- Chair of the GDCh Ortsverband Ruhr at the MPI for Chemical Energy Conversion and MPI für Kohlenforschung, DE, 2016-2019

Farès, C.

- Chemistry Show for Kindergarten Arche, Mülheim an der Ruhr, DE, June 2017
- NMR Experimental Project with Pupils from Luisenschule, Mülheim an der Ruhr, DE, June 2019

Fürstner, A.

- Chief-editor of “Science of Synthesis“, since 2017
- Chairman, Editorial Board “Angewandte Chemie” (2014-2018)
- Senior Editor "Bulletin of the Chemical Society of Japan" (BCSJ), since 2014
- Alexander-von-Humboldt Professorship Selection Committee

Klußmann, M.

- Organization of the Carnival Conference Session, University of Cologne, DE, February 2017
- Organization of the Carnival Conference Session, University of Cologne, DE, February 2018
- Organization of the Carnival Conference Session, University of Cologne, DE, February 2019

List, B.

- Member of the Institute for Molecular Science, Okazaki, JP, 2017
- Editor in Chief of Synlett (Thieme), since 2015
- Advanced Synthesis and Catalysis Academic Advisory Board, since 2011
- Nature Communications Editorial Advisory Panel, since 2010
- Editorial Advisory Board, Beilstein Journal of Organic Chemistry, since 2008
- Co-Editor of Synfacts (Thieme), since 2005

Neese, F.

- Scientific Chair of 9th Molecular Quantum Mechanics Conference (MQM19), Heidelberg, DE, June/July 2019
- Member of the Editorial Board of the review book series “Structure and Bonding”, since 2016
- Associate Editor Inorg. Chem., since 2015
- Advisory Board of Journal of Chemical Theory and Computation, since 2012

Pantazis, D. A.

- Scientific Chair of the 5th Quantum Bio-Inorganic Chemistry Conference (QBIC-V), Marseille, FR, July 2019

Prieto, G.

- Organization of the Meeting of the Spanish Catalysis Society (SECAT'17) Oviedo, ES June 2017
- Scientific Committee of the XVI Young Researchers Symposium of the Spanish Chemistry Society RSEQ-SIGMA ALDRICH, Valencia, ES, September 2019

Reetz, M. T.

- Inauguration of the “Reetz Laboratory” at the Tianjin Institute of Industrial Biotechnology, Tianjin, CN, November 2019

Ritter, T.

- C&EN webinar “Overcoming Synthetic Challenges through Recent Advances and Practical Approaches to Fluorination Chemistry”, US, October 2019
- Associate Editor “Organic Letters”, ACS, since 2018
- Chem Advisory Board, since 2016
- ACS Central Science Advisory Board, since 2016

Schrader, W.

- Organization of the 2nd Annual Meeting of the GDCh Division “Chemistry and Energy”, Mülheim an der Ruhr, DE, October 2018
- Organization of the Division Meeting 2019 of the GDCh Division “Chemistry and Energy” during the GDCh Wissenschaftsforum, Aachen, DE, September 2019

Schüth, F.

- Experimental Open Air Show, Mülheim an der Ruhr, DE, June 2019
- Easter Academy at a Local Secondary School, Mülheim an der Ruhr, DE
- Various Lectures at Primary and Secondary Schools, DE 2017-2019
- Junior University at the Institute, Mülheim an der Ruhr, DE, 2019

- Member of the Editorial Board “Sustainable Chemistry and Pharmacy”, since 2017
- Member of the Editorial Board “Advances in Catalysis”, since 2007
- Member of the Advisory Board “Chemistry-An Asian Journal”, since 2006
- Editor of “Chemistry of Materials”, since 2006
- Member of the Editorial Advisory Board “Chemical Engineering & Technology”, since 2005
- Member of the Editorial Board QSAR-Combinatorial Science, since 2003
- Member of the Editorial Board „Microporous and Mesoporous Materials“, since 1996
- Member of the Editorial Board „Advanced Materials“, since 1996

9.4 Courses Taught at Universities

All research group leaders are associated with a university at which the doctoral students receive their degrees. The group leaders as well as a few members of the Institute teach at universities. Official cooperations are established with the Ruhr University Bochum, the Louis Pasteur University de Strasbourg, and with the RWTH Aachen University. During the period of 2017-2019, the following lectures/workshops were taught.

Anderl, F.

- CaRLa Winter School, Heidelberg, DE, February 2018

Auer, A.

- Spektroskopie und Struktur, TU Chemnitz (Honorarprofessur), DE, SS 2017
- Accuracy in Electronic Structure Models and Introduction to Band Structure Theory - A Chemists View, IMPRS "Recharge" graduate school lectures on "Electron Correlation, 2017
- Spektroskopie und Struktur, TU Chemnitz (Honorarprofessur), DE, SS 2018
- Accuracy in Electronic Structure Models and Introduction to Band Structure Theory - A Chemists View, IMPRS "Recharge" graduate school lectures on "Electron Correlation, 2018
- Spektroskopie und Struktur, TU Chemnitz (Honorarprofessur), DE, SS 2019
- Accuracy in Electronic Structure Models and Introduction to Band Structure Theory - A Chemists View, IMPRS "Recharge" graduate school lectures on "Electron Correlation, 2019
- Kooperation Prof. S. Schulz, Zweitgutachter Promotion L. John und K. Dzialkowski, University Duisburg/Essen, DE

Fürstner, A.

- Givaudan-Karrer Guest Professorship, University of Zurich, CH, March 2018

Heinrich, M.

- BASF Summer School, Ludwigshafen, DE, August 2017

Helmich-Paris, B.

- Trial Lecture, TU Darmstadt, DE, March 2018
- Trial Lecture, University of Bremen, DE, July 2018

Klußmann, M.

- Kinetics and Mechanisms in Organocatalysis, Summer School "Advanced Organocatalysis" (ADVOCAT) of the University of Cologne, Bergisch-Gladbach, DE, August 2018
- „Calorimetry and Kinetics“, University of Cologne, DE, November 2019

Lehmann, C. W.

- Characterization of Materials and Surfaces, University of Wuppertal, DE, WS 2016/2017
- Inorganic Materials, University of Wuppertal, DE, SS 2017
- Characterization of Materials and Surfaces, University of Wuppertal, DE, WS 2017/2018
- Inorganic Materials, University of Wuppertal, DE, SS 2018
- Characterization of Materials and Surfaces, University of Wuppertal, DE, WS 2018/2019
- Synthesis and Characterization Methods for Solid Materials, University of Wuppertal, DE, SS 2019
- Advanced Spectroscopic Methods, University of Wuppertal, DE, WS 2019/2020

List, B.

