### **BIENNUAL REPORT**

2021 | 2022



Leibniz Institute for Catalysis



LIKAT Rostock

## Leibniz Institute for Catalysis

### **I**MPRINT

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Editorial: Dr. Martha Höhne Tel.: +49 381 1281-382 martha.hoehne@catalysis.de

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Leibniz Association

LIKAT Rostock

**BIENNUAL REPORT** 2021 | 2022



# Foreword



Prof. Dr. Matthias Beller, *Scientific Director* (right) and Dr. Mirko Kirschkowski, *Commercial Director* (Photo: LIKAT)

## Chemistry in Transition

The global community is pushing for a "green turn" to halt climate change and conserve natural resources. Renewable raw materials are to replace fossil fuels - in entire industries as well as in people's everyday lives. Germany is committed to climate neutrality by 2045. And the Leibniz Institute for Catalysis Rostock can contribute significantly to all these challenges. This is because catalysis is one of the key technologies for converting the economy, everyday life and society to a sustainable basis.

Catalysts enable new procedures and circular processes that are essential for a climateneutral economy.

At LIKAT, more than 300 employees are researching the fundamentals for this. In Germany, 97 percent of all products are created by chemical processes, and catalysts are involved in four out of five of these reactions. They succeed in converting raw materials, and increasingly from sustainable sources, into basic chemicals such as hydrogen and methanol, and into recyclable, circular chemicals and materials.

Let's take hydrogen. The gas is one of the hopes of the climate and energy transition, and LIKAT has a wide range of expertise in this field. For example, during the reporting period, members of the institute worked with industrial partners to develop a catalytic system that uses the battery principle to chemically store H<sub>2</sub> and release it in a highly purified form. This "hydrogen battery", combined with photovoltaics or wind power, can support climate-neutral concepts in rural regions, for example. It also recycles atmospheric CO<sub>2</sub>.

High-quality research on fundamental topics relevant to industry is one of LIKAT's strengths,

visible in several patents and pilot processes will be no solutions to the many technological filed jointly with industrial partners. Every year, and societal challenges without it. Improved the institute works on around 50 bilateral or chemical technologies and new improved camultilateral projects with industry participation. talysts are needed to sustainably manage the In 2021 and 2022, LIKAT researchers laid the economy, feed the world's population, treat foundation for a total of 55 patents and two future pandemics and currently incurable diseatransfers to industrial pilot scale or directly to ses, and achieve the climate goals mentioned at industrial production. The collaborations with the beginning. Evonik Industries, Henkel and Symrise deserve As an institute of the Leibniz Association, LIKAT special mentioning. In 2022, a framework agreewants to make its contribution to this for the ment was signed with Apex Energies, a regional benefit of our society. company specializing in hydrogen technologies.

In addition, LIKAT is expanding its research activities to promising new fields in order to bring fundamental research results into application. One example is electrochemistry, which can be used to obtain indispensable molecular building blocks from  $CO_2$  and green  $H_2$ , among other things.

And the institute's new *Catalysis2Scale* technical center offers members of our institute and partners a unique opportunity in northeastern Germany to test laboratory findings themselves on a pilot scale.

This will enable LIKAT to fulfill the mission enshrined in its statutes even better than before: To conduct cutting-edge basic research and to apply the findings to practical applications. And to do so even under difficult conditions, as we demonstrated during the Corona pandemic. Even in times of lockdown, LIKAT maintained its research operations in the laboratories with a staff from 36 countries.

In the public perception, chemistry is still criticized as an emitter of greenhouse gases and a major energy consumer, and yes, it has been part of the problem for many decades. Yet there

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Matthias Beller

and

Mirko Kirschkowski



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(Photo: LIKAT/Thomas Müller)

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## 2021 IN REVIEW

#### January

#### LIKAT Welcomes New Head of Department for "Electrochemistry & Catalysis" Robert Francke

At the beginning of January 2021, the department "Electrochemistry & Catalysis" headed by Heisenberg fellow Dr. habil. Robert Francke had started its work at LIKAT.

#### March

Alumni Meeting (virtual) Together, LIKAT alumni and current employees defied the pandemic: the regular alumni meeting was unceremoniously moved to the virtual world. In addition to contributions from the alumni, there was also the opportunity to exchange ideas at "virtual coffee tables".

### May

#### **Osama El-Sepelgy Moved** to LIKAT

As of May 1, Dr. Osama El-Sepelgy started his work at LIKAT as leader of the exploratory reseach group "Sustainable Excited-State Catalysis" in the department of "Applied Homogeneous Catalysis". Until then, he has been working at the Biotechnology Institute of RWTH Aachen University.

Chemie

#### July Jagadeesh Rajenahally **Received Visiting Pro-**

fessorship and Became Advisory Member at REVA University

Dr. Jagadeesh Rajenahally is awarded a visiting professorship and became an advisory member at REVA University in Yelahanka, Bengalore (India).

#### August

#### Stephan Bartling received HOT TOPIC Award for presentations

During the Cluster Meeting 2021 in Prague from July 18 to 23, Dr. Stephan Bartling (Analytical Department: Photoelectron Spectroscopy) received an award for one of the three best HOT TOPIC presentations.

#### September

#### Katrin Zschau und Julian **Barlen visited LIKAT**

Julian Barlen (MdL) and Katrin Zschau (MdB) informed themselves at LIKAT about possibilities for chemical energy storage, alternative fuels of the future and hydrogen technologies with a focus on the joint project "Research Factory Hdrogen MV".



### February

#### Conference with 5000 **Participants**

A better world succeeds only with women in science - The virtual workshop "International Day of Women and Girls in Science, drew about 5,000 participants: Female researchers and students from 350 universities in the Islamic world, as well as professors, Nobel laureates, politicians and motivators from all over the world participated in the conference organized by the Islamic World Organization for Education, Science and Culture (ICESCO), LIKAT in Rostock, Germany, and the Space Foundation, a non-profit organization promoting space technologies.

### May

#### Armin Börner Received Literature Award of VCI

Prof. Dr. Armin Börner. head of the department "Hydrogenations and Hydroformylations", received the Literature Award of the Chemical Industry Fund of the VCI for his book "Chemie - Verbindungen fürs Leben" published by wgb Theiss in 2019. In VCI's tribute to the award of the 2021 Literature Prize, it emphasized that Armin Börner gives his audience "a completely new view of the world".

#### Juni

NAL DAY OF

From Climate Gas to Raw Material: LIKAT Participa-

ted in the Week of the Environment with the project "CO<sub>2</sub>4 Future"

The goal of researchers at the Leibniz Institute for Catalysis in Rostock is to relieve the atmosphere of CO<sub>2</sub> and to make the climate gas directly usable for a hydrogen economy in the future. The institute presented concrete ways to achieve this in its contribution "CO<sub>2</sub>4 Future" as part of the "Week of the Environment", hosted by German President Frank-Walter Steinmeier and the German Environmental Foundation.

## July

#### Reappraisal of the NS Past of the LIKAT Founding Fathers

On behalf of LIKAT, the historian Dr. Florian Detjens has written a report on the Nazi past of the two LIKAT founding fathers Profs. Günther Rienäcker and Wolfgang Langenbeck. Their life stories are mirrors of German history - including the dark times of dictatorship and oppression. They show: Science is not an ivory tower of self-sufficient scientific activity. Scientists bear responsibility for society. LIKAT is committed to this responsibility, which includes dealing openly and transparently with its own past. The report is available on the LIKAT website.

#### August

#### Mirko Kirschkowski **Became Commercial** Director

On August 1, Dr. Mirko Kirschkowski took over the position of Commercial Director at LIKAT. Previously, he worked in various science management positions, such as Managing Director of the German Center for Heart Failure at the University Hospital Würzburg or Administrative Director of the Sigmund Freud Institute in Frankfurt am Main.

### September

#### Veronica Papa received Award of SCI

Veronica Papa received the prize of the Italian Chemical Society (Società Chimica Italiana, SCI) for her doctoral thesis, which she wrote in the research group "Sustainable Redox Reactions" of Dr. Kathrin Junge.



#### September

#### Back at it again:

After a break due to the pandemic, the "Open Night of Sciences" took place as a hybrid format in Rostock's Klostergarten.

#### November

#### **Together for Climate**

On the eve of the 26th UN Climate Change Conference in Glasgow, a good two dozen universities and research institutions from around the world have ioined forces to form an alliance for combating climate change. LIKAT is one of the founding members.

#### Oktober

#### Milica Feldt strengenths LIKAT

Since October 2021, Dr. Milica Feldt strengthens the portfolio of LIKAT as junior research group leader with her group "Theory of Homogeneous & Biocatalysis". She is dedicated to computational chemistry with a research focus on "Catalysis with transition metals". She is particularly interested in the study of non-heme iron complexes. Milica Feldt has a degree in physics and will enrich LIKAT with her expertise on the theoretical consideration of the phenomenon of catalysis.

#### November

#### Rüdiger Selke (1934 -2021)

LIKAT mourns the death of long-time colleague Prof. Dr. Rüdiger Selke. He pioneered catalysis research with transition metal complexes and was significantly involved in the development of the Isicom process, the world's second asymmetrically catalyzed process to be implemented on an industrial scale.

#### December

#### Matthias Beller has again been recognized as a Highly Cited Researcher.

The names on the "Who's Who" list rank in the top 1 percent of citations in the Web of Science<sup>™</sup> citation index for the respective field and publication year.

## 2022 IN REVIEW

#### Januar

#### P-Campus Publication Award 2021 for Thomas Werner

The P-Campus Publication Award 2021 went, among others, to LIKAT scientist Prof. Dr. Thomas Werner for the Ecotoxicology and Environmental Safety publication

"AMPA-<sup>15</sup>N – Synthesis and application as standard compound in traceable degradation studies of glyphosate" (DOI: 10.1016/j. ecoenv.2021.112768)

#### June

Thirsty for Knowledge: The "Open Night of Sciences"

Thirsty for knowledge: For the first time after the pandemic-related restrictions of the past years, we were again able to welcome visitors live on site during the "Open Night". The response was very great on both the visitor and LIKAT sides.

#### New Transmission Electron Microscope

July

The transmission electron microscope (TEM) operated jointly with the Interdisciplinary Faculty of the University of Rostock was inaugurated.

#### July

#### Grand Opening of the *Catalysis2Scale* Technical Center

In the institute's own transfer technical center, researchers will now be able to test the application readiness of their laboratory findings themselves on a pilot scale. This will bring basic research, in particular, closer to practice.

#### September

#### "Chemiker im Wortlabor"

On September 29th, a reading "CHEMISTS in the literary WORD LABORATO-RY" took place for the first time in the large seminar room of LIKAT. Three authors (and former

LIKAT chemists) read from their (non-scientific) works.



#### April

#### At Eye Level with the Academic "High Nobility" - Two LIKAT Chemists Traveled to the Nobel Laureate Meeting

With Thea Mayer (reseach group of J. Pospech) and Aija Gudkova (research group of R. Francke) two young female chemists from LIKAT were invited to the 71st Meeting of Nobel Laureates in Lindau at Lake Constance.

#### June

Mav

Award for Good Teaching

Dr. Jola Pospech was awar-

ded for very good teaching

performance at the Insti-

tute of Chemistry of the

University of Rostock.

#### Honor for Jagadeesh Rajenahally

Prof. Dr. Jagadeesh Rajenahally was honored for publishing research papers that are among the 1% of the most cited papers in European institutions.

#### June

#### **Best Poster Pitch**

At the 55th Annual Meeting of the German Catalysts, Stefan Peters (Department Wohlrab) was awarded a prize for the best poster pitch.

### July

Handing Over of the Notice of Approval "Research Factory Hydrogen MV"

With the award of the first funding to LIKAT, the joint project "Research Factory Hydrogen MV" started. Together with two other research institutions, LIKAT will explore and optimize processes and technologies for CO<sub>2</sub>-neutral production cycles on the basis of renewable energies and bring them to application maturity. In addition to LIKAT, the collaborative partners are the Rostock Fraunhofer Institute for Large Structures in Production Engineering, IGP, and the Leibniz Institute for Plasma Research and Technology, INP Greifswald.

#### August

#### ChemBioChem Early Career Award

Dr. Jola Pospech received the ChemBioChem Early Career Award at the 29th Young Scientist Symposium on Bioorganic Chemistry at KIT in Karlsruhe.

#### Oktober

#### "Young Researchers Award" der CGCA

Kangkang Sun, PhD student in the department of Prof. Matthias Beller (research group "Homogeneous Catalysis for Life Sciences" of Dr. Helfried Neumann), was awarded the "Young Researchers Award" of the Community of Chinese Chemists and Chemical Engineers in Germany (CGCA).

#### November

#### Eszter Baráth at Leibniz Programme for Women Professors

As one of five internationally outstanding scientists, Dr, habil. Eszter Baráth will be funded to establish a professorship with the Universitiy of Rostock within the framework of the "Leibniz Programme for Women Professors".

#### November

## Matthias Beller Awarded as Highly Cited Researcher

Prof. Dr. Matthias Beller has once again been listed as a "Highly Cited Researcher". According to Clarivate Analytics, this makes him one of the world's most influential researchers.

#### November

#### Matthias Beller Again in the Board of the Leibniz Association

Prof. Dr. Matthias Beller has been re-elected to the Leibniz Association's Executive Board. He is one of three vice presidents, along with Sebastian Lenz (Director of the Leibniz Institute for Regional Geography in Leipzig) and Stephan Junker (Managing Director of the Museum für Naturkunde Berlin - Leibniz Institute for Evolutionary and Biodiversity Research in Berlin).

#### Dezember

#### Professorship for Torsten Beweries

During the meeting of the Faculty Council of the MNF of the University of Rostock, Prof. Dr. Torsten Beweries was awarded the certificate of conferral of the title of Professor for gaining the title of Extraordinary Professor by the Dean of the MNF.

## LIKAT IN NUMBERS



13.3 | 13.5 **Basic Funding** 

7.5 | 7.2 **External Funding** 

2.8 | 2.5 thereof Industrial Funding

4.8 | 4.6 thereof Public Funding

5.8 | -**Construction Investment** 



2021 | 2022

**Scientists** 

100 | 110

**PhD Students** 



55 | 68

**Science Supporting Staff** 





316 318 2021 | 2022 **Publications** 

103 | 107 thereof OA

161 | 198 thereof IP>5

> 1 | 2 **Books**

11 | 13 **Book Chapters** 

## **ORGANIZATION CHARTS**





General Meeting . Ralf Ludwig / Univ. Rostock		Scientific & Industrial Advisory Board Chair Prof. Brigitte Voit / IPF Dresden				
r Baráth Prof. Robert Francke Dr. Mirko Kirschkowski						
<u>\</u>				Staff Unit Dr. S Hinze		
	o Top	ic 01 Structur-Reactivity Re-	Services			
	NN,	W. Baumann (Deputy)	Analytics Dr. W. Ba	umann		
00	Top Med	ic 02 Kinetics, Theory & hanisms	Chromatography • EA XPS • IR • MS • NMR			
	E. Ko	ondratenko, H. Jiao (Deputy)	I LIVI - AK	D·OV/VIS		
	Top & In	ic 03 Reaction Engineering	Administ Dr. M. Kir	<b>ration</b> schkowski		
0 0	D. L	inke, U. Armbruster (Deputy)	Project Management Finances · Purchase			
	Тор	ic 04 Renewable Resources	Law & Pe	ersonnel · IT		
	E. Ba (Dep	aráth, A. Abdel-Mageed puty)	Technical A. Schupp	Service		
0 0	Top R. F	ic 05 Energy & Environment rancke, H. Junge (Deputy)	Building Workshop	Services ps		
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	Topic 07 New Products & cesses T. Beweries, C. Hering-Jung (Denuty)		U. von Zv Occupatio Dr. N. Ro	veydorff onal Safety ckstroh (ASA)		
on • Dr. W. Baumann Dis qual Opportunities • Dr. S. Hir	sabled I	Persons • A. Simmula Dive PhD & PostDocs • T. Mayer,	ersity • U. vo P. Hünemö	on Zweydorff rder, C. Stein		

## **RESEARCH MISSION**

The Leibniz Institute for Catalysis (LIKAT) and its LIKAT conducts society-relevant state-of-the-art predecessor institutions have been dedicated to catalysis research for 70 years. It began with research efforts to produce artificial butter in the post-war period to secure society's food supply. Today, LIKAT in Rostock is one of the largest publicly funded research institutes in its field in Europe, occupying a place at the interface of fundamentals and applications.

The institute has undergone many changes since its founding in 1952. The original main claim of the work at the institute still exists today, in the spirit of the Leibniz Association: to transfer the results of basic research to chemical products or processes with application relevance.

catalysis research, which is applied to alternative energy technologies as well as in the material and life sciences, in addition to the classical areas of chemistry.

For this purpose, the entire range of modern research instruments is made available in one institute. Innovative research approaches arise less from a juxtaposition of individual research areas with outstanding expertise, but rather from the interdisciplinary, cross-disciplinary answering of relevant research questions. The holistic view of the phenomenon of catalysis enables the institute to make significant contributions to achieving the overarching strategic goal of closing material cycles with its research results.



Only the solid stem of basic research enables its investigation for possible applications. This applied research (green branches) bears fruit in the best case and results in real products or processes for industry or everyday life.

The Leibniz Institute for Catalysis researches at the interface of basic and applied research.



# **Research Structure**

The research work at LIKAT is assigned to seven Topics, which are regarded as future-oriented, socially relevant research areas.

They are cross-disciplinary and combine expertise from the different Research Departments (RD) or their Research Groups (RG).

This matrix structure promotes the exchange of different disciplines on research questions and allows to maximize the professional potential at LIKAT.

A total of seven Topic Fields have been identified, which are addressed by ten existing Research Departments and their individual Research Groups.

### Methodologically Oriented Topics:

Topic 01 Structure-Reactivity Relationships Speaker: N. N. Deputy: PD Dr. habil. Wolfgang Baumann



Topic 04 Renewable Resources Speaker: PD Dr. habil. Eszter Baráth Deputy: Dr. Ali Abdel-Mageed

Energy & Environment

Deputy: Dr. Henrik Junge

Speaker: Prof. Dr. Robert Francke

Materially Oriented Topics:

Topic 05



Topic 02 Kinetics, Theoriy & Mechanisms Speaker: Prof. Dr. Evgenii Kondratenko Deputy: Prof. Dr. Haijun Jiao





Topic 03 *Reaction Engineering* & Implementation Speaker: Dr. David Linke Deputy: Dr.-Ing. Udo Armbruster



Topic 06 More Efficient Processes Speaker: Dr. Sebastian Wohlrab Deputy: Dr. Bernd Müller



Topic 07 New Products & Processes Speaker: Prof. Dr. Torsten Beweries Deputy: Dr. Christian Hering-Junghans











# TOPICS





## Topic 01 - Structure-Reactivity-Relationships

N. N. PD Dr. habil. Wolfgang Baumann



## Topic 02 - Kinetics, Theory & Mechanisms

Prof. Dr. Evgenii Kondratenko Prof. Dr. Haijun Jiao

Topic 01 deals with the establishment and combination of modern experimental, mainly analytical, methods as a basis for knowledge-based catalyst design. This includes the development, optimization and application of innovative methods, procedures and setups for the investigation of catalytic reactions and catalyst syntheses. The goal is to accelerate the development of new catalytic processes and to make existing processes more efficient on a rational basis. A very illustrative example of the collaboration between different reseach groups in Topic 01 is the development of a special spin-trapping method that can selectively distinguish between different radicals. With the help of this method, groups working primarily in preparative chemistry can develop mechanistic

understanding and demonstrate whether radical intermediates play a role in the relevant reactions. Investigation of structural and electronic properties of heterogeneous and homogeneous photo- and electrocatalyst systems in CO<sub>2</sub> reduction, water splitting, and methanol oxidation revealed that known active sites from thermal catalysis can possess comparable activities in the novel reaction guides. The collaboration in Topic 01 enabled the more detailed investigation of these findings in temperature-dependent UV-Vis and Raman measurements and the deciphering of the relationships between optical, electronic and catalytic properties of the material. In the future, a new experimental advance will be made by combining operando FTIR spectroscopy with kinetics and chemometrics.

The focus of Topic 02 is on mechanistic and kinumerical analysis of time-resolved experiments netic aspects of heterogeneous, homogeneous, and density functional theory (DFT) calculaelectro- and photocatalysis. The subject of the tions. The combination provides a very detailed view of the mode of action of a wide variety of investigations are large-scale, future-oriented and sustainable catalytic processes. The aim catalysts. The collaboration in TF 02 promotes the rationalization of experimental results, on is to derive correlations between macroscopic observations in reactors with the microscopic the basis of which proposals can be made for structure of the catalytically active centers/ targeted catalyst development, optimization of phases and the reaction microkinetics at the reaction conditions, improvement of reaction most elementary level possible. To this end, sequences and planning of new experiments. mechanistic and microkinetic studies are used Topic 02 thus supports the research work in the to obtain fundamental relationships between material-oriented topics 04-07. For example, the the structure of the active sites and the kinetics elucidation of the mechanism for the formation of cyclic carbonates from epoxides and CO<sub>2</sub> enof the selective and nonselective reaction steps. These form the guidelines for controlled catalyst abled the optimization of reaction conditions so production and for the development of new or that cyclic carbonates can be isolated in yields of up to 99%. Future plans are to expand eximproved reactor concepts, which is particularly important in view of the changing raw material pertise to include theory of homogeneous and biocatalysis (junior research group, Milica Feldt). base and energy technologies. Topic 02 applies In addition, digitization and automation offer various methods for this purpose: transient (time-resolved) experiments with isotope-lagreat potential to improve existing methods beled molecules, steady-state kinetic and meand to develop new methods and techniques. chanistic measurements, spectroscopic catalyst characterization, mathematical modeling, and

INORGANIC FUNCTIONAL MATERIALS (Dr. Sebastian Wohlrab) CATALYSIS FOR ENERGY (Dr. Henrik Junge) CATALYSIS OF EARLY TRANSITION METALS (Dr. Fabian Reiß) CATALYSIS OF LATE TRANSITION METALS (Prof. Dr. Torsten Beweries) CATALYTIC FUNCTIONALIZATIONS (Dr. Jola Pospech) MAGNETIC RESONANCE- & X-RAY METHODS (Dr. Jabor Rabeah) MODERN ORGANIC CHEMISTRY (Dr. Osama El-Sepelgy) SUSTAINABLE REDOX REACTIONS (Dr. Kathrin Junge)

SURFACE CHEMISTRY IN APPLIED CATALYSIS (Dr. Ali Abdel-Mageed) OPTICAL SPECTROSCOPY & THERMOANALYTICAL METHODS (Dr. Christoph Kubis) REACTION MECHANISMS (Prof. Dr. Evgenii Kondratenko) SELECTIVE CATALYTIC SYNTHESIS METHODS (Dr. Sergey Tin, now: Dr. habil. Eszter Baráth) STRUCTURE-FUNCTION CORRELATIONS (Prof. Dr. Jennifer Strunk) THEORY OF HOMOEGENEOUS & BIOCATALYSIS (Dr. Milica Feldt) UNI IN LEIBNIZ (Prof. Dr. Björn Corzilius, Prof. Dr. Marko Hapke, Prof. Dr. Axel Schulz)

Catalysis of Early Transition Metals (Dr. Fabian Reiß)

CATALYSIS WITH PHOSPHOROUS CONTAINING MATERIALS (former: Activation of Small Molecules) (Dr. Christian Hering-Junghans)

Magnetic Resonance & X-ray Methods (Dr. Jabor Rabeah)

MECHANISMS OF HOMOGENEOUS CATALYSIS (Dr. Hans-Joachim Drexler, former: Prof. Dr. Detlef Heller)

Optical Spectroscopy & Thermoanalytical Methods (Dr. Christoph Kubis)



REACTION MECHANISMS (Prof. Dr. Evgenii Kondratenko) Synergies between Homo- & Heterogeneous Catalysis (Now: Catalysis for Sustainable Syntheses) (Prof. Dr. Jagadeesh Rajenahally) Theory of Homogeneous & Bio-Catalysis (Dr. Milica Feldt) Theory of Catalysis (Prof. Dr. Haijun Jiao) UNI IN LEIBNIZ (Prof. Dr. Ralf Ludwig, Prof. Dr. Klaus Neymeyr)

## **Topic 03 - Reaction Engineering &** Implementation

Dr. David Linke Dr.-Ing. Udo Armbruster



### With regard to reaction engineering in topic 03, the aim is to develop the best possible reactor design and operating regime for catalyzed chemical reactions. Different reactor concepts can be evaluated, but also reactor and process concepts can be developed together. In addition to the catalytic reaction, procedural aspects of catalyst synthesis are addressed. Implementation includes (i) the transfer of catalytic reactions from laboratory scale to pilot or technical scale and (ii) the transfer of methods from neighboring disciplines and information technology to catalysis, which have the potential to accelerate the transfer from research to technical application. The third focus in topic 03 is on Data Science. The NFDI4Cat project, in which LIKAT is the lead partner, aims to manage research data.

To realize these goals, research groups from different research areas are working together. Topic 03 is a competent partner for industry with respect to the transfer of new developments in catalysis from the laboratory to application in both fine and bulk chemistry. Several industrial projects deal with reaction engineering or upscaling issues for homogeneous and heterogeneous catalytic reactions. For example,

an industrially established fragrance synthesis could be modified to produce the product in fewer reaction steps and with higher yields. To support these activities, LIKAT researchers working in topic 03 experimental facilities of various scales (from microreactor to pilot plant scale) that provide data of high quality and significance. Here, the Catalysis2Scale transfer pilot plant plays an essential role. In contrast to topic 04 to 07, topic 03 focuses less on specific reactions and more on methodologies and technologies. As a result, the reactions studied in topic 03 are often also the subject of research in topic 04 to 07. However, not with the focus on fundamental catalyst development as there, but with emphasis on reaction engineering aspects. In the development of kinetic models, topic 03 works closely with topic 02 to provide a mechanistic basis for the models. In the future, the Catalysis2Scale technical center will enable topic 03 to focus, among other things, on faster transfer from laboratory to pilot plant scale. Further emphasis will be placed on the digitalization of the development chain and the development of more efficient reaction technology.

## **Topic 04 - Renewable Resources**

Dr. habil. Eszter Baráth Dr. Ali Abdel-Mageed

Topic 04 bundles expertise in the field of renefor example, to convert it into (poly)carbonates. wable raw materials and focuses on research In addition, fatty acids were converted into mointo catalytic conversions of renewable raw nomers for polymers by catalytic oxidation, carmaterials into basic chemicals for products used bonylation, hydroformylation or hydrogenation. in our daily lives. For example, lignocellulose For terpenes, modern catalytic methods of conobtained from wood waste and its compoversion are and have been developed, which are of particular interest for the fragrance industry. nents or fatty acids and terpenes can be used to produce various polymers, agrochemicals, Here, both molecularly-defined homogeneous solvents or flavorings. The first step is to convert and heterogeneous catalysts have been used. the biomass into so-called platform chemicals. Biocatalytic methods (in collaboration with the These can usually be produced in large quanti-University of Greifswald) and low-temperature ties in simple and profitable reactions and are plasma technologies (with INP Greifswald) were suitable as synthesis building blocks for numealso used through collaboration in the Leibniz rous other compounds. These platform chemi-Science Campus ComBioCat. cals (e.g. glycerol, levulinic or lactic acid, HMF, Electrochemical upgrading of renewable raw furfural) are converted in further catalyzed steps materials, which works without the use of stoiinto existing or new chemicals with the desired chiometric amounts of reducing or oxidizing properties. Since biomass contains an excess of agents, will play an increasing role in the future. oxygen, the following reactions are of great im-Likewise, investigations into the replacement of portance for the first steps: hydrogenation, hyundesirable solvents or uneconomical synthesis drogenolysis, dehydration, decarbonylation and strategies will be intensified. decarboxylation. During the reporting period, carbon dioxide was also used as a raw material.

APPLIED CARBONYATIONS (Dr. Ralf Jackstell) INORGANIC FUNCTIONAL MATERIALS (Dr. Sebastian Wohlrab) BIOCATALYSIS (Prof. Dr. Udo Kragl) **HIGH-THROUGHPUT TECHNOLOGIES** (Dr. Uwe Rodemerck) Homogeneous Catalysis for Life Sciences (Dr. Helfried Neumann) CATALYSIS FOR ENERGY (Dr. Henrik Junge)

SURFACE CHEMISTRY FOR APPLIED CATALYSIS (Dr. Ali Abdel-Mageed) POLYMER CHEMISTRY & CATALYSIS (PD Dr. habil Esteban Mejía) REACTION ENGINEERING (Dr. David Linke) Synergy between homo- & heterogeneous Catalysis (now: Catalysis for Sustainable Syntheses) (Prof. Dr. Jagadeesh Rajenahally) **TECHNOLOGY ORIENTED PROCESSES** (Dr. Udo Armbruster)

INORGANIC FUNCTIONAL MATERIALS (Dr. Sebastian Wohlrab) Homogene Katalyse mit erneuerbaren Rohstoffen (Dr. Sergey Tin) CATALYSIS WITH PHOSPHOROUS CONTAINING MATERIALS (former: ACTIVATION OF SMALL MOLECULES) (Dr. Christian Hering-Junghans) CATALYSIS OF HETEROCYCLES (Prof. Dr. Xiao-Feng Wu) MODERN ORGANIC CHEMISTRY (Dr. Osama El-Sepelgy) SUSTAINABLE REDOX REACTIONS (Dr. Kathrin Junge) SURFACE CHEMISTRY OF APPLIED CATALYSIS



(Dr. Ali M. Abdel-Mageed) POLYMER CHEMISTRY & CATALYSIS (PD Dr. habil. Esteban Mejía) SELECTIVE CATALYTIC SYNTHESIS METHODS (Dr. Sergey Tin, now: Dr. habil. Eszter Baráth) Synergy between homo- & heterogeneous Catalysis (now: Catalysis for Sustainable Syntheses) (Prof. Dr. Jagadeesh Rajenahally) THEORY OF HOMOGENEOUS & BIOCATALYSIS (Dr. Milica Feldt) Uni in Leibniz (Prof. Dr. Thomas Werner)

## Topic 05 - Energy & Environment

Prof. Dr. Robert Francke Dr. Henrik Junge

Topic 05 is concerned with basic and applied research aimed at using acidic and sustainable resources for future processes in the field of chemistry and alternative energy technologies. Activities focus on the use of sustainable energy sources, such as sunlight or regeneratively generated electricity, to drive chemical syntheses. One focus is on hydrogen production, its storage and reconversion into electrical energy, in particular the catalytic production and decomposition of liquid energy carriers (e.g. methanol, formic acid) from green hydrogen and CO<sub>2</sub>. The addition of the natural amino acid L-lysine to a Ru-based catalyst system made it possible to bind CO<sub>2</sub> directly from the air in the form of formates and to sustainably remove it from the atmosphere according to the CCU concept. In the future, catalyst systems based on readily available metals will be increasingly used in the processes studied. New mechanistic findings

in photocatalytic water splitting will enable the development of systems that operate in a much broader wavelength range. Another focus is on the recycling of greenhouse gases into chemical production. This includes, for example, the capture of CO<sub>2</sub> from the air in quantities significant for chemical reactions and its subsequent conversion to fuels, monomers and platform chemicals. In the last decade, processes for the purification of wastewater and exhaust gas streams have also been developed. For the latter, for example, new Ta and Mo catalysts have been introduced that convert up to 95% of NO with NH, at low temperatures. In the future, electrochemical catalysis will also play a greater role in Topic 05. It enables the direct use of green electrical energy and the avoidance of chemical oxidizing and reducing agents.

## **Topic 06 - More Efficient Processes**

Dr. Sebastian Wohlrab Dr. Bernd Müller

The aim of topic 06 is to optimize the energy of which has been pursued by industry and and resources of important, industrially relevant science for over 60 years: By means of direct dicatalytic processes. The focus is on developing carbonylation of 1,3-butadiene, adipates, signimore efficient catalysts and intensifying procesficant platform chemicals and monomers, which ses. With regard to the development of more are used on a million ton scale for the producefficient catalysts, completely new material tion of nylon, for example, can be synthesized in one step for the first time (Jackstell, Beller). concepts are important in addition to knowled-Crucial to this success was the development of a ge-based development. In order to realize more efficient process control, innovative technolonew P(III) ligand (Neumann, Beller). gies or alternative synthesis routes are explored. In the future, this topic area will also focus The core approach of this topic is the optimizaon the development of non-toxic and readily tion of catalytic parameters such as conversion, available 3d metal-based catalysts. In additiselectivity, activity and productivity. In addition, on, computer-aided data evaluation and new the increase of catalyst stability, but also already simulation methods will be used to conserve the reduction of process steps by direct syntheresources. Electrocatalysis offers the potential ses can mean a more efficient use of resources. to substitute chemical oxidizing and reducing An illustrative example is the realization of a agents with electrical energy. so-called Dream reaction, the implementation

CATALYSIS FOR ENERGY (Dr. Henrik Junge) MAGNETIC RESONANCE & X-RAY METHODS (Dr. Jabor Rabeah) MICRO REACTION ENGINEERING (Dr. Norbert Steinfeldt) MOLECULAR ELECTROCHEMISTRY (Prof. Dr. Robert Francke) OPTICAL SPECTROSCOPIC & THERMOANALYTICAL METHODS (Dr. Christoph Kubis) PHOTOCATALYTIC CO<sub>2</sub> REDUCTION (Dr. Tim Peppel) REACTION MECHANISMS (Prof. Dr. Evgenii Kondratenko) REACTION ENGINEERING (Dr. David Linke) TECHNOLOGY ORIENTED PROCESSES (Dr. Udo Armbruster) UNI IN LEIBNIZ (Prof. Dr. Wolfram Seidel, Prof. Dr. Klaus Neymeyr, Prof. Dr. Malte Brasholz)

APPLIED CARBONYATIONS (Dr. Ralf Jackstell) INORGANIC FUNCTIONAL MATERIALS (Dr. Sebastian Wohlrab) **HIGH-THROUGHPUT TECHNOLOGIES** (Dr. Uwe Rodemerck) Homogeneous Catalysis for Life Sciences (Dr. Helfried Neumann) **Hydroformylations** (Dr. Jens Holz) CATALYST DESIGN FOR ELECTROSYNTHESIS (Dr. Bernd Müller) MICRO REACTION ENGINEERING (Dr. Norbert Steinfeldt) MOLECULAR ELECTROCHEMISTRY (Prof. Dr. Robert Francke)



SUSTAINABLE REDOX REACTIONS (Dr. Kathrin Junge) REACTION MECHANISMS (Prof. Dr. Evgenii Kondratenko) REACTION ENGINEERING (Dr. David Linke) SYNERGY BETWEEN HOMO- & HETEROGENEOUS CATALYSIS (NOW: CATALYSIS FOR SUSTAINABLE SYNTHESES) (Prof. Dr. Jagadeesh Rajenahally) TECHNOLOGY ORIENTED PROCESSES (Dr. Udo Armbruster) UNI IN LEIBNIZ (Prof. Dr. Thomas Werner)

## Topic 07 - New Products & Processes

Prof. Dr. Torsten Beweries Dr. Christian Hering-Junghans

The aim of the investigations in topic 07 is the development, characterization and testing of new catalysts and products as well as the establishment of new processes. Research in topic 07 is based on the long-standing expertise of LIKAT researchers in both fundamental and applied aspects of homogeneous and heterogeneous catalysis. Expertise in organometallic and coordination chemistry is combined with main group chemistry, photocatalysis as well as organocatalysis and complemented by aspects of heterogeneous catalysis. For this reason, the expertise of many research groups is pooled in topic 07. Since the establishment of the matrix structure in 2019, it is currently the most strongly staffed topic with a total of 36 FTEs and delivers a correspondingly large number of publications. In addition to industry-related research pro-

jects, basic research takes up a large part of the activities in topic 07. The relevance of this work lies, among other things, in the investigation of reactivities and the discovery of new methods that allow conclusions to be drawn about catalysis-related issues. Basic investigations on the catalyzed fluorination of organic molecules are, for example, the basis for the development of new synthesis processes in the agro- or pharmaceutical industry.

In the future, renewable raw materials are to be increasingly integrated as substrates in the research activities of topic 07 within the framework of the LIKAT 2030 strategy. In the sense of a circular economy, emphasis will be placed, among other things, on the recovery and reuse of catalyst components, such as precious metals or phosphorus, and polymer building blocks.