- Asymmetric Organocatalysis, University of Cologne, DE, January 2019
- 28. Nachwuchswissenschaftler-Symposium Bioorganische Chemie, University Duisburg-Essen, DE, September 2019

Marlow, F.

- Photonik II, University Duisburg/Essen, DE, SS 2017
- Projektpraktikum Photonik, University Duisburg/Essen, DE, SS 2017
- Photonik I, University Duisburg/Essen, DE, WS 2017/2018
- Projektpraktikum Photonik, University Duisburg/Essen, DE, WS 2017/2018
- Photonik I, University Duisburg/Essen, DE, SS 2018
- Projektpraktikum Photonik, University Duisburg/Essen, DE, SS 2018
- Optical Properties of Solids, IMPRS SurMat T4-course, October 2018
- Analysis of Solids, IMPRS SurMat T4-course, October 2018
- Photonic Crystals, IMPRS SurMat T4-course, October 2018
- Photonik II, University Duisburg/Essen, DE, WS 2018/2019
- Projektpraktikum Photonik, University Duisburg/Essen, DE, WS 2018/2019
- Projektpraktikum Photonik, University Duisburg/Essen, DE, SS 2019
- Photonik I, University Duisburg/Essen, DE, WS 2019/2020
- Projektpraktikum Photonik, University Duisburg/Essen, DE, WS 2019/2020

Morandi, B.

- Modern Organotransition Metal Catalysis, Ruhr University Bochum, DE, SS 2017

Prieto, G.

- Introduction to General Chemistry, Ruhr University Bochum, DE, WS 2016/2017
- Advanced Chemical Reactor Design, University of Oviedo, ES, WS 2016/2017
- Introduction to General Chemistry, Ruhr University Bochum, DE, WS 2017/2018
- Advanced Chemical Reactor Design, University of Oviedo, ES, WS 2017/2018
- Advanced Chemical Reactor Design, University of Oviedo, ES, WS 2018/2019

Ritter, T.

- Catalysis for Modern Organic Synthesis, RWTH Aachen, DE, SS 2017
- Catalysis for Modern Organic Synthesis, RWTH Aachen, DE, SS 2018
- Catalysis for Modern Organic Synthesis, RWTH Aachen, DE, SS 2019

Rosca, D.-A.

- CaRLa Winter School, Heidelberg, DE, February 2017

Schmidt, W.

- Diffraction, Sorption, and Small Angle X-ray Scattering. Lectures for students in the training program of the IMPRS RECHARGE (Ruhr University Bochum, MPI CEC Mülheim, MPI KOFO Mülheim, MPI Düsseldorf, University of Bonn, University of Duisburg-Essen), WS 2019
- The structure of solids. Lectures for students in the training program of the IMPRS SurMat (Ruhr University Bochum, MPI KOFO Mülheim, and MPI Eisenforschung Düsseldorf), SS 2018
- Analysis of porous solids. Lectures for students in the training program of the IMPRS SurMat (Ruhr University Bochum, MPI KOFO Mülheim, and MPI für Eisenforschung Düsseldorf), SS 2018
- Basics of porosity determination and related methods. Lectures for students at the MPI für Kohlenforschung. WS 2017
- Characterization of Solid Catalysts. Guest Professorship, Shandong University, Jinan, CN, WS 2017

Schrader, W.

- Laboratory course (Fachpraktikum) Analytical Chemistry, University Duisburg/Essen, DE, 2017
- Laboratory course (Fachpraktikum) Research practical, University Duisburg/Essen, DE, 2017
- Advanced Mass Spectrometry, University Duisburg/Essen, DE, SS 2017
- Laboratory course (Fachpraktikum) Analytical Chemistry, University Duisburg/Essen, DE, 2018
- Laboratory course (Fachpraktikum) Research practical, University Duisburg/Essen, DE, 2018
- Advanced Mass Spectrometry, University Duisburg/Essen, DE, SS 2018
- Laboratory course (Fachpraktikum) Analytical Chemistry, University Duisburg/Essen, DE, 2019
- Laboratory course (Fachpraktikum) Research practical, University Duisburg/Essen, DE, 2019
- Advanced Mass Spectrometry, University Duisburg/Essen, DE, SS 2019

Schulze, P.

- General chemistry, University of Wuppertal, DE, WS 2019/2020

Schüth, F.

- Chemistry for engineers, Ruhr University Bochum, DE, WS 2019/2020
- Chemistry of Materials, Ruhr University Bochum, DE, WS 2019/2020

Theysen, N.

- Ruhr-Lehrverbund Katalyse, Ruhr University Bochum, DE, 2018

Tüysüz, H.

- Inorganic Chemistry III, Ruhr University Bochum, DE, WS 2016/2017
- Gen. Chemistry for Engineering Departments, Ruhr University Bochum, DE, WS 2018/2019
- Ruhr Catalysis Lecture Series, Ruhr University Bochum, DE, WS 2018/2019
- Gen. Chemistry for Engineering Departments, Ruhr University Bochum, DE, WS 2019/2020
- WDKL Catalysis Lecture Series, UA Ruhr, WS 2019/2020

Weidenthaler, C.

- Modern Diffraction Methods for Solid-State Analytics, University Duisburg/Essen, DE, WS 2016/2017
- Introduction to Modern Diffraction Techniques, Lectureship Shandong University, Jinan, CN: April 2017
- Inorganic Chemistry (IV), University Duisburg/Essen, DE, SS 2017
- Modern Diffraction Methods for Solid-State Analytics, University Duisburg/Essen, DE, WS 2017/2018
- Methoden der Pulverdiffraktometrie, University of Innsbruck, AT, WS 2017/2018
- Inorganic Chemistry (IV), University Duisburg/Essen, DE, SS 2018
- Introduction to Crystallography and Diffraction Techniques, IMPR SurMat, September 2018
- Modern Diffraction Methods for Solid-State Analytics, University Duisburg/Essen, DE, WS 2018/2019
- Inorganic Chemistry (IV), University Duisburg/Essen, DE, SS 2019
- Modern Diffraction Methods for Solid-State Analytics, University Duisburg/Essen, DE, WS 2019/2020

Van Gastel, M.