ACTIVATION OF SMALL MOLECULES (NOW: CATALYSIS WITH PHOSPHOROUS CONTAINING MATERIALS) (Dr. Christian Hering-Junghans) **APPLIED CARBONYATIONS** (Dr. Ralf Jackstell) INORGANIC FUNCTIONAL MATERIALS (Dr. Sebastian Wohlrab) Asymmetric Hydrogenations (now: Hydrogenations & Hydroformylations) (Dr. Jens Holz) **BIOINSPIRIERED CATALYSIS** (Prof. Dr. Paul Kamer) Homogeneous Catalysis for Life Sciences (Dr. Helfried Neumann) CATALYSIS OF EARLY TRANSITION METALS (Dr. Fabian Reiß) CATALYSIS FOR ENERGY (Dr. Henrik Junge) CATALYSIS OF LATE TRANSITION METALS (Prof. Dr. Torsten Beweries) CATALYSIS OF HETEROCYCLES

(Prof. Dr. Xiao-Feng Wu)

CATALYTIC FUNCTIONALIZATIONS (Dr. Jola Pospech) MODERN ORGANIC CHEMISTRY (Dr. Osama El-Sepelgy) SUSTAINABLE REDOX REACTIONS (Dr. Kathrin Junge) New Hydroformylation Catalysts (Dr. Detlef Selent) Organocatalysis (Prof. Dr. Thomas Werner) POLYMER CHEMISTRY & CATALYSIS (PD Dr. habil. Esteban Mejía) **REACTION MECHANISMS** (Prof. Dr. Evgenii Kondratenko) Selective Catalytic Synthesis Methods (vorm. Catalysis WITH RENEWABLE RESOURCES & PLATFORM CHEMICALS) (Dr. Sergey Tin)

Synergy between homo- & heterogeneous Catalysis (Prof. Dr. Jagadeesh Rajenahally)

UNI IN LEIBNIZ (Prof. Dr. Axel Schulz, Prof. Dr. Marko Hapke, Prof. Dr. Udo Kragl)







# **CURRENT PROJECTS**











## Tiny Species with Big Impact: High Activity of Cu Single Atoms on CeO<sub>2</sub>-TiO<sub>2</sub> Deciphered by *Operando* Spectroscopy

"More" does not always mean "better": Raising the copper content of a ceria-titania supported catalyst does not necessarily raise the catalytic activity for the oxidation of CO to CO<sub>2</sub>! This is surprising at first sight but can be explained after research combining a multitude of analytical methods, in particular spectroscopy under reaction conditions ("operando"). The optimal amount of copper was found to be 0.26 percent by weight, as under these conditions the distribution of the single atoms over the entire catalyst surface is at optimum.

This technically important reaction is realized predominantly with catalysts based on noble metals. Cost issues motivate research for alternatives and substitutes for those platinum-, rhodium-, palladium- or gold-based catalysts. A combination of cerium and copper oxides



Fig. 1: Relative Reactivity as function of the copper content in the catalyst. Overall CO conversion with the three catalysts (under identical conditions) amounts to 20%, 75% und 35% approximately, albeit the conversion (with respect to the mass of copper) is maximal for the catalyst on the left.

seems promising, and our research aimed at a better understanding and thus improvement of this system.

Catalysts were synthesized with a copper content between 0.06 and 0.86 percent by weight, supported on  $CeO_2$ -modified  $TiO_2$ . The catalytic performance was checked on a gas mixture of  $CO/O_2$ , heavily diluted with nitrogen. The catalyst was characterized extensively, prior to and after the use as well as during the reaction (in situ). The latter work was largely done using IR, EPR and X-ray photoelectron spectroscopy. The degree of conversion to  $CO_2$  was monitored by gas-liquid chromatography.

An optimum catalyst performance (Fig. 1) was found at 0.26 percent copper content, for a higher share of copper does favour aggregation (formation of copper/copper oxide clusters) on the support's surface. This clustering reduces the number of active centres. The observed photoelectron spectra let us conclude that there are electronic interactions (redox processes) between single copper and the cerium atoms, these are regarded beneficial for catalytic activity.

Our results<sup>[1]</sup> demonstrate the potential inherent in "single site catalysts", also known as "single-atom catalysts". These materials gain a lot of interest presently.<sup>[2]</sup> The reactivity of isolated atoms in interaction with their chemical surrounding (the catalyst support) requires more detailed investigation which is only possible if diverse methods and techniques are working together in a synergistic way as it is possible at LIKAT: The groups "Heterogeneous Catalytic Processes: Surface Chemistry", "Heterogeneous Catalytic Processes: Technology-Oriented Processes", "Heterogeneous Catalytic Processes: Inorganic Functional Materials", "Magnetic Resonance and X-ray Methods" and the Analytical Department contributed jointly to this work.

#### Scientific Contact: PD Dr. habil. Wolfgang Baumann

[1] J. Mosrati, A. M. Abdel-Mageed, T. H. Vuong, R. Grauke, S. Bartling, N. Rockstroh, H. Atia, U. Armbruster, S. Wohlrab, J. Rabeah, A. Brückner, *ACS Catalysis* 2021, *11*, 10933-10949. Tiny Species with Big Impact: High Activity of Cu Single Atoms on CeO<sub>2</sub>-TiO<sub>2</sub> Deciphered by Operando Spectroscopy.
[2] Special Issue on "Heterogeneous Single-Atom Catalysis": *Chemical Reviews* (Issue 21) 2020, *120*, 11699-12342.



Current Projects - Topic 01



## Preparation and Industrial Potential of Catalysts Based on Commercial ZnO and Oxidic Supports for Propane Dehydrogenation

Non-oxidative propane dehydrogenation to propene (PDH) is an important environmentally friendly alternative to oil-based cracking processes, to produce this vital platform chemical. The current PDH technologies using Pt- or Cr-containing catalysts suffer from high costs of Pt or toxicity of Cr(VI). Encouraged by the requirements of environmental sustainability, we developed a preparation method with a potential of large-scale applications to yield industrially relevant catalysts using commercially available ZnO and oxidic supports.

Motivated by low-costs and environmental compatibility of ZnO, our objective was to provide a preparation method, which is easily upscalable from grams to kilograms, to yield catalysts with industrially relevant PDH performance. We hypothesized that gas-phase metallic Zn atoms can be generated upon reduction of ZnO above the melting point of Zn and oxidized by support OH groups to form supported ZnO<sub>x</sub> species.

To prepare the catalysts, we simply mixed ZnO and SiO<sub>2</sub> supports or used a dual-bed approach

with ZnO being in the upstream bed (Fig. 1).<sup>[1,2]</sup> ZnO<sub>x</sub> species were generated on the surface of the support after treatment in a flow of H<sub>2</sub> at about 550°C. Their structure and concentration can be controlled through the topology of SiO<sub>2</sub> and the presence of defective OH groups. This conclusion was possible owing to combining



X(C<sub>3</sub>H<sub>8</sub>) / -0.0 STY(C<sub>3</sub>H<sub>6</sub>) / kg h<sup>-1</sup> kg<sup>-1</sup> cat 11111 ZnO was added ///// 0.0 100 200 250 50 150 300 350 400 Time on propane stream / h

Fig. 2: Propane conversion (X( $C_3H_8$ )) and space time yield of propene formation (STY( $C_3H_6$ )) over ZnO-S-1 (green) and K-CrO\_/Al\_2O\_3 (red) at 550 °C under different industrially relevant conditions

complementary methods from TG Kondratenko, TG Jiao, TG Linke, TG Rodemerck, TG Rabeah, TG Wohlrab and "Analytics" of LIKAT as well as groups of Prof. Grunwaldt (KIT, Karlsruhe), and Prof. Jiang (China University of Petroleum, Beijing). This approach is applicable to other commercial materials, e.g., Al<sub>2</sub>O<sub>2</sub>, AlSiO<sub>2</sub>, TiO<sub>2</sub>, ZrO<sub>2</sub>, TiZrO, and YZrO, that can anchor Zn atoms to form active ZnO species. Its industrial relevance was proven in a test with a physical mixture of ZnO and silicalite-1 (ZnO-S-1) over about 400 h on propane stream at 550°C under industrially relevant conditions (Fig. 2). In comparison with co-tested analogue of commercial K-CrO /Al<sub>2</sub>O catalyst, the mixture revealed about 3 times higher propene productivity with similar propene selectivity.

We are in contact with potential industrial partners. From a fundamental viewpoint, it is planned to further elucidate basics related to the effect of the kind of ZnO<sub>x</sub> species that can be controlled through the kind of support materials and defective OH groups on catalyst performance. The developed concept should also be extended to other metals. To this end, a DFG project is in preparation as well as internal studies are in progress.

Scientific Contact: Prof. Dr. Evgenii Kondratenko

[1] D. Zhao, X. Tian, D. E. Doronkin, S. Han, V. A. Kondratenko, J.-D. Grunwaldt, A. Perechodjuk, T. H. Vuong, J. Rabeah, R. Eckelt, U. Rodemerck, D. Linke, G. Jiang, H. Jiao, E. V. Kondratenko, *Nature* 2021, *599*, 234-238. *In-situ* formation of ZnOx species for efficient propane dehydrogenation.
[2] D. Zhao, K. Guo, S. Han, D. E. Doronkin, H. Lund, J. Li, J.-D. Grunwaldt, Z. Zhao, C. Xu, G. Jiang, E. V. Kondratenko, *ACS Catalysis* 2022, *12*, 4608-4617. Controlling Reaction-Induced Loss of Active Sites in ZnO./Silicalite-1 for Durable Nonoxidative

Propane Dehydrogenation.





## **Data Science Assisted Development of** CO, hydrogenation Catalysts for Hydrocarbon Production

Motivation: Carbon dioxide hydrogenation (CO<sub>2</sub>-Fischer-Tropsch (CO<sub>2</sub>-FT) to higher hydrocarbons is a potential solution to the CO<sub>2</sub> emission problem. Due to an increase in the number of scientific publications about this problem, it is becoming attractive to use modern methods for the analysis of the literature. It can help in the systematization and evaluation of the wide pool of data, extract latent knowledge as well as formulate new ideas. The main aim of the present study is to analyze the literature on CO. hydrogenation catalysts to find relationships between catalyst characteristics and performance as well as its experimental validation and usage for screening highly selective and active catalytic materials. Detailed information about catalytic performance, catalyst composition, reaction condition, etc. was extracted from scientific articles and converted into an SQL database. Because there are a lot of dependent catalytic parameters, we first developed an approach for transforming them into a small number of independent parameters to minimize correlation and thereby improve the significance of the analysis. Such parameters are the chain growth probability  $\alpha$  and excess

to CH, selectivity y estimated by the modified Anderson-Schulz-Flory distribution describing hydrocarbon selectivity [1]. The thermodynamic ratio  $n^{[2]}$  was estimated to analyze the approach to equilibrium of the reverse water gas shift (RWGS) reaction. Finally, random forest (RF) was applied to identify the most important parameters determining catalyst performance.

*Results*: It is generally accepted the process of CO<sub>2</sub> hydrogenation proceeds into two stages: the RWGS reaction followed by CO hydrogenation via the FT mechanism. In this case, the thermodynamic ratio  $\eta$  should be not higher than 1. However, when we estimated the ratio for all the catalysts from the obtained database, we found that around 20% data have the values of  $\eta$  higher than 1 (see Fig. 1A). The observed result can be explained by the presence of a direct route of CO<sub>2</sub> hydrogenation to higher hydrocarbons via the FT mechanism. To validate this 'hypothetical' pathway, we prepared the Fe-based catalyst using the organic combustion method and tested it under CO<sub>3</sub>-FT condition in a wide range of CO<sub>2</sub> conversion (see Fig. 1B).<sup>[3]</sup> It was found that for selectivity to C2+ hydrocarbons at zero CO<sub>2</sub> conversion estimated by the





data extrapolation is around 30 %. This indicates the presence of the direct pathway of CO<sub>2</sub> hydrogenation. In addition, XRD analysis of the spent catalyst allowed us to conclude that Fe<sub>c</sub>C<sub>2</sub> could be responsible for this direct hydrogenation of  $CO_2$  into  $C_2$ , hydrocarbons. The influence of reaction conditions and catalyst composition on parameters  $\alpha$  and  $\gamma$  which are the key parameters of catalyst selectivity were also analyzed. It was found that the parameters only slightly depend on the reaction conditions and, thus, are defined by the catalyst. Analysis of the parameters' importance showed that doping with alkali metals is the most effective measure for improving catalyst performance. The obtained results were used for developing the strategy of screening selective and active CO<sub>2</sub>-FT catalysts (our path in the catalyst development is presented in Fig. 1C) that confirmed the effectiveness of the data analysis.

Conclusions: The literature data analysis and the derived experiments expanded the understanding of the CO<sub>2</sub>-FT process. This led to the development of well-performing catalysts for producing hydrocarbons from CO<sub>2</sub>. In summary, modern ML and data science methods can be recommended for the analysis of literature data in catalysis. They can accelerate scientific work and help in formulating new ideas and hypotheses.

Financial support from BMBF through the project InnoSyn (FKZ: 03SF0616B) is gratefully acknowledged.

Scientific Contact: Dr. David Linke

[1] A. Fedorov, D. Linke, J. CO2 Util. 2022, 61, 102034. Data Analysis of CO2 Hydrogenation Catalysts for Hydrocarbon Production. [2] Y. Xu, P. Zhai, Y, Deng, J. Xie, X. Liu, S. Wang, D. Ma, Angew. 2020, 132, 21920-21928. Highly Selective Olefin Production from CO.

Hydrogenation on Iron Catalysts: A Subtle Synergy between Manganese and Sodium Additives. [3] A. Fedorov, H. Lund, V. A. Kondratenko, E. V. Kondratenko, D. Linke, Appl. Catal. 2023, 122505. Elucidating reaction pathways occurring in CO<sub>2</sub> hydrogenation over Fe-based catalysts.



## Development of Catalysts from (Rice) Biowaste



Rice, or padi, is by far the most important food crop for human consumption and the main food source for more than one-third of the world's population. Padi fields occupy more than 10% of the world's cultivated area, resulting in an estimated global production of 501.96 million tons in 2020. The management and disposal of non-edible rice by-products, mainly rice husks and straw, therefore poses an environmental challenge as traditionally large quantities of these products are burned in the open. While this practice is convenient for farmers, it releases large amounts of greenhouse gases and particulate matter into the atmosphere.

Therefore, developing strategies for sustainable management and utilization of agricultural rice waste is of great importance. Due to the high (Fig.: Esteban Mejía)

content of silica in rice husk (up to 25 wt%), many research efforts have been devoted to the extraction and use of this biogenic silica as a support material for heterogeneous catalysts. The objective of this work, the use of rice husk, which is an agricultural waste, for the synthesis of catalytically active materials, is both: 1) to utilize a resource that actually grows in the fields, and

2) to reduce the energy requirements of chemical processes by using a catalyst.

In summary, the use of rice husk for the development of hydrogenation catalysts was realized in this work. The preparation of the Ag-based catalyst for nitro group reduction showed that it is in principle possible to fix

metal ions to rice husk and to convert them particles and combines it with a simple and strainto catalytically active particles by carbotherightforward synthesis approach. mal reduction. The second step of the project In conclusion, the alternative ways of rice husk showed that the methodology can be transferutilization presented in this work can be apred to the use of other metals as active sites. plied to various hydrogenation reactions using Therefore, the Co-based catalyst was prepared different metals and the production of sanitary by introducing Co in the form of nitrogen-rich materials. complexes. In addition, the catalytic properties However, such alternative treatment methods as well as the recycling stability of the prepared must first gain the trust and acceptance of those catalyst were optimized by base etching the carmost affected: the rice farmers. Otherwise, the bon-silica composite structure of the rice husk traditional method of open burning will remain support. The catalyst was used for the reduction the applied solution to the waste problem, as of nitro groups. Finally, a Ni-based catalyst was it ensures smooth rice production and thus the used for the reductive conversion of epoxides to livelihood of about 4 million people in Vietnam anti-Markovnikov alcohols. The catalytic perforalone. Therefore, it is of utmost importance that mance of the three model systems was evaluaresearch such as the one presented here is not ted by reaction optimization, extensive substraonly discussed and presented within the scientite screening, and kinetic studies. In addition, the fic community, but also presented to the authostructure-activity relationships of the prepared rities and the staff of the affected communities. catalysts were investigated using various characterization methods such as XRD, XPS, TPD, BET- surface analysis, EA, IR, and SEM and STEM Scientific Contact: microscopy techniques. Thus, the catalytic active PD Dr. habil. Esteban Mejía sites were identified and the mode of action was revealed.

In addition, the prepared Ag-containing material was successfully tested as an antimicrobial agent. It was shown that the Ag nanoparticles on pyrolyzed rice husk possess antimicrobial activity against the ESKAP pathogens and pathogenic yeasts at extremely low levels. The presented method benefits from the wellknown antimicrobial mode of action of Ag nano





## Simple and Scalable Electochemical Approach to Hypervalent Bromine(III) Compounds

Recently, an electrochemical synthesis of unusual OCO pincer complexes of Br(III) has been reported. In general, hypervalent bromine(III) compounds have been little studied in contrast to the isoelectronic iodine(III) compounds, which may be due to the difficult-to-control reactivity as well as the conventional synthetic route via the highly toxic and corrosive bromine trifluoride. Given the wide range of catalytic and stoichiometric applications of iodine(III) compounds and the interesting properties of their Br(III) analogs (higher electrophilicity and oxidation potentials), the potential for application is expected to be high. Compared to the known highly reactive organobromine(III) compounds, the investigated OCO-pincer complexes offer the advantage that the intrinsic reactivity is locked by the triple coordination and can be released on demand by the addition of Lewis acids. The preparative utility has already been demonstrated by successful use in oxidative arene-arene and amide-arene couplings.

The first hypervalent iodine(III) compounds were synthesized as early as 1886 by Conrad Willgerodt, just 75 years after the discovery of the element iodine. However, it is only in the last few decades that synthetic chemists have become aware of the advantages of this class of compounds, which has led to an upsurge in count-



Electrosynthesis of hypervalent Br(III) compounds.



Comparison between conventional and electrochemical access to bromanes

less areas of application. The growing interest in these compounds is due to their mild properties combined with their environmentally friendly nature and ease of handling, but most importantly, their facile availability. A few of them are now also commercially available. Bromine(III) compounds promise a greatly expanded field of applications. So far, only the difficult synthesis and the resulting limited availability have prevented a similar development. A simplified, electrochemical approach to hypervalent Br(III) compounds could change that. A chelation-stabilized aryl- $\lambda^3$ -bromane has already been described by Martin et al. The product itself is stable to air and moisture. However, for its synthesis, bromine trifluoride must be used as an oxidizing agent. The highly toxic BrF, attacks even glass and is not a standard chemical in a synthetic laboratory. Electric current is to replace the "unloved chemical" BrF<sub>2</sub>.

The anodic oxidation of aryl bromides succeeds in an undivided cell with glassy carbon as working electrode, platinum as counter electrode, tetrabutylammonium tetrafluoroborate as supporting electrolyte and hexafluoroisopropanol (HFIP) as solvent. By scaling up the electrolysis, gram quantities of bromane are readily available in over 70% yield with a high purity.

The synthetic utility of these compounds has

already been demonstrated in oxidative biaryl and amide-arene couplings, as well as oxidative cyclization of Schiff bases to benzoxazoles.

The developed electrochemical synthesis for  $\lambda^3$ -bromanes offers significant advantages over existing methods that rely on highly toxic, hazardous, and difficult-to-handle BrF<sub>3</sub> as a key reagent. Therefore, we believe that our approach can open the door for the development of entirely new synthetic transformations that could benefit from the unique properties of hypervalent bromine(III) species.

#### Scientific Contact:

Prof. Dr. Robert Francke

N. Mohebbati, I. Sokolovs, P. Woite, M. Lokov, E. Parman, M. Ugandi, I. Leito, M. Roemelt, E. Suna, R. Francke, *Chem. Eur. J.* **2022**, *28*, e202200974. Electrochemistry and Reactivity of Chelation-stabilized Hypervalent Bromine(III) Compounds.
 I. Sokolovs, N. Mohebbati, R. Francke, E. Suna, *Angew. Chem. Int. Ed.* **2021**, *60*, 15832-15837. Electrochemical Generation of Hypervalent Bromine(III) Compounds.





# IREKA and SEGIWA to Implement the National Hydrogen Strategy

In 2020, the National Hydrogen Strategy was launched by the German government with the declared aim of establishing Germany as international pioneer and market leader in hydrogen technologies. In order to achieve this, three flagship projects have been funded by the BMBF.

The Topic 05 (RG Francke, RG H. Junge and RD Wohlrab) is involved with two different projects in the hydrogen flagship project "Upscaling and series production of electrolyzers" (H2Giga). The goal of H2Giga is the development and construction of 5 GW of electrolyzer capacity in Germany until 2030, to fulfil the continuously growing demand for hydrogen. In H2Giga's innovation pool, projects such as the network project IREKA, which is directed by LIKAT, are funded to investigate and develop processes, technologies and components related to electrolysis. Another LIKAT project is funded under the leadership of Siemens Energy in the joint project SEGIWA, a scale-up project to develop and establish technologies for the large-scale production of PEM electrolyzers. Both projects are coordinated by A.-E. Surkus.

The PEM electrolysis is based on the application of IrO, as anode catalyst. Until now, there is no real alternative for this electrocatalyst, since the highly acidic and oxidative conditions at the anode lead to rapid corrosion. With steadily increasing energy consumption, the demand for iridium will exceed the available resources in a few decades. As a result, the price of iridium as well as the technologies based on it will continuously increase. An enhancement of PEM electrolysis capacities on a large scale can therefore only be realized in the long term if the application of iridium is significantly reduced. The joint project IREKA therefore aims at reducing the iridium content of PEM anodes while maintaining catalytic activity and stability. In the LIKAT project SEGIWA, the most promising candidate will then be scaled up in its synthesis and made available to the collaborative partners as an alternative anode material for industrial application tests.

In the LIKAT subproject IREKA, the iridium content will be reduced by supporting it, and the morphology of the composite will be modified in such a way that the catalytically active centers are distributed more homogeneously and easier to reach for water oxidation. This should compensate for the activity setbacks that are otherwise to be expected due to the reduced iridium content. To compensate for the potential reduction in electrical conductivity, doping of the carrier is also envisaged, with the aim of improving corrosion resistance in the process. Another approach is the incorporation of an additional, readily available metal that is protected from corrosion by the presence of iridium and at the same time assists the iridium in catalysis.

Three LIKAT research groups are collaborating to implement these plans; the RG "Catalysis for Energy", which is concerned about examining ways and means of immobilizing the iridium on a support, the RG "Surface Chemistry in Applied Catalysis", which focuses on improving the morphological properties of the support and the composite, and the RG "Molecular Electrochemistry", which is investigating electrochemical testing for catalytic suitability for acid water oxidation.

An external partner in IREKA is the department of electroplating at IPA Stuttgart, who is utilizing its expertise to fabricate iridium-containing coatings.

The IREKA and SEGIWA projects were launched in spring 2021 with a four-year duration. In the previous project period, the synthesis of a supported Ir-Sn-oxide was successfully achieved, which exhibits a similarly low overvoltage compared to the IrO<sub>2</sub> materials that have been used industrially so far, and an improved exchange current density with respect to its iridium content, which has been significantly reduced.



Scientific Contact:

Prof. Dr. Robert Francke, Dr. Sebastian Wohlrab, Dr. Henrik Junge, Dr. Annette-Enrica Surkus

(Photo: Tobias Täufer)



## Development of Stable Heterogeneous Single-Atom Catalysts for Oxidation Catalysis

SACs (Pd, Ru and Pt) and examining their applicability for the above discussed reactions.

Scientific Contact: Dr. Ali Abdel-Mageed

Optimizing heterogeneous single-atom catalysts (SACs) is essential to step them up for industrial applications. This is done through the systematic modulation of their physicochemical properties, their catalytic testing in industrially relevant processes, and eventually characterization with operando methods to establish structure-reactivity relationship. We focus in this project on heterogeneous Cu-SACs for oxidation catalysis. First is CO oxidation which serve as test reaction and also applied in catalytic after-treatment, and in PEM fuel cells. Second is water-gas-shift (WGS) used in the production and cleaning of hydrogen after hydrocarbon reforming.

Objectives are (i) the synthesis of heterogeneous Cu-SACs supported on  $CeO_2$ -TiO<sub>2</sub>, (ii) the catalytic testing in CO oxidation and LT-WGS and (iii) *operando* characterization with different methods.

Guided by earlier results on Cu-SACs supported by Zr-based UiO-66 and understanding of their structure-reactivity relationship,<sup>[1]</sup> we optimized one-pot-synthesis of CeO<sub>2</sub>-TiO<sub>2</sub> supported Cu-SACs and studied their catalytic activity in CO oxidation and LT-WGS. The CO oxidation activity of Cu/CeO<sub>2</sub>-TiO<sub>2</sub> SACs can be fine-tuned by modulating the Ce/Ti ratio. The catalytic activity obeys a volcano-shaped dependence of Ce/Ti molar ratio with the catalytic activity culminating at Ce/Ti ratio around 0.18, while keeping at the same time Cu loading well below 0.1 wt.%.[2] Findings from a multitude of characterizations indicated that isolated Cu single sites build into small CeO, nanoparticles dispersed homogeneously on TiO<sub>2</sub>. The change in Ce/Ti ratio was found to modulate the redox properties of Cu1+/  $Cu^{2+}$  and  $Ce^{3+}/Ce^{4+}$  redox shuttles, and thus catalytic activity. These materials were further tested in the low-temperature water-gas-shift (WGS) reaction between 300 and 180°C. We found out that Cu/CeO<sub>2</sub>-TiO<sub>2</sub> (Ce/Ti  $\approx$  0.18) is in the same order of activity to the highly acti-



Fig.: Front cover of work published in *ChemCatChem* highlighting the structure relationship established for optimized heterogeneous Cu-SACs in CO oxidation.<sup>[2]</sup> DOI: 10.1002/cctc.202300441

ve supported Au catalysts.<sup>[3,4]</sup> Cu-SACs showed, however, higher stability during reaction on stream compared to Au-based catalysts which deactivate strongly during reaction (results prepared for submission).

Appling optimized materials for liquid phase solvent-free aerobic oxidation of primary alcohols to useful chemicals. Furthermore, similar synthetic methodologies shall be endeavored for the architecture of precious metal-based  A. Abdel-Mageed, B. Rungtaweevoranit, X. Pei, O. Yaghi, J. Behm, J. Am. Chem. Soc. 2019, 141, 5201-5210.
 A. Abdel-Mageed, S. Cisneros, J. Mosrati, H. Atia, T. Vuong, N. Rockstroh, S. Wohlrab, A. Brückner, J. Rabeah, ChemCatChem 2023, e202201669.
 A. Abdel-Mageed, G. Kučerová, J. Bansmann, J. Behm, ACS Catal. 2017, 7, 6471-6484.
 J. Carter, A. M. Abdel-Mageed, D. Zhou, D. J. Morgan, X. Liu,

[4] J. Carter, A. M. Abdel-Mageed, D. Zhou, D. J. Morgan, X. Liu, J. Bansmann, S. Chen, J. Behm, G. Hutchings, ACS Nano 2022, 16, 15197–15205.



## Synthesis of Fluor-containing Builing Blocks with CF<sub>2</sub> Function for Drug Discovery

It has been known for years, that fluorochemical drugs increase the activity and bioavailability. Characteristics like solubility, metabolic stability, hydrogen bonding ability, lipophilicity and chemical reactivity are strongly influenced by fluorochemical building blocks. Fluoroalkylations have gained in importance in the last years visible also by the big increase of publications in this field (Fig. 1a). Prominent examples for fluorination agents, which can transfer a CF<sub>3</sub> or CHF group, are summarized in Fig. 1b. Less known are reagents which contain a CF<sub>2</sub>-R unit. It is thus the objective to synthesize building blocks with a CF<sub>2</sub> function, which can be utilized in the synthesis of drugs.

In the last years we are focused our attention on the synthesis of fluorochemical compounds. We succeeded in preparing gem-difluoroallylammoniumsalts (DFAAs), which can be used as difluoromethylation agents.<sup>[1]</sup> Especially, the air and water stable 3,3-difluoropropen-1-yl piperidiniumtriflate is synthesized easily in a twostep procedure and is useful because a gem-difluoroallyl unit can be transferred to O-, N-, S-, C-

and Se-nucleophiles without any metal catalyst. The synthesis of 3,3-difluoropropen-1-yl piperidiniumtriflate starts from pipridine and 3,3,3-trifluoropropene, which are converted via base to  $\gamma$ ,  $\gamma$ -difluoroally lpiperidine. Subsequent N-methylation with methyl triflate gives the desired piperidinium salt, which can be prepared in gram scale.<sup>[1]</sup> Especially, interesting is the allylic substitution with O and N nucleophiles, since the structure motifs RCF<sub>2</sub>-O und RCF<sub>2</sub>-N can be easily formed, that otherwise is not simply accessible.<sup>[2]</sup> Now, the allylic function is used for building up analogous active agents. More specifically, we were able to prepare the drugs Pramocaine und Aripripazole containing the gem-CF<sub>2</sub> unit.<sup>[3]</sup>

It shall be demonstrated, that the 3,3-difluoropropen-1-yl piperidiniumtriflate agent is useful in other drug syntheses. For example, the allylic double bond is epoxidized and the formed epoxide is opened by a piperazine derivative. The resulting structure motif occurs in many drugs (Fig. 2). Finally, the modified drugs were tested for biological activity.



Fig. 1: a) Increase in publications on fluoroalkylation reactions. b) Important examples of fluorinating agents that can transfer a CF<sub>2</sub> or CH<sub>2</sub>F group.



#### Fig. 2: Preparation of difluoromethylation reagent (bo S-, C, and Se-nucleophiles without metal catalyst.

The study has shown, that 3,3-difluoropropen-1-yl piperidiniumtriflate can be produced with piperidine and industrial used 3,3,3-tri-fluoropropene in a base catalyzed reaction. The compound is air and water stable and can be employed as a difluoromethylation agent. The agent reacts with O-, N-, S-, C- and Se-nucle-ophiles in exclusively  $\gamma$ -regioselectivity to gem-difluoroallyl compounds without usage of a metal catalysts. Some products can be used for setting up modified active agents.



Fig. 3: Epoxidation of allylic function and subsequent opening of the resulting epoxide with piperazine derivatives.

Scientific Contact: Dr. Helfried Neumann

[1, 2, 3] F. Ye, Y. Ge, A. Spannenberg, H. Neumann, L-W. Xu, M. Beller, *Nat. Commun.* **2021**, *12*, 3257. [4] S. Kopf, F. Ye, H. Neumann, M Beller, *Chem. Eur. J.* **2021**, *27*, 9768 –9773. [5] P. Wang, Y. Wang, H. Neumann, M. Beller, *Chem. Sci.* **2022**, *13*, 13459-13465. [6] P. Wang, J. Yang, K. Sun, H. Neumann, M. Beller, *Org. Chem. Front.* **2022**, *9*, 2491.

Fig. 2: Preparation of difluoromethylation reagent (box) and transfer of a gem-difluoroallyl group to O-, N-,



**Research Groups** 

## **Applied Carbonylations**

#### Dr. Ralf Jackstell ralf.jackstell@catalysis.de

The research group "Applied Carbonylations" is equally dedicated to basic research [e.g. within the framework of BMBF, BMWI and EU projects (PlasCO<sup>2</sup>, Cooperate, EWiMe4) as well as in cooperation with other university institutions (e.g. University of Aarhus, Oslo) and industry] and application-oriented research (cooperation with industry, e.g. Evonik, BASF, Astra Zeneca, Creative Quantum, Miltiz Aromatics, Rafflenbeulanlagenbau, Ils, etc.).

The focus is on hydroformylation, alkoxycarbonylation, hydroxycarbonylation and hydroaminomethylation with industrially relevant raw materials (such as olefins, alkynes, alcarbons, carbon dioxide) to industrially relevant products (such as aldehydes, carboxylic acids, esters, amines, alcohols) for applications in polymer chemistry (monomers, plasticizers, alternative fuels, etc.).

The hydrogenation of CO to methanol is investigated until it is ready for application in mini-plant plants.

Another research topic is dedicated to the low-temperature plasma-induced hydrogenation of CO<sub>2</sub> to CO as well as the low-temperature plasma-induced "dry reforming" of CO<sub>2</sub> and methane to CO as a C1 building block. In order to contribute the transfer into industrial applications, process-accompanying research is one of our tasks. This includes, for example, the investigation of activity, stability and selectivity behavior of new catalysts in new reactions to known and new products of industrial significance as well as the production of product samples for application-related investigations in industry in the kilogram range.

Another focus is on the development and testing of new homogeneous and heterogeneous catalysts for carbonylation reactions and CO<sub>2</sub> hydrogenations with known precious metals and alternative catalyst metals such as iron, cobalt, manganese, ruthenium or iridium. The direct co-development and test runs of small demonstration plants in cooperation with industrial partners and university institutions are also part of the research activities. They are used to validate important process parameters in hydrogenation reactions of carbon monoxide and carbon dioxide.

(Photo: ©Eikelpoth/Evonik AG)



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## Sustainable Redox Reactions

Dr. Kathrin Junge kathrin.junge@catalysis.de



Fig. 1: Cover for Cobalt catalyzed formation of ethers (left, DOI: 10.1002/chem.202200379) and for nickel catalyzed hydrodehalogenation (right, DOI: 10.1002/cssc.202200247).

In the topic "Sustainable Redox Reactions", catalysts are developed for various model reactions in the field of oxidation and reduction reactions (hydrogenation of carboxylic acid derivatives). Here, the focus is particularly on base metals such as iron, cobalt, manganese, nickel and, more recently, molybdenum (Fig. 1-2).<sup>[1, 2]</sup>

Based on our homogeneous background the research group is aspecially focused on the synthesis of pincer type complexes which allow a very efficient tuning of catalyst properties. But also, heterogeneous catalyst systems are studied for more than 10 years.<sup>[3]</sup> The aspect of sustainability plays an important role, which is reflected in the choice of readily available and inexpensive catalyst metals as well as in the establishment of novel catalyst support from industrial waste. The catalysts are tested using autoclave technology, whereby both parallel screening on a ml scale and upscaling experiments up to a 2-liter scale can be realized (Fig. 2). For the synthesis of homogeneous catalysts, Schlenk and glovebox techniques are used,

[1] W. Li, J. Rabeah, F. Bourriquen D. Yang, C. Kreyenschulte, N. Rockstroh, S. Bartling, A.-E. Surkus, K. Junge, A. Brückner, A. Lei, M. Beller, *Nature Chemistry* **2022**, *14*, 334–341, Scalable and Selective Deuteration of (Hetero)arenes. [2] F. Bourriquen, N. Rockstroh, S. Bartling, K. Junge, M. Beller, *Angew. Chem.* **2022**, *137*, e202202423, *Angew. Chem. Int. Ed.* **2022**, *61*, e202202423, Manganese catalysed deuterium labelling of anilines and electron-rich (hetero)arenes. [3] N. F. Both, A. Spannenberg, K. Junge, M. Beller, *Organometallics* **2022**, *41*, 1797–1805, Low-valent Molybdenum PNP Pincer Complexes as Catalysts for the Semihydrogenation of Alkynes (Special issue).

Research Groups

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while heterogeneous materials are produced using pyrolysis.

As part of the recent, growing significance of sustainability and the shortage of resources, industry has an increasing interest in the development of environmentally benign, non-noble metal catalysts. The research group has longstanding experiences with industrial collaborations in various fields (pharmaceuticals, life science, agrochemicals). We are working on application-oriented problems in the field of redox reactions with high flexibility. In a European cooperation with partners from research and industry, catalysts for deuteration reactions have recently been developed.



Fig. .2: Device for parallel reactions in the autoclave. (Photo: K. Junge/LIKAT)

## **Theory of Catalysis**

#### Prof. Dr. Haijun Jiao haijun.jiao@catalysis.de

In the past two years we have been involved in several internal projects and international cooperation from physical organic chemistry, organometallics, homogeneous and heterogeneous catalysis and published 34 scientific papers. Our goal was the understanding and rationalization of the mechanisms of catalytic reactions. Some selected results are summarized and emphasized.

The first example is the conversion mechanisms of  $CO_2$  and  $H_2$  in methanol to dimethoxymethane catalyzed jointly by metallic  $[P_3Co-H]^+$ catalyst and HNTf<sub>2</sub> acid co-catalyst in a domino sequence.<sup>[1]</sup> The full conversion has the steps of Co-catalyzed hydrogenation of  $CO_2$  and HCOOCH<sub>3</sub>, and acid-catalyzed methylation of HCOOH and  $CH_3OCH_2OH$ . Our study shows the individual role of metal and acid and the need of their combination.

The second example is a joint investigation into the reaction mechanism of the regio-divergent reductive opening of epoxides by catalytic hydrogenation using a CpFe(CO)<sub>3</sub> complex.<sup>[2]</sup> DFT study rationalized the different activity and selectivity of aryl and aliphatic epoxides and explained role of a Lewis acid co-catalyst in the reaction of aliphatic epoxide. A multistep reaction mechanism was proposed on the basis of kinetic analysis, deuterium labeling and computational studies.