- Allgemeine Chemie für Physiker und Nanoengineering, University Duisburg/Essen, DE, in Kollaboration mit Prof. E. Spohr und Prof. S. Schlücker, WS 2017/2018
- PCIII, Kinetik und Elektrochemie, University Duisburg/Essen, DE, in Kollaboration mit Prof. S. Schlücker, SS 2018
- Allgemeine Chemie für Physiker und Nanoengineering, University Duisburg/Essen, DE, in Kollaboration mit Prof. E. Spohr, WS 2018/2019

- PCIII, Kinetik und Elektrochemie, University Duisburg/Essen, DE, in Kollaboration mit Prof. S. Schlücker, SS 2018
- Allgemeine Chemie für Physiker und Nanoengineering, University Duisburg/Essen, DE, in Kollaboration mit Prof. S. Schlücker, WS 2019/2020

9.5 Scientific Talks Given by Guests

2017

- January 10th Alina Arslanova (University of Moscow, RU)
Materials for Fuel Cells: Electrocatalysts and Membranes
- January 10th Dr. Virginie Peneau (University of Ottawa, CA)
Chemistry in Nanocatalysis
- February 21st Dr. Sara Zamanian (University of Teheran, IR)
Catalytic Olefin Activations by Heterogeneous Catalysts
- February 21st Dr. Jordi Burés (The University of Manchester, UK)
Better Understanding for Better Reactions
- March 9th Dr. Yassine Bouhoute (University Lyon, FR)
Well-defined silica-supported tungsten oxo alkyl derivatives as models of WO₃/SiO₂ olefin metathesis catalysts
- March 10th Özgül Agbaba (Aalto University of Espoo, FI)
Microfluidics and Catalysis
- March 10th Hannah Kirsch (Karlsruher Institute for Technology, DE)
Overview of Research Projects – Nanoparticles, Refrigeration and Catalysis
- March 14th Alexander Bodach (University of Frankfurt, DE)
Syntheses and Crystal Structures of Organolithium Compounds
- March 17th Srimanta Manna (Max-Planck Institute for Molecular Physiology Dortmund, DE)
Development of Novel Oxidative Annulation via C–H Bonds Functionalization in the Syntheses of Biologically Relevant Compounds
- March 20th Prof. Dr. Ronny Neumann (Weizmann Institute for Science Tel Aviv, IL)
Polyoxometalates – Towards Sustainable Catalysis and Transformations in Dense Phases

- March 22nd Dr. Mathias Fischer (University Bonn, DE)
Applying XRD and XAFS to nanoparticle samples
- March 27th Olena Vozniuk (University of Bologna, IT)
Chemical-loop approach in bio-alcohols reforming
- March 28th Jochen Ortmeier (University of Paderborn, DE)
Bioinspired Coordination Chemistry with Phenanthroline Guanidine, Camphor-like Guanidine and Imidazolium Dithiocarboxylate Ligands
- April 25th Prof. Dr. László Kürti (Rice University Houston, US)
Practical Direct Electrophilic Amination of Olefins and Aromatic Systems
- April 28th Prof. Dr. Ben Feringa (University of Groningen, NL)
Dynamic Molecular System
- May 4th Volker Berg and Michael Engels (The Boston Consulting Group)
Consulting – Career Opportunities for Chemists
- May 11th Prof. Dr. Bernhard Breit (University Freiburg, DE)
Rhodium-Catalyzed Addition of Pronucleophiles to Alkynes & Allenes: An Atom-Economic Alternative to the Tsuji-Trost Reaction
- May 15th Felix vom Bruch (University Aachen, DE)
Phase Change Materials – Fabrication and characterization of metastable cubic Sb₂Te₃
- May 15th Dr. Michael Hirscher (MPI for Intelligent Systems Stuttgart, DE)
Separation of hydrogen isotopes in porous materials
- May 26th Tristan Delcaillau (Actelion Basel, CH)
Palladium-Catalyzed Direct C–H Arylation of heterocycles and total synthesis of a terpene
- June 6th Prof. Dr. Jorge Gascon (University of Delft, NL)
Towards new concepts in the design of heterogeneous catalysts
- June 6th Prof. Dr. Patrick Holland (University of Yale, US)
GDCh-Lecture: *Breaking N–N, C–N, and C–H Bonds with Low-Coordinate Metal Complexes*

- June 13th Simone Gallus (RWTH Aachen, DE)
Materials inspired by nature: synthesis and characterisation of the perryite-related compounds Ni_{8-x}Fe_xSi₃ with 0 ≤ x ≤ 8
- June 14th Prof. Dr. Paula Diaconescu (University of California Los Angeles, US)
Redox switchable catalysis
- June 14th Dr. Carla Obradors (The Scripps Research Institute La Jolla, US)
Transition-Metal Catalysis: Mechanistic Studies for More Efficient Designs. Application into Total Synthesis
- June 19th Prof. Dr. Rong-Zhen Liao (University of Science and Technology Huazhong, CN)
Quantum chemical modeling of homogeneous water oxidation catalysis
- June 19th Prof. Tomislav Rovis (Columbia University New York, US)
Controlling Catalysis with Visible Light
- June 28th Prof. Dr. Robert Knowles (Princeton University, US)
Proton-coupled electron transfer in organic synthesis
- July 4th Jeffrey Bruffaerts (Technion – Israel Institute of Technology Haifa, IL)
Promoting the Remote functionalization of Alkenes as a Powerful Synthetic Tool
- July 5th Prof. Dr. Amir H. Hoveyda (Boston College, US)
Increasing Challenges in Catalytic Chemistry: Implications Regarding the Future
- July 6th Prof. Dr. Amir H. Hoveyda (Boston College, US)
Sulfonate-Containing NHC Ligands for Enantioselective Catalysis
- July 7th Prof. Dr. Amir H. Hoveyda (Boston College, US)
Small-Molecule Organoboron Catalysts for Enantioselective Synthesis
- July 19th David Dailler (University of Basel, CH)
Developments and applications of the C(sp³)-H functionalization
- July 25th Prof. Dr. Connie Lu (Max-Planck-Institute for Coal Research Mülheim, DE)
Bio-inspired bimetallic complexes for activating H₂ and CO₂