The third example is a joint investigation into the reaction mechanism of propane dehydrogenation.<sup>[3]</sup> DFT study identified the reduced binuclear  $Zn_2O_x$  cluster on the defect surface zeolite as the active catalyst and rationalized observed activity and selectivity. A reasonable reaction mechanism was proposed (Fig below).

## **Catalysis for Energy**

#### Dr. Henrik Junge henrik.junge@catalysis.de

Since 2003, the "Catalysis for Energy" group has been working on the production of hydrogen from renewable energies and raw materials, chemical storage, and the use of green hydrogen for carbon dioxide utilization through the synthesis of energy carriers and industrially relevant products (e.g. carbon monoxide, formic acid, methanol).

This is in line with a globally important research focus. In order to make practical contributions to the use of renewable energies as well as carbon dioxide as a C1 building block, we are currently working together with other partners on two projects to realize demonstration plants in LIKAT's pilot plant. Catalysts and technologies developed in our group for hydrogen production from methanol as well as hydrogen storage in aqueous formate solutions are used. Another



[1] Z. Wei, X.-X. Tian, M. Bender, M. Beller, H. Jiao, ACS Catal. 2021, 11, 6908-6919. [2] L. Tadiello, B. M. Stadler, S. Tin, H. Jiao, J. G. de Vries, T. Gandini, L. Pignataro, C. Gennari, ACS Catal. 2022, 12, 235-246. [3] D. Zhao, X.-X. Tian, D. E. Doronkin, S. Han, V. A. Kondratenko, J.-D. Grunwaldt, A. Perechodjuk, T. H. Vuong, J. Rabeah, R. Eckelt, U. Rodemerck, D. Linke, G. Jiang, H. Jiao, E. V. Kondratenko, Nature 2021, 599, 234-238.



[1] E. Alberico, T. Leischner, H. Junge, A. Kammer, R. Sang, J. Seifert, W. Baumann, A. Spannenberg, K. Junge, M. Beller, *Chem. Sci.* **2021**, *12*, 13101-13119; HCOOH Disproportionation to MeOH promoted by Molybdenum PNP Complexes. [2] J. Schneidewind, Miguel A. Argüello Cordero, H. Junge, S. Lochbrunner, M. Beller, *Energy Envir. Sci.* **2021**, *14*, 4427-4436; Two-photon, visible light water splitting at a molecular ruthenium complex. [3] D. Wei, R. Sang, P. Sponholz, H. Junge, M. Beller, *Nature Energy* **2022**, *7*, 438-447; A carbon-neutral chemical hydrogen battery based on formic acid.



highlight from the reporting period is the successful use of amino acids (lysine, arginine, their salts, amino acid-based ionic liquids) for carbon dioxide capture from air and subsequent hydrogenation to formate. This work enables the development of a CO<sub>2</sub>-based cycle for hydrogen storage (hydrogen battery) without the release of carbon dioxide and without the use of toxic amines or corrosive bases. In further work, molybdenum-catalysed formic acid disproportionation to carbon dioxide, methanol and methyl formate was developed. So far, only noble metals (Ir, Ru) have been used for this reaction. For our chemical conversions we develop and synthesize organometallic complexes as well as supported nanoparticles and "single atoms", which are then used in classical thermal as well as photocatalytic reactions. In particular, non-precious metals also play a crucial role. To realise our goals, we are working together with various partners from science and industry.

## **Catalysis for Life Sciences**

#### Dr. Helfried Neumann helfried.neumann@catalysis.de

One goal is the synthesis of fluorochemical building blocks for drug research, which are utilizing the preparation of pharmaceutical products. It has been known for years, that fluorochemical drugs increase the activity and bioavailability. Beside fluorine chemistry the other goal is the deuteration of arenes via CH activation. Deuterium in drugs have a positive influence, like fluorine on activity and bioavailability. In cooperation with Evonik our goal is the industrial application of efficient catalysts in the methoxycarbonylation of octene mixtures to esters. The resulting products are precursors for plasticizer. Currently a pilot plant is testing the stability of the catalysts. We are also interested in the optimization of classical coupling reactions like aminocarbonylation and alkoxycrbonylation with inert chloroarenes.

In the last years we are focused our attention on the synthesis of fluorochemical compounds



as well deuteration reactions. Deuterium und fluorochemical compounds play an important role in the drug research. We are successful in the syntheses of a difluoromethylation agent,<sup>[1]</sup> which can transfer a gem-difluoroallyl unit on O, N, S, C and Se nucleophiles without metal catalyst.<sup>[2]</sup> In subsequent reaction sequences analogous pharmaceuticals can be synthesized.<sup>[3]</sup> In the second main research we have developed H/D ruthenium-catalyzed exchange reactions of aromatic carbonyl compounds. This kind of reaction is possible in the presence of a transgene amine as an auxiliary, which is removed after the deuteration.<sup>[4]</sup> Finally, we have developed for the classical alkoxycarbonylation a palladium<sup>[5]</sup> and for aminocarbonylation a ruthenium catalyst,<sup>[6]</sup> which can convert in combination with Nal respective CsCl inert chloroarenes.





[1],[2],[3] F. Ye, Y. Ge, A. Spannenberg, H. Neumann, L-W. Xu, M. Beller, *Nat. Commun.* **2021**, *12*, 3257. [4] S. Kopf, F. Ye, H. Neumann, M Beller, *Chem. Eur. J.* **2021**, *27*, 9768 –9773. [5] P. Wang, Y. Wang, H. Neumann, M. Beller, *Chem. Sci.* **2022**, *13*, 13459-13465. [6] P. Wang, J. Yang, K. Sun, H. Neumann, M. Beller, *Org. Chem. Front.* **2022**, *9*, 2491.

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#### Prof. Dr. Torsten Beweries torsten.beweries@catalysis.de

The group investigates fundamentals of catalyses of late transition metal complexes on the basis of preparative and mechanistic organometallic chemistry. The aim is to gain insights into the optimisation of catalytic processes by studying structure-activity relationships. The focus is on various aspects of the activation and transformation of amine boranes as well as small, unreactive molecules such as H<sub>2</sub>O, N<sub>2</sub>,  $CO_2$ , or  $H_2$ .

In recent years, work has focused on the development of new catalysts with PCP and PNP pincer ligands for the catalytic dehydrocoupling and polymerisation of amine-borane adducts to oligo- and polyaminoboranes. These compounds are isovalence electronic to ubiquitous polyolefins and show great potential as molecular precursors for new B-N materials.

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Thus, dehydropolymerisation with a rhodium-bis(thiophosphinite) complex of the type  $[(^{R}PSCSP^{R})Rh(H)(Cl)]$  (R = Ph, *i*Pr) could be realised and investigated mechanistically in detail. <sup>[1a]</sup> Furthermore, the synthesis of analogous iridium complexes<sup>[1b]</sup> succeeded, which can be used for further organic coupling and hydroelementation reactions. In collaboration with the Hering-Junghans group, the coordination chemistry of P,N-based phosphaalkene ligands on rhodium and iridium was investigated.<sup>[2]</sup> The complexes are subject to interesting activations of the phosphaalkene ligand, which lead to the formation of a series of novel phophane-phosphaalkene complexes. Currently, the main focus is on the development and use of cooperative pincer ligands<sup>[3]</sup> for the activation and coupling of amine-boranes.



[1a] P. Hasche, J. Haak, F. Anke, C. Kubis, W. Baumann, H. J. Drexler, H. J. Jiao, T. Beweries, Catal. Sci. Technol. 2021, 11, 3514-3526. [1b] A. Linke, D. Decker, H.-J. Drexler, T. Beweries, Dalton Trans. 2022, 51, 10266-10271. [2] a) P. Gupta, T. Taeufer, J.-E. Siewert, F. Reiß, H.-J. Drexler, J. Pospech, T. Beweries, C. Hering-Junghans, Inorg. Chem. 2022, 61, 11639-11650; b) P. Gupta, H.-J. Drexler, R. Wingad, D. Wass, E. Baráth, T. Beweries, C. Hering-Junghans, Inorg. Chem. Front. 2023, 10, 2285-2293. [3] D. Decker, Z. Wei, J. Rabeah, H.-J. Drexler, A. Brückner, H. Jiao, T. Beweries, Inorg. Chem. Front. 2022, 9, 761-770.

## **Catalysis of Early Transition Metals**

Dr. Fabian Reiß fabian.reiss@catalysis.de



Our group investigates the fundamentals of This class of compounds was investigated in our catalytic processes that occur at early transition research group with regard to their catalytic acmetal complexes. Our main focus is on the rich tivity for the dehydrocoupling of amine-borane chemistry of sandwich complexes of titanium, adducts<sup>[2]</sup> and silanes.<sup>[3]</sup> zirconium and hafnium, so-called metallocenes. This type of compounds allows us to explore the limits of experimentally feasible binding motives and to stabilise highly strained 1-metallacyclobuta-2,3-dienes, which are organometallic analogues of the non-existent 1,2-cyclobutadiene. We succeeded in the synthesis and complete characterisation of two representatives of the previously unknown 1-zirconacyclobuta-2,3-dienes. Unprecedented intramolecular C-H activation was revealed and reactivity studies of this new class of compounds were performed.<sup>[1]</sup> The reactivity of these compounds is so far largely dominated by classical insertion reactions. Detailed quantum mechanical bond theory analyses revealed the structure-property relationships of this class of compounds and identified the ansa-metallocenes as the only type of complexes that can stabilise them. Classical metallocenes, under the same synthesis conditions, lead to bimetallic complexes in which two group 4 metals are bridged via an allene unit.

[1] X. Shi, S. Li, M. Reiß, A. Spannenberg, T. Holtrichter-Rossmann, F. Reiß, T. Beweries, Chem. Sci. 2021, 12, 16074-16084. 1-Zirconacyclobuta-2,3-dienes: synthesis of organometallic analogs of elusive 1,2-cyclobutadiene, unprecedented intramolecular C-H activation, and reactivity studies. [2] K. Lindenau, N. Jannsen, M. Rippke, H. Al Hamwi, C. Selle, H. J. Drexler, A. Spannenberg, M. Sawall, K. Neymeyr, D. Heller, F Reiß, T. Beweries, Catal. Sci. Technol. 2021, 11, 4034-4050. Mechanistic insights into dehydrocoupling of amine boranes using dinuclear zirconocene complexes. [3] K. Lindenau, A. Spannenberg, F. Reiß, T. Beweries, RSC Adv. 2022, 12, 26277-26283. T. Mono- and dinuclear zirconocene(iv) amide complexes for the catalytic dehydropolymerisation of phenylsilane.



## **Mechanisms of Homogeneous Catalysis**

## **Catalytic Functionalizations**

#### Dr. Hans-Joachim Drexler hans-joachim.drexler@catalysis.de

Our group investigates catalyst activation and deactivation phenomena as well as its impact for homogeneously catalysed reactions, aiming at a transfer of this knowledge for improving existing and developing new catalytic transformations. In addition to a method for online registration of gas consumption and development under isobaric conditions, we use stopped-flow UV/vis spectroscopy under anaerobic conditions for kinetic analysis of very fast reactions. Furthermore, in situ UV/vis spectroscopy is used and improved. Recently, a new analytical tool, an 80 MHz <sup>31</sup>P/<sup>1</sup>H-NMR benchtop spectrometer (Magritek), equipped with a flow cell, has been further developed so that individual components of a catalytic reaction can be followed under inert conditions.<sup>[1]</sup>

In the area of fundamental research, we focus on the organometallic chemistry of rhodium bis(phosphine) complexes in homogeneous catalysis. Examples include the influence of solvents on the activation of these complexes<sup>[2]</sup> as well as studies of catalyst deactivation in



propargylic C-H activation. The latter topic was investigated together with the Breit group (Freiburg) as part of a DFG project.<sup>[3]</sup> In cooperation with industrial partners (e.g., Hansen & Rosenthal, DSM) we have studied hydrogenation reactions as well as systems that can replace toxic solvents, e.g., in extraction processes. Lately, for the latter project, transfer of a lab process the into the industrial pilot scale was accomplished.

#### Dr. Jola Pospech jola.pospech@catalysis.de

The group investigates strategies for the catalytic functionalization of biologically active organic molecules through ground and light-driven excited-state chemistry. The aim is to develop functional group transfer reactions and gain insights into and the underlying mechanistic paradigms. The focus lies on photo-mediated hydrofunctionalizations, oxygen atom transfer, carbon dioxide activation and C-H bond functionalization.

In recent years, the research efforts have focused on the development of new organic photoredox catalysts based on a pyrimidopteridinetetraone scaffold.<sup>[1]</sup> The heteroaromatic catalysts have been successfully applied in additive-free photo-mediated C-N, C-H/D, C-C, and C-O bond formations that traditionally require the addition of redox-active co-catalysts.<sup>[2]</sup> A strategy for the formation of C-H and C-D bonds in the context of photo-mediated hydro- and deuterodecarboxylation was developed using a DoE approach.<sup>[3]</sup> This decarboxylation method was tested in the context of deactivation of drug residues, e.g., in wastewater. Under optimized reaction conditions, the conversion



[1] L. Tadiello, H.-J. Drexler, T. Beweries, Organometallics 2022, 41, 2833-2843. Low-field flow <sup>31</sup>P NMR spectroscopy for organometallic chemistry: on-line analysis of rhodium diphosphine complexes. [2] N. Jannsen, C. Fischer, C. Selle, C. Pribbenow, H.-J. Drexler, F. Reiß, D. Heller, T. Beweries, Dalton Trans. 2022, 57, 18068-18076. How Solvents Affect the Stability of Cationic Rhodium(I) Diphosphine Complexes: A Case Study of Acetonitrile Coordination. [3] S. Möller, N. Jannsen, J. Rüger, H.-J. Drexler, M. Horstmann, F. Bauer, B. Breit, D. Heller, Chem. Eur. J. 2021, 27, 14034-14041. Catalyst Deactivation During Rhodium Complex-Catalyzed Propargylic C-H Activation.

CO2 PrPPT Ö K<sub>3</sub>PO<sub>4</sub> MeCN:H<sub>2</sub>O (94:6) 396 nm, 50 °C, 24 h 26 examples 14-99% isol. yield • Optimization via Experimental Design

photo-mediated decarboxylation

Applicable to commercially available NSAIDs in tablet form

[1] T. Taeufer, M. A. Argüello Cordero, A. Petrosyan, A.-E. Surkus, S. Lochbrunner, J. Pospech, ChemPhotoChem 2021, 5, 999-1003. [2a] T. Taeufer, R. Hauptmann, F. El-Hage, T. S. Mayer, H. Jiao, J. Rabeah, J. Pospech, ACS Catal. 2021, 11, 4862-4869. [2b] A. Petrosyan, L. Zach, T. Taeufer, T. S. Mayer, J. Rabeah, J. Pospech, Chem. Eur. J. 2022, 28, e202201761. [3] T. S. Mayer, T. Taeufer, S. Brandt, J. Rabeah, J. Pospech, J. Org. Chem. 2022, 10.1021/acs.joc.2c01664.

CO<sub>2</sub>H

of commercially available nonsteroidal anti-inflammatory drugs (NSAIDs) in tablet form and on gram-scale was realized. Furthermore, the methodology allows for the deuterium-labelling of organic compounds using D<sub>2</sub>O as inexpensive deuterium source. Moreover, a photo-mediated formal addition of carboxylic acids to activated alkenes was reported.<sup>[2b]</sup> The decarboxylation of aliphatic carboxylic acids upon single-electron oxidation is countered in the presence of electron-rich alkenes and a hydroacetoxylation is the preferred reaction pathway. All studies are accompanied by detailed mechanistic studies considering structure-reactivity relationships using various spectroscopic techniques. Currently, the group focuses on the development of oxygen atom transfer reactions and the development of new PPT-based photoredox offering the opportunity of stereocontrol through non-covalent interactions.

photo-mediated hydroacetoxylation Bu 5.0 mol% BuPPT Cs<sub>2</sub>CO<sub>3</sub> (0.75 to 1.5 equiv.) MeCN:H<sub>2</sub>O (9:1, 0.1 M) 41 examples 396 nm. 30 °C. 24 h 15-94% isol. yield

Hammett-plot analysis

Mechanistic insights by CV, luminescence quenching and EPR



## **Reaction Engineering**

#### Dr. David Linke david.linke@catalysis.de

The group has been working at the interfa-Within LIKAT a local system "CaReD" will be dece between chemistry, engineering, and data veloped that assists in producing FAIR data. science with a special focus on the development Another important part of the work are expeand improvement of catalytic gas-phase procesrimental studies. We use parallel reactors for catalyst development and kinetic studies. We ses. explore reactions related to using alternative raw materials (e.g. bioethanol) or alternative reaction pathways (e.g. CO, based fuel production). The group has many years of experience in the design and construction of fully automated laboratory reactors from milligram to miniplant scale. In the last years, we cooperated with an industrial partner the development of a new fixed-bed process for a large commodity chemical. We operated and optimized our Miniplant to support the process and catalyst development. Runs up to 4500 hours were performed at a high degree of reliability despite demanding process conditions (70 bar).

The aim is to support development and scale-up of new processes of through provision of data and models. Another direction of work is related to data management and the extraction of information and knowledge from data. As a group interested in innovative data usage, we have always wished that data would be made available in machine readable form including all relevant metadata. Therefore, we significantly invested in establishing the initiative NFDI4Cat (we coordinated proposal writing).<sup>[1]</sup> NFDI4Cat, which started in Oct-2020, will address creation of machine-interpretable data applying principles that have been recently summarized under the term FAIR (Findable, Accessible, Interoperable, Reusable).<sup>[3]</sup>



Fig. 1: ChemCatChem cover picture "A Unified Research Data Infrastructure for Catalysis Research - Challenges and Concepts, (C. Wulf et al.) (DOI: 10.1002/cctc.202001974)

[1] Wulf, C. et. al. ChemCatChem 2021, 13, 3223-36. doi: 10.1002/cctc.202001974. A Unified Research Data Infrastructure for Catalysis Research - Challenges and Concepts. [2] NFDI for Catalysis-Related Sciences - NFDI4Cat, http://www.nfdi4cat.org/ [3] Wilkinson, M., Dumontier, M., Aalbersberg, I. et al., Sci Data 3 2016, 160018. https://doi.org/10.1038/sdata.2016.18. The FAIR Guiding Principles for scientific data management and stewardship.

**Research Groups** 

# **\***

#### Prof. Dr. Evgenii Kondratenko evgenii.kondratenko@catalysis.de

In the group "Reaction Mechanisms", we are dealing with the development of heterogeneous catalysts and reactor concepts for challenging reactions with alternative raw materials and commercial processes with a focus on their sustainability and environmental friendliness. The development is supported by mechanistic and kinetic studies. The goal is to identify generic descriptors that determine catalyst activity/ selectivity and use them for catalyst development.

Our approach is as follows. In catalyst preparation, we develop methods that enable the production of materials with well-defined phases or supported metal(oxide) species in order to establish direct relationships between these structural characteristics and catalytic properties. The catalysts are tested under industry-relevant conditions. Deeper insights into the reaction mechanism are gained from temporal (from sub milliseconds to minutes resolution) product analysis and from temporal/spatial-resolved



operando UV-Vis spectroscopic investigations. We are currently working on the production of platform chemicals from CO<sub>2</sub> and CH<sub>4</sub>, which are present in biogas. In CO<sub>2</sub> research, the focus is on the production of higher hydrocarbons (fuels and lower olefins),<sup>[1]</sup> methanol or propanol.<sup>[2]</sup> In the frame of a Sino-Germany DFG project, we are developing reaction engineering solutions to increase the selectivity to  $C_2H_4/C_2H_c$  in the oxidative CH, coupling. Our long-standing activities in the field of non-oxidative propane dehydrogenation to propene are continued to develop cost-effective and environmentally friendly catalysts as an alternative to the Cr- or Pt-based commercial catalysts.<sup>[3]</sup> We also support industry in the development of catalysts for the ammoxidation of CH<sub>4</sub> to HCN.



Fig.: Setups for spatially resolved (left) and parallel time-resolved (right) catalyst characterization by UV-vis spectroscopy under industrially relevant conditions with simultaneous analysis of reaction products. (Photos: E. Kondratenko)



## **High-Throughput Technologies**

Dr. Uwe Rodemerck uwe.rodemerck@catalysis.de



High-throughput technologies are effective tools for speeding-up R&D in catalysis since high numbers of potentially active catalytic materials can be automatically synthesized, characterized, and tested for their catalytic performance.

In our research group high-throughput technologies are developed as well as applied in searching for new, more effective heterogeneous catalysts for improved catalytic processes. Presently, the following high-throughput equipment is used:

- Effective search strategies for new catalysts (statistical methods, evolutionary strategy using genetic algorithms; co-operation with TG Linke)
- 2 synthesis robots, automated calcination apparatus (64 parallel reactors, calcination under different gas atmospheres)
- Automatic catalytic performance tests in fixed-bed reactors with 15 or 50 parallel reactors each (GC analytics, operation up to

[1] U. Rodemerck, E.V. Kondratenko, M. Stoyanova, D. Linke, J. Catal. 2020, 389, 317-327. Study of reaction network of the ethylene-to-propene reaction by means of isotopically labelled reactants. [2] M. Stoyanova, U. Bentrup, H. Atia, E.V. Kondratenko, D. Linke, U. Rodemerck, Catal. Sci. Technol. 2019, 9, 3137-48. The role of speciation of Ni<sup>2+</sup> and its interaction with support for selectivity and stability in conversion of ethylene to propene. [3] T. Otroshchenko, G. Jiang, V. A. Kondratenko, U. Rodemerck and E.V. Kondratenko, Chem. Soc. Rev. 2021, 50, 473-527. Current status and perspectives in oxidative, non-oxidative and CO\_-mediated dehydrogenation of propane and isobutane over metal oxide catalysts. (co-operation with TG Kondratenko)

# **\***@ 14

(Photo: U. Rodemerck)

750 °C and 20 bar)

- Automated apparatus with 8 reactors for temperature-programmed experiments (TPO, TPR, TPD)
- Automatic calculation of catalytic data from GC analyses (co-operation with TG Linke)

The methods and equipment have been successfully applied to the development of catalysts for different reaction types such as dehydrogenation, oxidation, condensation, isomerization, metathesis, C-C coupling, methane reforming, CO<sub>2</sub>-based Fischer-Tropsch synthesis and others.

Presently, the high-throughput technology is mainly applied to catalyst development for reactions which use CO<sub>2</sub> as raw material (CO<sub>2</sub>-based Fischer-Tropsch synthesis in co-operation with TG Kondratenko, CO<sub>2</sub>-mediated propane dehydrogenation) or hydrogen generation (NH, splitting). For the latter reaction one 50-channel reactor has been adapted in respect of material compatibility and safety device.

(now: Catalysis with Phosphorous Containing Materials)

## Dr. Christian Hering-Junghans

christian.hering-junghans@catalysis.de





In our group, we address the fundamental issue of ligand design for small molecule activation. The focus is on the synthesis of ligand architectures with phosphaalkene units. Phosphaalkenes are molecules with a P=C double bond and offer multiple coordination possibilities and should be particularly suitable for stabilizing electron-rich metals. Using the phospha-Wittig reaction, we were able to present a variety of pyridine-based phosphaalkenes and, in particular, have studied guinoline-substituted phosphaalkenes, bidentate P,N-type ligands, in detail. It has been shown that unusual distorted trigonal-bipyramidal Rh(I) and Ir(I) complexes are formed with these ligands (Figure 1, left),<sup>[1]</sup> with the Ir(I) complexes being identified as precatalysts for the Guerbet reaction of ethanol with methanol, with the potential green fuel

iso-butanol obtained in high selectivities (Fig. 1, right).<sup>[2]</sup>

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We have recently shown that phospha-reagents can be used not only for the synthesis of phosphaalkenes, but also represent potent phosphinide carriers. We have now succeeded in activating N-H bonds with ArP(PMe<sub>2</sub>),<sup>[3]</sup> to afford a variety of variously substituted secondary aminophosphanes, which are ideal precursors for P-chiral ligands (Fig. 2). In addition, we showed that O-H and E-O bonds can also be activated.<sup>[4,5]</sup> In particular, the deoxygenation of SO<sub>2</sub> has potential applications in the treatment of exhaust gas streams.<sup>[5]</sup>



#### Dr. Sergey Tin sergey.tin@catalysis.de

Due to the increasing scarcity of fossil resour-Selective oxidation of HHD leads to 2,5-dioces and environmental concerns of the society, xohexanal (DOH), a reactive compound with 3 more and more attention goes to the convercarbonyl groups.<sup>[3]</sup> DOH was converted to useful sion of renewable raw materials into basic and aromatic compounds, such as N-substituted fine chemicals every year. One of the biggest di-2-methyl-5-hydroxypyridine salts.<sup>[4]</sup> These pyrirections is the catalytic conversion of non-edible dine salts can serve as precursors for pharmaplant materials such as cellulose, lignin or ligceutical compounds. Apart from that, 1,4-subnocellulose into a range of platform chemicals. stituted benzene rings with hydroxy or tertiary These platform chemicals are then converted to amine groups were synthesized.<sup>[5]</sup> While it is valuable compounds for chemical industry. typically very challenging to prepare benzenoid molecules from renewable resources in good One of these platform chemicals, 5-hydroxyyields and selectivities, the desired molecules methylfurfural, a very promising platform chewere obtained in up to 88% yield.

mical,<sup>[1]</sup> can be converted to 1-hydroxy-2,5-hexanedione (HHD).<sup>[2]</sup>



[1] R. J. van Putten, J. C. van der Waal, E. de Jong, C. B. Rasrendra, H. J. Heeres, J. G. de Vries, Chem. Rev. 2013, 113, 1499-1597. Hydroxymethylfurfural, a versatile platform chemical made from renewable resources. [2] B. Wozniak, A. Spannenberg, Y. Li, S. Hinze, J. G. de Vries, ChemSusChem 2018, 11 (2), 356-359. Cyclopentanone derivatives from 5-hydroxymethylfurfural via 1-hydroxyhexane-2,5-dione as Intermediate. [3] S. Zheng, W. Smit, A. Spannenberg, S. Tin, J. G. de Vries, Chem. Commun. 2022, 58 (29), 4639-4642. Synthesis of alpha-keto aldehydes via selective Cu(I)-catalyzed oxidation of alpha-hydroxy ketones. [4] S. Zheng, S. Chakrabortty, E. Baráth, S. Tin, J. G. de Vries, ACS Sustain. Chem. Eng. 2022, 10 (48), 15642-15647. Synthesis of N-substituted 3-hydroxypyridinium salts from bioderived 5-hydroxymethylfurfural in water. [5] S. Zheng, Z. Wei, B. Wozniak, F. Kallmeier, E. Baráth, H. Jiao, S. Tin, J. G. de Vries, Nat. Sustain., article submitted. A new strategy for the synthesis of valuable benzenoid aromatics from bioderived 5-hydroxymethylfurfural (HMF) under mild conditions.



Abb. 2: N-H bond activation with phospha-Wittig reagents.

[1] P. Gupta, T. Täufer, J.-E. Siewert, F. Reiß, H.-J. Drexler, J. Pospech, T. Beweries, C. Hering-Junghans, Inorg. Chem. 2022, 61, 11639-11650. [2] P. Gupta, H.-J. Drexler, R. Wingad, D. Wass, E. Baráth, T. Beweries, C. Hering-Junghans, Inorg. Chem. Front. 2023, 10, 2285-2293. [3] F. Dankert, J.-E. Siewert, P. Gupta, F. Weigend, C. Hering-Junghans, Angew. Chem. Int. Ed. 2022, e202207064. [4] F. Dankert, M. Fischer, C. Hering-Junghans, Dalton Trans. 2022, 51, 11267-11276. [5] F. Dankert, P. Gupta, T. Wellnitz, W. Baumann, C. Hering-Junghans, Dalton Trans. 2022, 51, 18642-18651.

## Synergy between Homo- and Heterogeneous Catalysis

(now: Catalysis for Sustainable Syntheses)

## Prof. Dr. Jagadeesh Rajenahally jagadeesh.rajenahally@catalysis.de

The group's research focuses on (i) the development of inexpensive, durable and practical catalysts with the activity and selectivity of the homogeneous ones, and the stability and recyclability of the heterogeneous ones, and (ii) on the development of more sustainable and environmentally beneficial catalytic processes for the synthesis of fine and bulk chemicals, life science molecules as well as for the valorization of renewable feedstocks and plastics-waste.



The group works on the development of both homogeneous and heterogeneous catalysts for sustainable and advanced organic synthesis. In general, homogeneous catalysts are highly selective but not stable, while heterogeneous catalysts are stable but not selective. Our mission is to combine homogeneous and heterogeneous catalysis to develop "ideal" catalysts. We focus on the preparation of catalysts based on nanoparticles (NPs) and single atoms (SACs) by immobilization and pyrolysis of homogeneous metal complexes or metal-organic frameworks on inorganic supports. These materials consti-



tute highly active and selective as well as stable and reusable catalysts for amination, hydrogenation and oxidation process giving access to essential chemicals.

Applying suitable catalysts, we perform advanced organic synthesis in a more sustainable, efficient and selective manner. In particular we focus on the development of sustainable and cost-effective processes for the synthesis of industrial fine and bulk chemicals, functionalized and structurally diverse molecules, pharmaceuticals and agrochemicals as well as for the valorization of renewable feedstocks (CO<sub>2</sub> and biomass) and plastics-waste. For these syntheses, we use catalytic C-N, C-C, C-O and C-X (X=F, CI and Br) bond forming and cleaving reaction.



[1] V. G. Chandrashekhar, W. Baumann, M. Beller, R. V. Jagadeesh, *Science* 2022, *376*, 1433-1441. Nickel-catalyzed hydrogenative coupling of nitriles and amines for general amine synthesis. [2] V. G. Chandrashekhar, T. Senthamarai, R. G. Kadam, O. Malina, J. Kašlík, R. Zbořil, M. B. Gawande, R. V. Jagadeesh, M. Beller, *Nature Catalysis* 2022, *5*, 20-29. Silica supported Fe/Fe-O nanoparticles for the catalytic hydrogenation of nitriles to amines in the presence of aluminium additives. [3] T. Senthamarai, V. G. Chandrashekhar, N. Rockstroh, J. Rabeah, S. Bartling, R. V. Jagadeesh, M. Beller, *Chem.* 2022, *8*, 508-531. A "universal" catalyst for aerobic oxidations to synthesize (hetero)aromatic aldehydes, ketones, esters, acids, nitriles and amides. [4] J. Gao, L. Feng, R. Ma, B. J. Su, A. M. Alenad, Y. Liu, M. Beller, R. V. Jagadeesh, *Chem Catalysis* 2022, *2*, 178-194. Cobalt single-atom catalysts for domino reductive amination and amidation of levulinic acid and related molecules to N-heterocycles.



#### Prof. Dr. Jennifer Strunk jennifer.strunk@catalysis.de

In this research group we focus on gaining a deep understanding of the underlying photophysical, catalytic and electrochemical processes to create a basis for the targeted development of photocatalysts and application concepts with regard to potential large-scale implementation. In addition to reactions relevant for energy storage (carbon dioxide reduction, water splitting), we also deal with selective oxidation reactions of alcohols or of nitrogen.

Various methods of spectroscopy, particularly IR spectroscopy under reaction conditions and optical spectroscopy, as well as electrochemical characterization are used to study the optoelectronic and catalytic properties and to follow the



these parameters, the group also cooperates with other research groups that have the appropriate, specialized methodologies, for example transient optical spectroscopy. The aim is to identify precisely those structural and electronic properties of the photocatalyst that are responsible for a high photocatalytic activity. With this knowledge more efficient photocatalysts should be synthesized in a targeted way.



## **Micro Reaction Engineering**

#### Dr. Norbert Steinfeldt norbert.steinfeldt@catalysis.de

The input of environmentally harmful substances into the water resources available to us is a serious problem, the importance of which will increase in the future.

One focus of the Micro Reaction Engineering group is therefore the development of photocatalytically active materials with the help of which these substances (e.g. phenols, antibiotics, painkillers) can be completely degraded to CO<sub>2</sub> and water under the influence of light. The catalysts are tested in batch reactors<sup>[1]</sup> as well as in photoreactors, which allow a continuous reaction. While mainly suspensions are used in the batch reactor, the photocatalysts are applied as a thin layer to appropriate support materials in continuous processes in order to ensure the greatest possible irradiation of the available surface with light.

In the present example, TiO, nanotubes were electrochemically produced from a titanium sheet. These are amorphous and, in order to be photocatalytic, must be converted into a crystalline TiO<sub>2</sub> modification by thermal post-treatment. Our studies have shown that the presence of water vapor during crystallization positively affects both the forming structure and the photocatalytic activity of the TiO<sub>2</sub> films.<sup>[2]</sup> In addition, the films prepared with the participation of water vapor showed higher stability against deactivation, which is often observed.

Another area of work of the research group is the development of continuously guided multiphase processes taking place in a liquid phase for the production of fine chemicals. On this topic, there was collaboration with both the "Liquid Phase Oxidation" research group (Dr. Köckritz) and the "Modern Organic Chemistry" junior research group (Dr. El-Sepelgy). A problem that has not yet been adequately solved for heterogeneously catalyzed liquid-phase proces-

[1] S. Ding, T. Dong, T. Peppel, N. Steinfeldt, J. Hu, J. Strunk, J. Colloid and Interface Sci. 2022, 607 (2022), 1717-1729. Construction of amorphous SiO, modified  $\beta$ -Bi<sub>2</sub>O, porous hierarchical microspheres for photocatalytic antibiotics degradation. [2] M. Sebek, T. Peppel, H. Lund, I. Medic, A. Springer, P. Mazierski, A. Zaleska-Medynska, J. Strunk, N. Steinfeldt, Chem. Eng. J. 2021, 425, 130616. Thermal annealing of ordered TiO, nanotube arrays with water vapor-assisted crystallization under a continuous gas flow for superior photocatalytic performance. [3] M. Sebek, H. Atia, N. Steinfeldt, J. Flow. Chem. 2021, 11, 333-344. Synthesis of flow-compatible Ru-Me/Al<sub>2</sub>O<sub>2</sub> catalysts and their application in hydrogenation of 1-iodo-4-nitrobenzene.

ses is the stability of the catalysts used. For this purpose, commercially available Al<sub>2</sub>O<sub>2</sub> spheres were coated with Ru or Ru-M (M= Sn, Zn, Cu, or Fe) nanoparticles and used for the hydrogenation of 1-iodo-4-nitrobenzenes.<sup>[3]</sup> For all catalysts studied, the activity decreased with time.



## Photocatalytic CO, Reduction

#### Dr. Tim Peppel tim.peppel@catalysis.de

It is well known that photocatalytic conversion of CO<sub>2</sub> and H<sub>2</sub>O to products such as CH<sub>4</sub> and CO is possible in principle. However, the conversions achieved so far are much too low for an application on an industrial scale. The focus of our work is on the implementation of reliable, reproducible experimental procedures for photocatalytic CO<sub>2</sub> reduction in order to establish a basis that allows elucidation of mechanistic details of the reaction pathway.

The key challenge is the complete exclusion of carbonaceous impurities in any reactor system. Since CO<sub>2</sub> is thermodynamically extremely stable, any impurity would react faster to form (apparent) products than CO<sub>2</sub> itself. Yields would thus be overestimated and incorrect conclusions https://twitter.com/PeppelLab drawn with respect to product distribution. (Trace) gas analysis is based on both gas chromatography and mass spectrometry. In 2021/22, by spreading the reaction conditions,

both qualitative and quantitative conclusions could be drawn about the usability of a wide variety of semiconductor materials (e.g. TiO<sub>2</sub>,  $g-C_{2}N_{4}$ , SiC, GaN), plasmonic systems, but also Z-scheme photocatalysts, whose mode of operation is inspired by natural photosynthesis, for energy storage reactions. Thus, experiments at up to 180 °C, with molecular photocatalysts and using H<sub>2</sub> or CH<sub>4</sub> as reaction partners are now possible as standard. All work was carried out in close coordination with the "structure-activity relationships" group, so that in situ studies on ", single site" and "single atom" catalysts could also be carried out.



measurements must be done under extremely pure conditions. That's the only way to garantee that all C containing products result from CO<sub>2</sub> instread of any impurities.