- September 1st Dr. Ben Sherry (Merck, US)
Development of Efficient Processes to Nitrogen Heterocycles
- September 4th Yan Xiong (Max-Planck-Institute for Coal Research Mülheim, DE)
Nano-sized BaTiO₃ and TiO₂ in Photochemical Energy Conversion Systems
- September 6th Christian Fischer (Merck Boston, US)
Working at Merck
- September 13th Prof. Dr. Robert Grubbs (California Institute of Technology Pasadena, US)
Synthesis of large and small molecules using olefin metathesis
- September 14th Prof. Dr. Rolf Breinbauer (TU Graz, AT)
Insanity in Science
- September 19th Dr. Changlong Wang (University of Toulouse, FR)
Design of efficient transition metal-based nanocatalysts in aqueous solution
- September 21st Prof. Dr. Kuiling Ding (Shanghai Institute of Organic Chemistry, CN)
A Story of SKP/Pd Catalyst: Mechanistic Understanding, Process Innovation & Drug Discovery
- September 28th Prof. Dr. Takuya Hashimoto (Kyoto University, JP)
Pursuit of New Catalyst Designs
- September 29th Dr. Christoph Roosen (SABIC Geleen, NL)
Introduction to Steam Cracking
- October 9th Prof. Dr. Felix Studt (Karlsruhe Institute of Technology, DE)
From fundamental understanding to catalyst design: Hydrogenation of CO and CO₂ to methanol and Beyond
- October 11th Prof. Dr. Tomoki Ogoshi (Kanazawa University, JP)
*Synthesis of Pillar-Shaped Macrocyclic Compounds 'Pillar[n]arenes'
Providing Supramolecular Assemblies*
- October 18th Diane Bécart (Université de Bordeaux, FR)
Bioinspired Catalysis Using Oligourea Helical Foldamers

- October 18th Prof. Dr. Martin Head-Gordon (UC Berkeley, US)
Modeling electrocatalytic reduction of carbon dioxide on copper electrodes
- October 26th Muammer Yusuf Yaman (Bilkent University, TR)
The synthesis of a photo-anode electrode for quantum dot sensitized solar cells with a new approach
- November 7th Prof. Dr. Gaunt (Department of Chemistry University of Cambridge, UK)
New strategies for chemical synthesis – from C–H activation to protein functionalization
- November 16th Dr. Joanna Jankowska (University of Southern California, US)
Local electric field slows down photogenerated charge recombination in hybrid perovskites: non-adiabatic molecular dynamics exploration of the photovoltaics 'dream-material' secrets
- November 21st Dr. Bernd Schmidt (Humboldt-Universität Berlin, DE)
Crystalline Sponge & Beyond
- November 22nd Dr. Ryan Wang (UCL London, UK)
Controlled engineering of nanostructures for applications in catalysis and beyond
- November 22nd Dr. Jimmy Faria (Twente University, NL)
Catalytic Strategies for Biomass Conversion into Chemical Platforms
- November 28th Prof. Dr. Ruben Martin (ICIQ Tarragona, ES)
Turning simplicity into complexity via Nicatalyzed cross-coupling reactions
- December 4th Prof. Dr. Benoit Louis (University of Strasburg, FR)
Biomass-assisted zeolite synthesis: from a real mess... to rationalized acid catalysis
- December 4th Dr. Amol Amrute (ETH Zürich, CH)
Catalyst design for halogen recycling in polymer manufacture and light alkane upgrading
- December 7th Prof. Dr. Klaus Roth (FU Berlin, DE)
The Chemical Secret of Christmas Scent

2018

- January 12th Prof. Dr. Thomas Riedl (University Wuppertal, DE)
Organic and Perovskite Lasers
- January 15th Prof. Dr. Debabrata Maiti (Indian Institute of Technology-Bombay, IN)
Designing of templates to reach the distal C–H bond
- January 18th Clara Eisebraun (TU Munich, DE)
Investigation of Copper Aluminate Hydrogenation Catalysts with Respect to Reaction Mechanism
- January 26th Prof. Dr. An-hui Lu (Dalian University, CN)
From precise materials synthesis to designed adsorbents and catalysts
- January 29th Marco Zuccarello, (University of Basel, CH)
New approaches to catalytic CH activation
- February 5th Maximilian Stangier (WWU Münster, DE)
New approaches regarding efficient photon upconversion processes in water and macrolactonization reactions under low dilution conditions
- February 6th Tim Görlich (University of Würzburg, DE)
Steps towards cationic Rhodacyclopentadienes
- February 6th Prof. Dr. M. Hassan Beyzavi (University of Arkansas, US)
Molecularly Tunable Porous Materials
- February 6th Dr. Monica Pérez Temprano (ICIQ Tarragona, ES)
Trapping Reaction Intermediates: Knowledge Building Blocks for Rational Design
- February 6th Prof. Dr. Christian Ochsenfeld (Ludwig-Maximilians-Universität Munich, DE)
GDCh-Lecture: *Schrödinger's World: From Quantum-Chemical Method Development to Understanding DNA Repair*
- February 9th Michael Buchsteiner (TU Graz, AT)
Biomimetic models for acetylene hydratase: alkyne activation on tungsten centers

- February 12th Dr. Tamal Ghosh (ICIQ Tarragona, ES)
From Photoredox Catalysis to Enantioselective Photo-Organocatalysis in Organic Synthesis
- February 12th Prof. Dr. Matteo Maestri (Polytechnic University of Milan, IT)
Escaping the trap of complication and complexity in multiscale microkinetic modelling of heterogeneous catalytic processes
- February 26th Ana Morais (NOVA Universität Lissabon, PT)
Overview of high-pressure technologies for lignocellulosic biomass conversion
- March 7th Prof. Dr. Joshua Telser (Roosevelt University Chicago, US)
Electronic structure, EPR-Spectroscopy and Catalytic Activity of Transition Metal Ketimide Complexes
- March 7th Davide Spinnato (University of Milan, IT)
DFT study on CO₂ activation and New developments in Lewis-base catalyzed reactions
- March 13th Jessica Gonzalez (FH Münster, DE)
Inorganic phosphors for PC-leds
- March 13th Dr. Nico Fischer (University of Cape Town, ZA)
Operando XRD and magnetic methods in catalysis research
- March 19th Joo Hyunho (Tokyo, JP)
Molecular Design for New Nanoarchitectures Construction and Apply to Water Splitting Photocatalyst
- April 3rd Verena Perner (TU Graz, AT)
Synthesis of CuInS₂ nanocrystals and their application in solar cells
- April 6th Yitao Dai (Aarhus University, DK)
Mechanistic Exploration and Rational Design in Heterogeneous Photocatalysis
- April 11th Stephan Hess (LMU Munich, DE)
Untersuchung der Palladium-katalysierten asymmetrischen Allylierung verschiedener stickstoffhaltiger Heterozyklen
- April 13th Dr. Gunnar Werncke (University of Marburg, DE)
Bond and Element Activation by Two-Coordinate 3d-Metal(I) Complexes