Fig.: Set-up in the Lab . The photo reactor is

directly connected to the gas

analytics. The

[1] N. G. Moustakas, F. Lorenz, M. Dilla, T. Peppel, J. Strunk, Chem. Eur. J. 2021, 27, 17213-17219. Pivotal Role of Holes in Photocatalytic CO., Reduction on TiO., [2] F. Lorenz, N. G. Moustakas, T. Peppel, J. Strunk, Chem. Ing. Tech. 2022, 94, 1776-1783. Comparative Studies of Oxygen-Free Semiconductors in Photocatalytic CO, Reduction and Alcohol Degradation. [3] P. Naliwajko, T. Peppel, J. Strunk, Reac. Kinet. Mech. Cat. 2022, 135, 2291-2305. Thermal and light induced infrared blackening of ZnO revisited: rediscovery of fundamental scientific knowledge



## Magnetic Resonance & X-ray Methods

#### Dr. Jabor Rabeah jabor.rabeah@catalysis.de

Our fundamental understanding of catalytic reactions has been significantly enhanced from the simultaneous monitoring of the dynamic behavior of catalytically active sites under reaction conditions. One of our research interests is the adaptation and use of EPR for real-time monitoring of various catalytic reactions. It has been used, in combination with other spectroscopic techniques, to elucidate different reaction mechanisms and proven to play an important role in determination the relationship between the chemical structural of the active sites and their catalytic activity. For instance, CO<sub>2</sub> methanation over supported Ru catalysts,<sup>[1]</sup> CO oxidation and PROX reaction over supported Cu single-atom catalysts,<sup>[2]</sup> reverse water-gas



shift reaction over supported-Au catalysts, and N-formylation of amines with C3 biomass-based platform molecules.<sup>[3]</sup> We are continuing our interest in establishing collaborative scientific relationships with national and international partners for example, with the group of Prof. Arne Thomas, TU-Berlin to study the photocatalytic H<sub>2</sub>O<sub>2</sub> production over COF-based catalysts. Since some of the catalytic reactions involve electrons transfer between catalyst and substrate, which usually occur on the time scale of <1 milliseconds (valence changes of transition metal ions and formation of short-lived radical intermediates), a rapid scan instrument for in situ EPR measurements has been used to enable real-time kinetic analysis of such processes.



The *operando* electron spin resonance spectroscopy (ESR, EPR) is ideally suited for tracking catalytic processes involving species with unpaired electrons, such as supported and unsupported transition metal oxide catalysts and/or free-radical intermediates. (Fig.: J. Rabeah)

S. Cisneros, A. Abdel-Mageed, J. Mosrati, S. Bartling, N. Rockstroh, H. Atia, H. Abed, J. Rabeah, A. Brückner, *Iscience* 2022, 25. [2]
 J. Mosrati, A. M. Abdel-Mageed, T. H. Vuong, R. Grauke, S. Bartling, N. Rockstroh, H. Atia, U. Armbruster, S. Wohlrab, J. Rabeah, A. Brückner, *ACS Catalysis* 2021, *11*, 10933-10949. [3] X. Dai, X. Wang, J. Rabeah, C. Kreyenschulte, A. Brückner, F. Shi, *Chem.Eur.J.* 2021, 27, 16889-16895.

## **Optical Spectroscopic & Thermoanalytical Methods**

#### Dr. Christoph Kubis christoph.kubis@catalysis.de

intermediate MoO<sub>2</sub>C<sub>2</sub>H<sub>2</sub> phases in metal molyb-The focus of the research group lies on in situ date containing molybdenum oxide catalysts for and operando spectroscopic investigations into the HDO of anisole are performed in the DFG heterogeneous and homogeneous catalytic reactions to elucidate mechanistic and kinetic project (442613239). aspects. A variety of analytical techniques In situ characterization of adsorbate species are applied, in particular, FTIR (Transmission, during CO<sub>2</sub> Fischer-Tropsch over supported iron oxide catalysts HP DRFITS are performed in the DRIFTS, ATR), Raman, UV-vis and NMR spectros-DFG project (406695057) embedded in the Priocopy as well as thermoanalytical methods. rity Program SPP2080.



Operando DRIFTS/MS coupling for studies on iron-based catalysts for the Fisher-Tropsh synthesis with CO<sub>2</sub>.

Simultaneous coupling of multi-spectral methods and product analysis tools (MS, GC) are performed to derive a maximum information output for deriving structure-reactivity relationships.

This approach is additionally enhanced by the combination of experiment design strategies and chemometric data evaluation. Current scientific interests are CO<sub>2</sub> valorization, alkene carbonylation, hydrodeoxygenation of lignin derivatives and alkene oligomerization. Within the BMBF project PlasCO2 (033RC030) a NT-plasma DRIFTS/MS apparatus is being constructed together with INP Greifswald for the study of adsorbate species during plasma induced CO<sub>2</sub> conversion to CO. Studies on the formation of

*In situ* FTIR and NMR spectroscopic studies combined with chemometric data processing on rhodium and cobalt catalyzed hydroformylation are conducted to understand fundamental and industrial relevant aspects within the project with Evonik Oxeno GmbH & Co. KG.

<sup>[1]</sup> J. Weiß, C. Rautenberg, T. Rall, C. Kubis, E. Kondratenko, U. Bentrup, A. Brückner, *Chemistry–Methods* 2021, *1*, 308-314. [2] Y. Hu, Z. Wei, A. Frey, C. Kubis, C.-Y. Ren, A. Spannenberg, H. Jiao, T. Werner, *ChemSusChem* 2021, *14*, 363-372. [3] P. Kucmierczyk, S. Behrens, C. Kubis, W. Baumann, Z. Wei, H. Jiao, K. Dong, A. Spannenberg, H. Neumann, R. Jackstell, A. Börner, R. Franke, M. Beller, *Catal. Sci. Technol.* 2022, *12*, 3175-3189. [4] B. Zhang, C. Kubis, R. Franke, *Science* 2022, *377*, 1223-1227. [5] J. Weiß, Q. Yang, U. Bentrup, E. V. Kondratenko, A. Brückner, C. Kubis, *ChemCatChem* 2022, *14*, e202200577. [5] H.-J. Ai, B. N. Leidecker, P. Dam, C. Kubis, J. Rabeah, X.-F. Wu, *Angew. Chem. Int. Ed.* 2022, *61*, e202211939. [6] B. Spiegelberg, H. Jiao, R. Grauke, C. Kubis, A. Spannenberg, A. Brandt, A. Taden, H. Beck, S. Tin, J. G. de Vries, *Adv. Synth. Catal.* 2022, *364*, 1251-1263

#### Dr. Sebastian Wohlrab sebastian.wohlrab@catalysis.de

The research group is dedicated to the development of new functional materials for the intensification of sustainable circular flows. This includes the following focal points:

#### Utilization of renewable carbon sources

In order to counteract a future carbon shortage, we are investigating possibilities of direct catalytic conversion of biomethane and carbon dioxide.

During the selective oxidation of methane, the influence of added water on the reaction was particularly noticeable. The dependencies of methane activation and formaldehyde decomposition found during this process may lead to selectivity enhancement of the reaction under investigation.<sup>[1]</sup>

We are also developing a new method for timeand spatially-resolved characterization using XANES with the "Bundesanstalt für Materialforschung" (BAM). The goal is to understand catalysts for methane activation and thus make knowledge-based adjustments to the catalyst material to enable long-term stable and more efficient processes.





We continue to develop concepts for the removal of carbon dioxide from the air (DAC - Direct Air Capture) or for its concentration. For downstream utilization, synthesis gas generation by reverse water gas shift reaction is being tested in particular. An interesting discovery are Ni-Cu core-shell particles. These are size-independent selective for CO generation, while pure Ni catalysts preferentially promote methanation.

#### Chemical hydrogen storage

The operating principle of a chemical hydrogen battery involves two reactions: The fixation of hydrogen to a basis, such as  $CO_x$  or N, and the release by decomposition of the storage structure. We are specifically working on problems related to the release of hydrogen from such molecules. Using ammonia as a storage molecule as an example, we recently presented the state of the art.<sup>[2]</sup>

#### Membrane technologies

We model properties of new materials for use in mass separation. For example, the separation properties of mixed matrix membranes are simulated using Monte Carlo, molecular dynamics and quantum mechanics,<sup>[3]</sup> in order to transfer them into a real application. Future membrane processes are envisaged for substance separation, to reduce energy requirements, and in catalytic reaction control for equilibrium shifting.

(Fig. DOI: https://doi/10.1002/cctc.202201604.)

[1] B. Kunkel, S. Wohlrab, *Catal. Commun.* **2021**, *155*, 106317. Enhancement and limits of the selective oxidation of methane to formaldehyde over V-SBA-15: Influence of water cofeed and product decomposition. [2] S. Peters, A. M. Abdel-Mageed, S. Wohl-rab, *ChemCatChem* **2023**, *15*, e202201185. Thermocatalytic Ammonia Decomposition – Status and Current Research Demands for a Carbon-Free Hydrogen Fuel Technology. [3] I. Salahshoori, M. N. Jorabchi, M. Asghari, S. Ghasemi, S. Wohlrab, *J. Mater.* **2023**, *23*, 1862-1886. Insights into the morphology and gas separation characteristics of methylene diisocyanate (MDI)-functionalized nano-TiO<sub>2</sub> polyurethane: quantum mechanics and molecular simulations studies.

## **Technology Oriented Processes**

#### Dr.-Ing. Udo Armbruster udo.armbruster@catalysis.de

The research group develops heterogeneous catalysts and synthesis routes for the material or energetic use of renewable raw materials, platform chemicals as well as CO<sub>2</sub>. The long-standing experience of the group on high-pressure reactions is ideally utilized here. We aim to design such conversions preferably in continuous processes and to gain knowledge for technical application at an early stage. The flexible equipment enables catalyst tests under various reaction conditions, even in larger reactors and with shaped catalysts (tablets) and is increasingly in demand for industrial collaborations.

For the characterization of solid catalysts for the elucidation of their mode of action, the group operates its own sorption laboratory, in which various methods (BET, TPX-MS coupling) are combined. This expertise is also available to other scientists in the institute as well as to external research partners.

Current key topics in publicly funded projects (BMWi, BMBF) are the conversion of platform chemicals such as levulinic acid or glycerol and the utilization of CO<sub>2</sub>. Particularly noteworthy are methanol synthesis, Fischer-Tropsch synthesis and dry reforming of CO<sub>2</sub> with methane. New test plants with expanded options for each of the latter two processes were commissioned in 2021. These ongoing projects also focus on shaping the catalysts. All this work and the experience gained from current industrial collaborations on ammonia and methanol synthesis and from environmental catalysis (denitrification and desulfurization) will provide valuable input for the operation of the new *Catalysis2Scale* technical center at LIKAT.

[1] Q. L. M. Ha, H. Atia, C. Kreyenschulte, H. Lund, S. Bartling, G. Lisak, S. Wohlrab, U. Armbruster, *Fuel* **2022**, *312*, 122823. Effects of modifier (Gd, Sc, La) addition on the stability of low Ni content catalyst for dry reforming of model biogas. (https://10.1016/j. fuel.2021.122823) [2] S. Nieß, U. Armbruster, S. Dietrich, M. Klemm, *Catalysts* **2022**, *12*, 374. Recent Advances in Catalysis for Methanation of CO<sub>2</sub> from Biogas. (https://doi.org/10.3390/catal12040374) [3] M.T. Le, S. Singh, M. Nguyen-Quang, A.B. Ngo, A. Brückner, U. Armbruster, Sci. Tot. Environ. 2021, 784, 147394. (https://doi.org/10.1016/j.scitotenv.2021.147394)



# Fig. : New Fischer-Tropsch pilot plant with online-GC for operation with conventional tubular reactor or membrane reactor. (Foto: U. Armbruster)


### Surface Chemistry in Applied Catalysis

#### Dr. Ali Abdel-Mageed ali.abdel-mageed@catalysis.de

### Development heterogeneous single-atom catalysts

The development of single-atom catalysts (SACs) is deemed as the ultimate design priciple of heterogeneous catalysts with the main target to rationalize the use of expensive metals. To step up these materials for industrial applications, their activity and stability should be significantly enhanced. We focus here on the development of CeO<sub>2</sub>-TiO<sub>2</sub> supported metal-SACs (Cu, Pd and Ru) using one-pot sol-gel method and their subsequent use in selected catalytic processes. We show that the activity for CO oxidation and water-gas-shift on Cu/CeO<sub>2</sub>-TiO<sub>2</sub> SACs can be significantly controlled by modulating the Ce/Ti ratio. The activity obeys a volcano-shaped dependence of Ce/Ti molar ratio, with the reaction rates culminating at Ce/ Ti ratio around 0.18.<sup>[1]</sup> These paves the way for the optimization of SACs based on different precious metals.

#### Ambient-pressure CO<sub>2</sub> reduction

The drastic effects associated with climate changes mandate the introduction of green alternatives for the standing carbon-based energy technologies. Diverting the air-captured CO, either to methane or to syngas via reverse-water-gas-shift (RWGS) reaction is considered an efficient option to circumvent and utilize this greenhouse gas in a closed energy loop. Supported Ru catalysts, in particular Ru/TiO<sub>2</sub>, are highly active at low temperatures (< 200°C) and their properties can be controlled to fine-tune the selectivity for a specific product. Recent findings indicated that high-surface-area Ru/TiO<sub>2</sub> catalysts (> 200 m2-g-1) can prodcue CO at 100% selectivity at temperatures < 200°C. [2] In contrast catalysts based on low-surface area supports (< 100 m2-g-1) show a 100%



selectivity for methane, where in this case the catalytic activity is controlloed by the interplay of Ru particle size and the support reducibility. <sup>[3]</sup> Further enancement of these catalysts for the application at lower reaction temperatures are topics of running studies in our group.

A. M. Abdel-Mageed, S. Cisneros, J. Mosrati, H. Atia, T. H. Vuong, N. Rockstroh, S. Wohlrab, A. Brückner, J. Rabeah, *ChemCatChem* 2023, e202201669.
 A. M. Abdel-Mageed, K. Wiese, A. Hauble, J. Bansmann, J. Rabeah, A. Brückner, R. J. Behm, *J.Catal.* 2021, 400.
 S. Chen, A. M. Abdel-Mageed, *Int. J. Hydrog. Energy* 2023.
 A. M. Abdel-Mageed, B. Rungtaweevoranit, S. Impeng, J. Bansmann, J. Rabeah, S. Chen, T. Häring, S. Namuangrak, K. Faungnawakij, A. Brückner, R. J. Behm, *Angew. Chem. Int. Ed.* 2023, 62, e2023019.



Prof. Dr. Robert Francke robert.francke@catalysis.de

One focus of the thematic group is the development of electrochemical syntheses of organic compounds. Our extensive equipment and expertise allow us to adapt the experimental setup and the type of reaction control to a variety of different synthetic challenges. Thus, divided and undivided cells are used as required, which can be operated in potentiostatic or galvanostatic mode. If necessary, the preparative work is supplemented by electroanalytical studies, which provide both mechanistic insights and information that is useful for the optimization of reaction parameters. As a further tool, we use homogeneous electrocatalysts (mediators) or catalytically active electrode materials if needed. This approach allows both selectivity control and lowering of the kinetic overpotential. To accelerate optimization, screening setups are



used that allow up to eight electrolyses to be carried out simultaneously per apparatus. For up-scaling of the reaction, various flow cells are available, which can be coupled with different analytical methods for online product analysis.



Fig. 1: Divided Cell (left), Undivied Cell (right), (Photos: R. Francke)

R. Francke, "Concepts for Sustainable Organic Electrosynthesis", Curr. Opin Electrochem. 2022, 36, 101111. R. Francke, M. Májek, "Mediated Electron Transfer in Electrosynthesis: Concepts, Applications, and Recent Influences from Photoredox Catalysis" in Sustainable and Functional Redox Chemistry (Ed.: S. Inagi), 2022, Royal Society of Chemistry, Cambridge. R. Francke, P. Enders, "Methods and Materials Applied in Electrosynthesis" in Science of Synthesis: Electrochemistry in Organic Synthesis (Ed.: L. Ackermann), Thieme, Stuttgart, 2022, 33-72.

### **Catalyst Design for Electrosynthesis**

Dr. Bernd H. Müller bernd.mueller@catalysis.de

One way to carry out electrochemical syntheses is to use homogeneous catalysts ("medi-The aim is to explore the mechanisms of alreaators"). These are redox-active species that can dy known mediated electrosyntheses and to be regarded as electrochemically regenerable develop new syntheses that follow this design reagents. Electron transfer first takes place principle to the point of application maturity. between the electrode and the catalyst under formation of the active species. The latter reacts with a substrate, which then converts to the donors desired product. This indirect electron trans-- σ-donor fer usually allows large overpotentials to be - π-acceptor avoided and selectivities to be controlled. The **backbone** mediator as electron carrier is always recovered metal center at the electrode and is not consumed during  $[\mathsf{M}]$ - bite angle - transition metal electrosynthesis. The reaction of the mediator - chirality with the substrate takes place in homogeneous phase.



#### Mediated Electrocatalysis

The electrode material usually plays a major role in the design of electrosyntheses. However, in mediated electrochemistry, the electrodes are no longer the site of the primary substrate reaction. Analogously to classical homogeneous catalysis, the mediator can be tailored via the choice of transition metal and ligand structure to meet the needs of the desired reaction. This expands the possibilities of electrosynthesis in terms of selectivity and possible reaction mechanisms.

[1] R. Francke, M. Roemelt, B. Schille, Chem. Rev. 2018, 118, 4631–4701. [2] L. F. T. Novaes, J. Liu, Y. Shen, L. Lu, J. M. Meinhardt, S. Lin, Chem. Soc. Rev. 2021, 50, 7941-8002.



#### Catalyst Optimization / Rational Ligand Design



### **Polymer Chemistry & Catalysis**

PD Dr. habil. Esteban Mejía esteban.mejia@catalysis.de

Chemistry, as one of the main players of progress and (arguably) the culprit of most of its evils, has been called to tackle these problems, head-on, for which a "complete makeover" on the way chemists design their processes and manage their outcomes was necessary. The paradigm shift came with the development of the concept of "green chemistry" and its twelve principles, having catalysis at its core. Guided by Green Chemistry's principles, the application of catalytic technologies towards the development of sustainable processes and products are the main research motivation at the Mejía's group.

Our main research activities include: (i) The development of safe polymerization catalysts for consumer products (silicones), together with novel base-metal systems to produce biodegradable polymers and the sustainable synthesis of  $CO_2$ -epoxide copolymers. (ii) Novel copper-based catalytic systems for the synthesis of enynes and heterocycles, improving over existing technologies, refraining from the use of noble metals and pre-functionalized substrates. These systems include molecular coordination compounds and artificial metalloenzymes.



(iii) The development of metal-free catalyst for aerobic oxidation reactions, including heterogeneous carbocatalysts and persistent radical cations.

(iv) The synthesis and application of heterogeneous catalysts derived from waste rice husk, establish an alternative route for the valorization of agricultural rice bio-waste, resulting in high added-value products (the catalysts) with potential immediate impact in the chemical industry.