- April 17th Prof. Dr. Tristan Lambert (Columbia University New York, US)
Catalyst Design with Aromatic Ions
- April 18th Prof. Dr. Zhenggang Lan (Chinese Academy of Sciences Qingdao, CN)
Theoretical description of nonadiabatic dynamics
- April 30th Gereon Behrendt (University of Rostock, DE)
From Theatre Effects to Research in Solid State Chemistry and Catalysis
- May 2nd Joyce Grimm (University of Hamburg, DE)
Towards the validation of stereochemical assignment in polyketide natural products
- May 8th Prof. Dr. Guy Lloyd-Jones (University of Edinburgh, UK)
An in situ Journey from Reactants to (side)Products
- May 11th Prof. Dr. Gopalan Rajaraman (IIT Bombay, IN)
Synergy Between Experiment and Theory: Examples from Lanthanide Based Molecular Magnets and Metal Mediated Catalytic Reactions
- May 18th Martin Scott (RWTH Aachen, DE)
From Lewis Acids to Multi-Phasic Catalysis
- May 23rd Gabriela Gerosa (Instituto de Química Rosario, AR)
Development and application of chiral organocatalysts derived from biomass
- May 24th Dr. Dr. Tom Sheppard (University College London, UK)
Dehydration Reactions for Sustainable Synthesis
- May 29th Dr. Juan Miguel López del Amo (CIC energigune Villodas, ES)
Solid-state NMR studies of the structure and dynamics of polymers, ceramics, porous solids, paramagnetic materials, metals, alloys and organometallic compounds
- June 1st Lucie Finck (School of Chemistry of Montpellier, FR)
Micelles-Enabled Photo-Assisted Selective Oxyhalogenation of Alkynes in Water Under Mild Conditions
- June 7th Prof. Dr. Petra de Jongh (Utrecht University, NL)
Supported Ag and Aucatalysts – take care of the support

- June 11th Gereon Behrendt (University of Rostock, DE)
From Theatre Effects to Research in Solid State Chemistry and Catalysis
- June 12th Philipp Pracht (University of Bonn, DE)
Recent Development and Application of the extended Tight-Binding Model
- June 18th Prof. Dr. Noah Z. Burns (Stanford University, US)
Selective Halogenation and the Study of Noncanonical Lipids
- June 19th Philip Boehm (TU Munich, DE)
Synergistic Iridium and Copper Catalysis for Stereodivergent Allylic Substitution & Copper-mediated Fluorination of Arylsilanes
- June 27th Prof. Dr. Petra de Jongh (Utrecht University, NL)
Light metal hydrides – from hydrogen storage to batteries
- June 28th Prof. Dr. Keary M. Engle (The Scripps Research Institute La Jolla, US)
Catalytic Methods for Selective Functionalization of C–C π -Bonds
- July 5th Prof. Dr. Evelino Colacino (University of Montpellier, FR)
From one Jar / one compound preparation to high throughput parallel mechanochemistry
- July 5th Prof. Dr. Martin Oestreich (TU Berlin, DE)
Wheland Intermediates In Catalysis
- July 9th Jacobo de Bellis (University of Pisa, IT)
Synthesis and post-synthetic modification of a chosen metal-organic framework
- July 12th Dr. Johannes Panten (Symrise AG Holzminden, DE)
History and Recent Developments in Fragrance Chemistry
- July 13th Prof. Dr. Galen Stucky, Prof. Dr. Brad Chmelka, Prof. Dr. Thomas Bein, Dr. Harun Tüysüz, Dr. Karin Möller, Prof. Dr. Peter Behrens, Prof. Dr. Alec Wodtke, Prof. Dr. Ferdi Schüth
Workshops Interfaces and pores in solids
- July 26th Prof. Dr. Graham Hutchings (University of Cardiff, UK)
Catalysis using Nanomaterials

- July 30th Dr. Takashi Niwa (RIKEN Center for Biosystems Dynamics Research Hyogo, JP)
Molecular Renovation Strategy: A Novel Synthetic Methodology for Expeditious Development of Molecular Probes
- August 1st Prof. Dr. Ming-Yu Ngai (State University New York, US)
Development of Novel Chemical Tools for Accessing Unexplored Chemical Spaces
- August 3rd Dr. Alvaro Gutierrez-Bonet (University of Pennsylvania, US)
Nickel/Photoredox Dual Catalysis for the Rapid Construction of Molecular Complexity
- August 8th Manuel Scharf (Stanford University, US)
Zinc-ProPhenol catalyzed asymmetric Mannich-additions
- August 22nd Dr. Quentin Dherbassy (University of Strasbourg, FR)
- August 29th Julia Kopp (University of Freiburg, DE)
Synthesis of Monomeric and Dimeric Naphthoquinonopyrone gamma lactones
- September 3rd Prof. Dr. Frank Glorius (University of Muenster, DE)
On discovery in catalysis
- September 14th Prof. Dr. Robert Schlögl (Max-Planck-Institute for Chemical Energy Conversion Mülheim, DE)
Sonne im Tank – Die Treibstoffe der Zukunft und das Potential synthetischer Kraftstoffe
- September 20th Dr. Suzanne Tobey (Senior Editor at Angewandte Chemie, DE)
The Editorial Office – Demystifying the Black Box
- September 26th Prof. Dr. Pablo Arnal (Centro de Tecnología de Recursos Minerales y Cerámica La Plata, AR)
Simple synthesis of biochar for decontamination of water
- October 9th Prof. Dr. Dean Toste (University of California Berkeley, US)
Organic Chemistry Inspired by the Organometallic Chemistry of Gold
- October 10th Dr. Naoya Kumagai (Institute of Microbial Chemistry Tokyo, JP)
Chemistry Empowered by Unique Heterocycles

- October 16th Prof. Dr. Brad Carrow (University Princeton, US)
Mechanism-driven catalyst design for sustainable chemistry
- October 29th Prof. Dr. Kyoko Nozaki (University of Tokyo, JP)
Coordination copolymerization of propylene with polar monomers
- October 30th Prof. Dr. Kyoko Nozaki (University of Tokyo, JP)
Homogeneous Catalysis toward Utilization of Renewable Resources
- October 31st Prof. Dr. Kyoko Nozaki (University of Tokyo, JP)
Sequential Bond Formation Reactions for the Synthesis of Novel π -conjugated Molecules
- November 12th Dr. Jussara Carneiro (Federal University of São Carlos, BR)
Synergistic catalysts with high selectivity for H₂O₂ electrogeneration
- November 15th Prof. Dr. Siegfried Waldvogel (University of Mainz, DE)
GDCh-Lecture: *Electrifying Organic Synthesis – Disruptive and Innovative*
- November 21st Prof. Dr. Ralf Tonner (University of Marburg, DE)
Concepts for functional materials from computational chemistry
- November 23rd Benjamin Mitschke (University Leipzig, DE)
ortho-Quinone Methide Imines – Templates for the Construction of N-Heterocycles
- November 27th Hilke Petersen (University Bremen, DE)
Synthesis and characterization of new Sodalites, Cancrinites and their intermediate phase
- November 27th Dr. Ahmed Faried Abdel-Hakim Ahmed (Assiut University, EG)
New trends in Chromatographic and Electrophoretic Pharmaceutical Analysis
- November 27th Prof. Dr. Jürgen Caro (University of Hannover, DE)
MOF, COF and 2D nanosheets as smart gas separation membranes
- November 28th Dr. Tynchtyk Amatov (Ludwig-Maximilians-University Munich, DE)
From Amino Acids to Alkaloids via Radicals and RNA-Programmed Peptide Synthesis
- November 28th Erika Michela Dematteis (University of Turin, IT)
Thermodynamics of Boron-Based Complex Hydrides for Energy Storage

- December 5th Dr. Xiao Wang (University of Singapore, SG)
Structuring Core@Shell Material for Catalytic Applications
- December 5th Prof. Dr. Thomas Magauer (University of Innsbruck, AT)
Construction and Deconstruction of Three-Dimensional Molecules
- December 6th Prof. Dr. Stephen Newman (University of Ottawa, CA)
New Pathways for Ni-Catalyzed Coupling Reactions: A High Throughput Approach to Reaction Discovery
- December 7th Prof. Dr. Susannah Scott (University of California Santa Barbara, US)
Looking for active sites in heterogeneous catalysts: Lessons in catalyst design from olefin polymerization and metathesis
- December 11th Kunyuan Xu (University of Utrecht, NL)
Optical spectroscopy of manganese doped perovskite nanocrystals
- December 12th Jürgen Kaube (Editor of the Frankfurter Allgemeine Zeitung, DE)
GDCh-Lecture: *Gesellschaftliche Voraussetzungen für Wissenschaft*
- December 19th Dr. Ali Mansouri (University of Alberta, CA)
Towards Earth-Abundant Metals in Hydrotreating Catalysts; Structure-Controlled Synthesis
- December 19th Joel Britschgi (TU Munich, DE)
A sustainable nitrogen-doped carbon catalyst for the synthesis of 2,5-dimethylfuran

2019

- January 24th Prof. Dr. Eric Meggers (University of Marburg, DE)
New Chemical Space for the Design of Asymmetric Transition Metal Catalysts
- January 29th Prof. Stefanie Dehnen (University of Marburg, DE)
Multinary Clusters: From Exotic Structures to Potential Use
- February 6th Jakob Seibert (University of Bonn, DE)
From circular dichroism for proteins to non-linear optical properties - an update on sTD(A)-xTB
- February 7th Prof. Dr. Cristina Nevado (University of Zurich, CH)
Harvesting Radicals to Functionalize π -Systems
- February 12th Dr. Pengyi Tang (University of Barcelona, ES)
Bottom-up Engineering of Hematite Nanowire Heterostructures for Photoelectrochemical Water Splitting
- February 13th Prof. Dr. Dr. h.c. L. Tietze (University of Göttingen, DE)
Domino Reactions. The Green and Economical Art of Chemical Synthesis
- February 19th Steffen Reichle (University of Tübingen, DE)
Upscaling of UiO-66 synthesis in millistructured reactors
- February 22nd Dr. Deniz Tuna (Stanford University, US)
Excited States, Conical Intersections and Photochemistry: Benchmarks of Quantum-Chemical Methods and Applications to Biomolecules
- February 26th Ma Yangbo (University of Beijing, CN)
Microwave Synthesis, Characterization and Oxygen Reduction Reaction Performance of Platinum Alloy Nano-octahedron
- February 27th Klara Sophia Kley (ETH Zürich, CH)
Mechanism and kinetics of CO₂ hydrogenation to methanol on indium oxide
- February 27th Dr. Tobias Gensch (University of Utah, US)
Quantitative analysis of catalytic transformations – examples from C–H activation and phosphine-based catalysis

- March 5th Dr. Shilpi Ghosh (University of Tokyo, JP)
Selective Oxidation Reactions over Single Metal Sites and Supported Metal Nanoparticles Catalysts
- March 7th Prof. Dr. Bettina Lotsch (Max-Planck-Institute for Solid State Research Stuttgart, DE)
2D or not 2D? Molecular frameworks as platforms for light-driven hydrogen evolution
- March 8th Symposium on Perspectives in Theoretical Chemistry
- March 12th Prof. Dr. Udayan De (University Kolkata, IN)
Materials for Sensors & Actuators – Quench-free preparation of an engineering piezoelectric material
- March 14th Prof. Dr. Paul Chirik (Princeton University, US)
Catalysis with Earth Abundant Metals for the Upgrading of Hydrocarbons
- March 18th Raphael Zachmann (Albert-Ludwigs-University Freiburg, DE)
Photoredox-katalysierte C–C Bindungsspaltung
- March 25th Prof. Dr. Paolo Melchiorre (ICIQ Tarragona, ES)
Organic Synthesis in the Excited State - Enhancing the Potential of Organocatalysis with Light
- March 27th Dr. Constanze Neumann (Massachusetts Institute of Technology, US)
Facilitating Access to PET Probes and Advanced Biofuels
- April 10th Alexander Hopf (University of Darmstadt, DE)
Ultrasound Attenuation Spectroscopy of Carbon Black Dispersions
- April 10th Prof. Dr. Hosea Nelson (University of California Los Angeles, US)
Twists and Turns Along The Path of Reactivity-Driven Methodology Development
- April 16th Tuğçe Beyazay (Koç University Istanbul, TR)
Self-standing Graphene Papers Electrodeposited with Manganese Oxide Nanostructures as Electrodes for Electrochemical Capacitors
- April 23rd Prof. Dr. Regina Palkovits (RWTH Aachen, DE)
Design of Solid Catalysts for the (Electro)Catalytic Valorisation of Renewable Carbon Sources

- April 30th Malte Stienecker (Max-Planck-Institute of Plasma Physics Munich, DE)
Hydrogen Permeation through Tungsten Visualised by Hydrogenography
- May 13th Prof. Dr. Barry M. Trost (Stanford University, US)
A Challenge for Total Synthesis: Atom Economy
- May 15th Prof. Dr. Jean C. Tremblay (Université de Lorraine, FR)
Quantum Dynamics in the Condensed Phase: from High-Dimensional Spectroscopy to Electronic Currents
- May 20th Prof. Dr. Tomislav Friscic (McGill University Montreal, CA)
Mechanochemistry: a tour de force of solvent-free materials and molecular synthesis
- May 27th Simon Rundstrom (Retsch GmbH Haan, DE)
The Art of Milling
- May 28th Dr. Michael E. Beck (Bayer AG Monheim, DE)
Quantum Theory meets the Field: Electronic reasoning in support of a fungicide
- June 13th Prof. Dr. Varinder Aggarwal (University of Bristol, UK)
Assembly Line Synthesis
- July 2nd Raphael Abolivier (ALBA Synchrotron Barcelona, ES)
Investigation and modelling of supported nanoparticles for catalysts via synchrotron GISAXS
- July 2nd Fei Wang (Utrecht University, NL)
Synthesis of FDCA from biomass-derived molecules over supported gold/silver/palladium nanoparticles
- July 4th Dr. Johannes Lehmann (Simon Fraser University Burnaby, CA)
Development of small molecular probes for high-affinity protein binding and target elucidation
- July 10th Prof. Dr. Klaus Kümmerer (Leuphana University Lüneburg, DE)
Beyond Green Chemistry-Sustainable Chemistry!
- July 11th Dr. Lisa Roy (Institute of Chemical Technology Mumbai, IN)
Theoretical Insights into The Nature of Oxidant and Mechanism in Bioinspired Non-Heme Iron Catalyzed Reactions

- July 12th Dr. Debasis Koley (Indian Institute of Science Education and Research Kolkata, IN)
Computational Studies on Some Selected Pd-catalyzed Organic Transformations
- July 24th Minhao Zhang (York University Toronto, CA)
The Total Synthesis of (±)7-HDHA
- July 30th Dr. Ruiyan Sun (RWTH Aachen, DE)
The Sustainable Production of Polyols From Cellulose Enabled by Bifunctional Catalysts
- July 31st Dr. Timo Ott (Grillo-Werke AG Duisburg, DE)
Sulfonation of Methane in Industry – Development of a Scalable Process
- August 9th Johannes Fessler (Universität Munich, DE)
Towards the asymmetric synthesis of quinolizidines via transannular iodoamination of octahydroazecines
- October 7th Mental Health Day: Dr. Ayscha Lucas-Gesing (Erfahrungsraum Achtsamkeit)
Stressbewältigung durch Achtsamkeit
- October 7th Career Day:
Discussion on Job Hunting and Career perspectives with MPI alumni and external guests
- October 10th Dr. Marcos Suero (ICIQ Valencia, ES)
New Carbon Reactivity Rules
- October 23rd Dr. Chris Armbruster (The Drivery Berlin, DE)
CV writing and skills gap analysis for a Digital Career
- October 28th Prof. Dr. Bert Weckhuysen (University of Utrecht, NL)
Catalysts Live and Up Close: Hunting for the Hidden Chemistry in Catalysis
- October 29th Prof. Dr. Bert Weckhuysen (University of Utrecht, NL)
Catalyst Images, Imaging and Imagination: Visualizing Molecules and Atoms in Action on Catalytic Surfaces
- October 30th Prof. Dr. Bert Weckhuysen (University of Utrecht, NL)
Spectroscopy of Solid Catalysts: A Tutorial Lecture on Catalysts Characterization and Related Challenges & Opportunities

- October 31st Dr. Tatiana Gorelik (University of Ulm, DE)
TEM structural characterization from a different perspective: electron diffraction
- November 8th Dr. Marc de Wergifosse (University of Bonn, DE)
New developments in a simplified time-dependent density functional theory (sTD-DFT) framework
- November 11th Prof. Dr. Dirk Trauner (New York University, US) (Ernst Haage Symposium)
Reflections on Racemates
- November 12th Ernst Haage Symposium
- November 13th Ernst Haage Symposium
- November 26th Xiaoran Liu (GRINM Beijing, CN)
Dehydrogenation properties of two phases of LiNH₂BH₃
- November 27th Prof. Aiko Fukazawa (Kyoto University, JP)
Exploring Stable Yet Unusual π -Electron Materials by Making Use of Phosphorus and Sulfur
- December 3rd Isabella Kappel (LMU Munich, DE)
Crystal Imperfections in Industrial VPO Catalysts
- December 4th Peter Wasserscheid (University of Erlangen, DE)
Liquid Organic Hydrogen Carrier systems – towards a hydrogen-free hydrogen economy
- December 5th Prof. Nicolai Cramer (EPFL Lausanne, CH)
The Quest for Efficient Ligands in Asymmetric C–H Functionalizations
- December 13th Sebastian Brunen (Philipps-Universität Marburg, DE)
Metal-Centered Chirality in Asymmetric Catalysis: Synthesis and Application of Novel Chiral-only-at-Metal Iridium(III)-Complexes

9.6 List of Publications 2017 - 2019

During the period 2017-2019, a total of 543 scientific articles and book sections have been published by scientists from the institute. For individual publication lists, please see our website: www.kofo.mpg.de/en.

2017

Abis, L.; Freakley, S. J.; Dodekatos, G.; Morgan, D. J.; Sankar, M.; Dimitratos, N.; He, Q.; Kiely, C. J.; Hutchings, G. J. Highly Active Gold and Gold-Palladium Catalysts Prepared by Colloidal Methods in the Absence of Polymer Stabilizers. *ChemCatChem* **2017**, *9* (15), 2914-2918.

Acevedo, J. P.; Reetz, M. T.; Asenjo, J. A.; Parra, L. P. One-Step Combined Focused epPCR and Saturation Mutagenesis for Thermostability Evolution of a New Cold-Active Xylanase. *Enzyme Microb. Technol.* **2017**, *100* (5), 60-70.

Ausfelder, F.; Beilmann, C.; Bertau, M.; Bräuninger, S.; Heinzl, A.; Hoer, R.; Koch, W.; Mahlendorf, F.; Metzelthin, A.; Peuckert, M.; Plass, L.; Räuchle, K.; Reuter, M.; Schaub, G.; Schiebahn, S.; Schwab, E.; Schüth, F.; Stolten, D.; Teßmer, G.; Wagemann, K.; Ziegahn, K.-F. Energy Storage as Part of a Secure Energy Supply. *ChemBioEng Rev.* **2017**, *4* (3), 144-210.

Barnes, R.; Sun, S.; Fichou, Y.; Dahlquist, F. W.; Heyden, M.; Han, S. Spatially Heterogeneous Surface Water Diffusivity around Structured Protein Surfaces at Equilibrium. *J. Am. Chem. Soc.* **2017**, *139* (49), 17890-17901.

Barrado, A. G.; Bayne, J. M.; Johnstone, T. C.; Lehmann, C. W.; Stephan, D. W.; Alcarazo, M. Dicationic phosphonium salts: Lewis acid initiators for the Mukaiyama-aldol reaction. *Dalton Trans.* **2017**, *46* (46), 16216-16227.

Barrado, A. G.; Zielinski, A.; Alcarazo, M.; Goddard, R. Regio- and Stereoselective Chlorocyanation of Alkynes. *Angew. Chem., Int. Ed.* **2017**, *56* (43), 13401-13405.

Beyzavi, M. H.; Mandal, D.; Strebl, M. G.; Neumann, C. N.; D'Amato, E. M.; Chen, J.; Hooker, J. M.; Ritter, T. ¹⁸F-Deoxyfluorination of Phenols via Ru π -Complexes. *ACS Cent. Sci.* **2017**, *3* (9), 944-948.

Bhawal, B. N.; Morandi, B. Shuttle Catalysis—New Strategies in Organic Synthesis. *Chem. – Eur. J.* **2017**, *23* (50), 12004-12013.

Bier, D.; Mittal, S.; Bravo-Rodriguez, K.; Sowislok, A.; Guillory, X.; Briels, J.; Heid, C.; Bartel, M.; Wettig, B.; Brunsveld, L.; Sánchez-García, E.; Schrader, T.; Ottmann, C. The Molecular Tweezer CLR01 Stabilizes a Disordered Protein–Protein Interface. *J. Am. Chem. Soc.* **2017**, *139* (45), 16256-16263.

Brambilla, M.; Tredwell, M. Palladium Catalyzed Suzuki-Miyaura Cross-Coupling of Secondary α -(Trifluoromethyl)benzyl Tosylates. *Angew. Chem., Int. Ed.* **2017**, *56* (39), 11981-11985.

- Calvaruso, G.; Burak, J. A.; Clough, M. T.; Kennema, M.; Meemken, F.; Rinaldi, R. On the Reactivity of Dihydro-p-coumaryl Alcohol towards Reductive Processes Catalyzed by Raney Nickel. *ChemCatChem* **2017**, *9* (14), 2627-2632.
- Calvaruso, G.; Clough, M. T.; Kaufman-Rechulski, M. D.; Rinaldi, R. On the Meaning and Origins of Lignin Recalcitrance: A Critical Analysis of the Catalytic Upgrading of Lignins Obtained from Mechanocatalytic Biorefining and Organosolv Pulping. *ChemCatChem* **2017**, *9* (14), 2691-2700.
- Calvaruso, G.; Clough, M. T.; Rinaldi, R. Biphasic extraction of mechanocatalytically-depolymerized lignin from water-soluble wood and its catalytic downstream processing. *Green Chem.* **2017**, *19* (12), 2803-2811.
- Campbell, M. G.; Mercier, J.; Genicot, C.; Gouverneur, V.; Hooker, J. M.; Ritter, T. Bridging the gaps in ¹⁸F PET tracer development. *Nat. Chem.* **2017**, *9* (1), 1-3.
- Cao, Z.; Engelhardt, J.; Dierks, M.; Clough, M. T.; Wang, G.; Heracleous, E.; Lappas, A.; Rinaldi, R.; Schüth, F. Catalysis Meets Nonthermal Separation for the Production of (Alkyl)phenols and Hydrocarbons from Pyrolysis Oil. *Angew. Chem., Int. Ed.* **2017**, *56* (9), 2334-2339.
- Cao, Z.; Ouyang, L.; Wang, H.; Liu, J.; Felderhoff, M.; Zhu, M. Reversible hydrogen storage in yttrium aluminum hydride. *J. Mater. Chem. A* **2017**, *5* (13), 6042-6046.
- Casitas, A.; Rees, J. A.; Goddard, R.; Bill, E.; DeBeer, S.; Füstner, A. Two Exceptional Homoleptic Iron(IV) Tetraalkyl Complexes. *Angew. Chem., Int. Ed.* **2017**, *56* (34), 10108-10113.
- Chang, X.-P.; Gao, Y.-J.; Fang, W.-H.; Cui, G.; Thiel, W. Quantum Mechanics/Molecular Mechanics Study on the Photoreactions of Dark- and Light-Adapted States of a Blue-Light YtvA LOV Photoreceptor. *Angew. Chem., Int. Ed.* **2017**, *56* (32), 9341-9345.
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- Chen, K.; Schünemann, S.; Tüysüz, H. Preparation of Waterproof Organometal Halide Perovskite Photonic Crystal Beads. *Angew. Chem., Int. Ed.* **2017**, *56* (23), 6648-6652.
- Clough, M. T. Organic electrolyte solutions as versatile media for the dissolution and regeneration of cellulose. *Green Chem.* **2017**, *19* (20), 4754-4768.
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- Damm, T.; Pattathil, S.; Günl, M.; Jablonowski, N. D.; O'Neill, M.; Grün, K. S.; Grande, P. M.; Leitner, W.; Schurr, U.; Usadel, B.; Klose, H. Insights into cell wall structure of *Sida hermaphrodita* and its influence on recalcitrance. *Carbohydr. Polym.* **2017**, *168*, 94-102.
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Max-Planck-Institut für Kohlenforschung

Kaiser-Wilhelm-Platz 1

45470 Mülheim an der Ruhr

Germany

www.kofo.mpg.de