[1] X. Guo, F. Unglaube, U. Kragl and E. Mejía, *Chem. Commun.* **2022**, *58*, 6144 – 6147.  $B(C_6F_5)_3$ -Catalyzed transfer hydrogenation of esters and organic carbonates towards alcohols with ammonia borane. [2] F. Unglaube, J. Schlapp, A. Quade, J. Schäfer, E. Mejía, *Catal. Sci. Technol.* **2022**, *12*, 3123-3136. Highly active heterogeneous hydrogenation catalysts prepared from cobalt complexes and rice husk waste. (Included in the themed collection: Emerging Investigator Series) [3] X. Guo, J. Rabeah, R. Sun, D. Wang, E. Mejía, *ACS Appl. Mater. Interfaces.* **2021**, *13*, 42889-42897. Fluorescent Hybrid Porous Polymers as Sustainable Heterogeneous Photocatalysts for Cross-Dehydrogenative Coupling Reactions.

### **Biocatalysis**

#### Prof. Dr. Udo Kragl udo.kragl@catalysis.de

One focus is the production of oligomers and polymers that are used as precursors for adhesives, sealants and coatings. Together with cooperation partners, new catalysts are developed and process engineering issues are addressed. Sample quantities are produced for testing in formulations. The aim is to avoid toxic or environmentally hazardous substances in the adhesive formulations. The production of polymers with low polydispersities, through characterization and optimization of process parameters and further development of catalysts, is at the forefront of the work. In addition, processes for multiphase catalysis as well as derivatization of renewable raw materials are investigated.

[1] J. Romischke, A. Scherkus, M. Saemann, S. Krueger, R. Bader, U. Kragl, J. Meyer, *Gels* **2022**, *8* 296. Swelling and Mechanical Characterization of Polyelectrolyte Hydrogels as Potential Synthetic Cartilage Substitute Materials. [2] A. Jastram, T. Lindner, C. Luebbert, G. Sadowski, U. Kragl, *Polymers* **2021**. Swelling and Diffusion in Polymerized Ionic Liquids-Based Hydrogels. [3] (218) M. Gronbach, L. Kraußer, T. Broese, C. Oppermann, U. Kragl, *Food Anal. Methods* **2021**. Sublimation for Enrichment and Identification of Marker Compounds in Fruits. [3] A. Jastram, J. Claus, P. A. Janmay, U. Kragl, *Polymer Testing* **2021**, *93*, 106943. Rheological properties of hydrogels based on ionic liquids.



Research Groups



Current research topics are:

- multiphase catalysis
- C-C coupling reactions such as Heck, Suzuki or Stille coupling, hydroformylation
- Catalyst development for stereoselective polymerization in the field of polyols
- Reactors & autoclaves for multiphase reactions; use of synthesis gas (CO/H2)
- Silicone-based polymers
- Polyether-based functional materials

### **Catalysis of Heterocycles**

#### Prof. Dr. Xiao-Feng Wu xiao-feng.wu@catalysis.de

Carbonylation is among the center of modern chemistry, with the transformation of CO, both academic research and industrial applications are benefited from it. Alkenes are interesting structure moiety with important synthetic applications in various areas. Hence, the using of abundant and non-expensive copper catalyst for the carbonylative transformation of alkenes is even more attractive. During last two years, we have been working on copper-catalyzed carbonylation of alkenes. In our catalytic systems,





[1] F.-P. Wu, H.-Q. Geng, X.-F. Wu, Angew. Chem. Int. Ed. 2022, 61, e202211455. [2] F.-P. Wu, Y. Yang, D. P. Fuentes, X.-F. Wu, Chem. 2022, 8, 1982. [3] H.-Q. Geng, T. Meyer, R. Franke, X.-F. Wu, Chem. Sci. 2021, 12, 14937. [4] Y. Yuan, F.-P. Wu, X.-F. Wu, Chem. Sci. **2021**, *12*, 13777.

### **Hydroformylations**

#### Dr. Jens Holz jens.holz@catalysis.de

Aspects of asymmetric and homogeneous the long-term project with Evonik Operations hydrogenation found attention in two projects GmbH. Control of the Rh-catalyzed hydroformylation with defined distribution ratios with Idorsia Pharmaceutical Ltd. (Switzerland). In these, proposals were made that on the one between the *n*- and *iso*-aldehydes should be hand enable the substitution of a commercially achieved through the preferred synthesis of nodifficult to access bisphosphine ligand in the vel bisphosphite compounds. Other important Rh-catalyzed hydrogenation of an  $\alpha$ -amino acid aspects are the selectivity to be achieved (no side reactions) and the speed of the reaction. precursor by simpler and more readily available bisphospholane compounds and on the other By varying steric and electronic parameters in hand, ways could be shown, as in another interthe bisphosphites used, some potential ligands mediate step in the synthesis of a precursor, the could be prepared. This is manifested in numetechnically more demanding reduction of a carrous patents filed.<sup>[1]</sup> bonyl compound with excess of boron hydrides In addition to Rh-catalysis, hydroformylation with cobalt catalysts was also investigated. Here can be replaced by a homogeneously catalyzed hydrogenation with Ru-precatalysts (Fig. 1). it could be shown that even with unmodified





In-depth studies on the iridium-catalyzed hydrogenation of TMQA to (R)-THQA using in situ and ex situ NMR spectroscopy were carried out with Bayer AG. The main focus was on the investigations into the recycling of the iridium catalysts used (Fig. 2).

After taking over the topic "hydroformylation", the main focus of activities continues to be on investigations into the regioselective hydroformylation of internal olefins as part of



Fig. 2: Iridium catalyzed hydrogenation of TMQA to (R)-THQA.

[1] some examples: EP 4 059 939 A1 (18.03.2021), EP 4 0599 18 A1 (18.03.2021). EP 4 098 646 A1 (02.06.2021) u.a. [2] B. Zhang, C. Kubis, R. Franke Science 2022, 377, 1223-1227.

**Research Groups** 

(phosphine-free) cobalt carbonyl complexes, the hydroformylation of olefins proceeds with high regioselectivity and activity even under comparatively mild conditions (50 bar, 140°C).<sup>[2]</sup>



Fig. 3: Dynamic in situ HP-NMR spectra during the hydrogenation of TMQA.

JUNIOR RESEARCH GROUPS

### **Theory of Homogeneous & Biocatalysis**

Dr. Milica Feldt milica.feldt@catalysis.de



The research group of "Theory & Catalysis" is interested in investigating the reactivity of iron catalysts, with the focus on non-heme iron-oxo species. The idea is to use highly accurate computational protocols to study reactivity of biomimetic non-heme iron-oxo complexes as well as non-heme iron enzymes and the influence of different spin states and metal environment on the reactivity. The end goal is to use knowledge obtained from theoretical and experimental studies of non-heme iron complexes and enzymes to computationally design an artificial metalloenzyme based on iron which should be able to selectively activate C-H bonds of various substrates.

Furthermore, the enzymatic reactivity and homogeneous catalysis will be studied not only

in the case of non-heme iron complexes, but in general. Understanding what are the key factors which are responsible for a high/low reactivity of enzymes and transition metal catalysts can help in designing new improved catalysts. To reach this understanding theory can play an important role since it can probe the aspects of enzymes and homogeneous catalysts which are not or hardly accessible by experiments. Additionally, we will work on testing and developing different hybrid approaches for the application on these systems. The main goal will be to find an approach with the desired accuracy while keeping computational costs affordable.

Modern Organic Chemistry

#### Dr. Osama El-Sepelgy osama.elsepelgy@catalysis.de

Innovative fundamental research is crucial to face urgent challenges posed by our current societal, environmental and economic demands. Among the most pressing challenges of the 21st century is the utilization of abundant but amides/imides ACS Catal 2022 enamides/enimides valuable synthons one step from feedstock unreactive feedstock as development of these technologies would enable the sustainable formal (Z)-hydroxymethylation of alkenes production of vitally important fine and bulk chemicals. To pursue this goal, our group focuses on the development of unprecedented hen Tamao oxidation sustainable concepts through the merger of tethered alcohols Chem Comm 2023 one step from feedstock base-metal catalysis with the visible light available from the sun. We believe that shining visible light on base-metal catalysts can change the strategies, which mainly focus on the photoexreaction outcome through unpredictable catacited base-metal catalysis. We aim at the dislytic pathways. The main goal of our group is to covery of new reactivities that are not possible redefine the synthetic chemistry, by using novel with ground-state chemistry.



Fig. 1: Junior Research Group "Modern Organic Chemistry" of Dr. Osama El-Sepelgy (right) (Photo: O. El-Sepelgy)

[1] Z. Amanollahi, L. Lampe, M. Bensberg, J. Neugebauer and M. Feldt, Phys. Chem. Chem. Phys. 2023, 25, 4635-4648. On the accuracy of orbital based multi-level approaches for closed-shell transition metal chemistry. [2] Feldt and Q. M. Phung, Eur. J. Inorg. Chem. 2022, https://doi.org/10.1002/ejic.202200014. Ab Initio Methods in First-Row Transition Metal Chemistry. [3] M. Feldt, C. Martín-Fernández and J. N. Harvey, Phys. Chem. Chem. Phys. 2020, 22, 23908-23919. Energetics of Non-Heme Iron Reactivity: Can Ab Initio Calculations Provide the Right Answer? [4] M. Feldt, Q. M. Phung, K. Pierloot, R. A. Mata and J. N. Harvey, J. Chem. Theory Comput. 2019, 15, 922-937. Limits of Coupled-Cluster Calculations for Non-Heme Iron Complexes.

[1] C. Wang, L. M. Azofra, P. Dam, E. J. Espinoza-Suarez, H. T. Do, J. Rabeah, A. Brückner, O. El-Sepelgy, Chem. Commun. 2023, 59, 3862-3865. Photoexcited cobalt catalysed endo selective alkyl Heck reaction. [2] C. Wang, L. M. Azofra, P. Dam, M. Sebek, N. Steinfeldt, J. Rabeah, O. El-Sepelgy, ACS Catal. 2022, 12, 8868-8876. Catalytic Desaturation of Aliphatic Amides and Imides Enabled by Excited-State Base-Metal Catalysis. [3] C. Wang, O. El-Sepelgy, Curr. Opin. Green Sustain. 2021, 32, 100547. Reductive depolymerization of plastics catalyzed with transition metal complexes.



As early as the summer of 2006, LIKAT signed a far-reaching cooperation agreement with the University of Rostock, which has been steadily expanded in recent years and from which both LIKAT and the university benefit equally. The contract enables LIKAT to involve research groups from the University of Rostock to a large extent in the institute's research work: from the natural science institutes, the interdisciplinary faculty, the engineering sciences or the medical field.

Cooperation within the framework of *Uni in Leibniz* was reorganized at the beginning of 2020 as a competition for ideas. Researchers from the universities can formulate proposals

## UNI IN LEIBNIZ Associated University Research Groups

Photochemistry & Photocatalysis Prof. Dr. Malte Brasholz

Magnetic Resonance in the Solid State Prof. Dr. Björn Corzilius

Catalytic Cycloadditions Prof. Dr. Marko Hapke

Vibrational Spectroskopy in Catalysis Prof. Dr. Ralf Ludwig

### **Cooperation with the University**

on predefined questions and submit them to LIKAT. The prerequisite is their cooperation with LIKAT staff, e.g. through the joint supervision of PhD students, for whom LIKAT provides resources.

Such an idea competition promotes exchange between universities and LIKAT and enables internal start-up funding for high-risk research that can and should lead to future joint research projects. The pre-definition of the research question by the LIKAT ensures the research orientation of these collaborations according to the research strategy of the institute. There are currently eight associated university research groups from three different universities.

Numerical Analysis Prof. Dr. Klaus Neymeyr

#### Material Design

Prof. Dr. Axel Schulz

Intermetallic Cooperativity Prof. Dr. Wolfram Seidel

Organocatalysis Prof. Dr. Thomas Werner

### **Photochemistry & Photocatalysis**

Prof. Dr. Malte Brasholz University of Rostock Organic Chemistry malte.brasholz@uni-rostock.de

Our central research interest is the development of new synthesis processes using the methods of photochemistry and photocatalysis, because these often open up access to unusual product structures that are not accessible using conventional thermal reaction control. In particular, photocatalysis with visible light makes the classic elementary steps of photochemical transformations usable in catalytic



processes. These include photoelectron transfer reactions, atom and group transfer reactions, and processes induced by energy transfer.

Among the most important reaction types we are investigating are photoinduced radical additions and mul-



ChemPhotoChem

ticomponent couplings, as well as various types of cycloadditions, especially those that occur under dehydrogenating conditions.

Another focus is on green oxidation reactions involving reactive oxygen species, in particular for the functionalization of heterocyclic compounds. The application of synthetic methodology developed in the group has also been demonstrated in the synthesis of natural products and in the development of biologically highly active alkaloid derivatives, which form a new class of antitumor agents. Concerning to this, we cooperate closely with scientists from the fields of oncology and cell biology at the University Medical Center Rostock. Furthermore, we investigate the heterogenization of homogeneous photocatalytic processes using selected examples.

(Photo.: M. Brasholz)

[1] P. Seefeldt, R. Dasi, A. Villinger, M. Brasholz, ChemPhotoChem 2021, 5, 979-983. Photoredox-induced deaminative radical-cationic three-component couplings with N-alkylpyridinium salts and alkenes. [2] M. Frahm, A. Voss, M. Brasholz, Chem. Commun. 2022, 58, 5467-5469. A short total synthesis of (±)-mersicarpine via visible light-induced cascade photooxygenation. [3] R. Dasi, A. Villinger, M. Brasholz, Org. Lett. 2022, 24, 8041-8046. Photocatalytic Azetidine Synthesis by Aerobic Dehydrogenative [2 + 2] Cycloadditions of Amines with Alkenes. [4] A. Eichhorst, M. Gallhof, A. Voss, A. Sekora, L. Eggers, L. T. Huyen, C. Junghanss, H. Murua Escobar, M. Brasholz, ChemMedChem 2022, 17, e20220016. Spirooxindol-1,3-oxazine alkaloids: highly potent and selective antitumor agents evolved from iterative structure optimization.

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### Magnetic Resonance in the Solid State

Prof. Dr. Björn Corzilius University of Rostock Physical Chemistry bjoern.corzilius@uni-rostock.de

### Magic-Angle Spinning NMR and Dynamic Nuclear Polarization

In collaboration with several groups from LI-KAT, nuclear magnetic resonance spectroscopy (NMR) is used to elucidate the structure and electronic state of the active sites of various heterogeneous catalyst systems.

NMR spectroscopy is particularly well suited for this purpose, as it can resolve the structure of molecules and solids at the atomic level without requiring long-range structural order. Thus, solid-state NMR is the methodology of choice for the investigation of amorphous solids, materials, (bio)polymers, or colloidal suspensions. A special focus is placed on the elucidation of the reaction mechanism of catalytic butene dimerization using nickel-supported mesoporous silicon aluminum oxides. In addition to studies on the surface acidity, investigations are carried out on the paramagnetic Ni centers in order to determine the distribution of various acid centers and their interplay with the active sites.

However, an inherent problem of NMR is its low sensitivity, since only a tiny fraction (1 in 10 000) (Fig.: M. Schröder) of the nuclear spins contribute to the signal. Using dynamic nuclear spin polarization (DNP), the population difference of nuclear spins can be increased by adding special paramagnetic polarizing agents to the sample and irradiation with high-frequency microwaves. In addition to signal amplification, specific hyperpolarization of nuclear spins can be used to specifically stu-Thus, NMR spectroscopy has been used to chady the spatial folding of proteins.<sup>[1]</sup> In addition racterize highly specifically the binding site in a to functionalization with paramagnetic polarizribonucleoprotein.<sup>[2]</sup> ation markers, the dynamics of methyl groups Currently, this newly developed methodology is can also be exploited to illuminate other atoms being combined with frequency-selective dipoand functional groups in their vicinity by heterolar recoupling to generate further specificity in nuclear cross-relaxation. solid-state NMR spectroscopy.





<sup>[1]</sup> T. Biedenbänder, V. Aladin, S. Saeidpour, B. Corzilius, Chem. Rev. 2022, 122, 9738-9794. [2] V. Aladin, A. K. Sreemantula, T. Biedenbänder, A. Marchanka, B. Corzilius, Chem. Eur. J. 2023, 29, e202203443

### **Cycloadditions**

Prof. Dr. Marko Hapke Johannes-Kepler-University Linz Institute for Catalysis (INCA) marko.hapke@jku.at

The activation and selective transformation of substrates with (single and multiple) bonds is a central concern in our group. In recent years, we have particularly advanced the development of new cobalt-based catalyst systems for the conversion of C-C or C-N triple bonds such as alkynes and nitriles by means of [2+2+2] cycloaddition reactions, which can also be stereoselective with the appropriate catalyst system.<sup>[1, 2]</sup> In addition to cobalt(I) systems, which are generally used, we succeeded in identifying cobalt(III) precatalysts that can also catalyze the cyclization of triynes or diynes and nitriles to the arene and pyridine derivatives.<sup>[3]</sup> Precatalysts in such high oxidation states without added reducing agent were previously unknown.

The investigation of different and unusual oxidation states of a catalyst metal such as cobalt in catalytic transformations is a highly interesting field and not trivial, especially in in situ-generated systems.<sup>[1b]</sup> We focused on the conversion of phosphaalkynes,  $R-C\equiv P$ , as P-homologues of nitriles, R-C≡N, to study such oxidation states and found that, remarkably, a cobalt(II) bisphosphane catalyst is able to efficiently generate the corresponding phosphinines (phosphabenzenes) from the phosphaalkynes and functionalized diynes at relatively high temperatures (160- 210 °C).<sup>[4]</sup> Interestingly, the catalyst tolerates nitrile groups in the substrate and selectively converts the phosphaalkynes. The phosphinines are a very interesting class of compounds, for example as ligands for transition metals or heterocyclic aromatics. We are currently studying other 3d metal complexes such



(Fig.: M. Hapke)

as those of iron and manganese as precatalysts and have also encountered interesting reactivities in cyclotrimerizations.

For the reactions, we are using microwave technology, photochemical reactors, and increasingly flow chemistry (in cooperation with the JKU Linz).

In addition, we are currently interested in stereoselective C-H functionalization reactions and the chemical recycling of polyolefins.<sup>[5]</sup>

### Vibrational Spectroscopy in Catalysis

Prof. Dr. Ralf Ludwig University of Rostock Physical and Theoretical Chemistry ralf.ludwig@uni-rostock.de

Professor Ludwig's research group is located at the University of Rostock as well as at the Leibniz Institute for Catalysis.

The research program at the Leibniz Institute for Catalysis is focused on establishing vibrational spectroscopy in catalysis. This includes the implementation of high-pressure in-situ infrared spectroscopy and the optimization of the experimental set-up, as well as the development and application of programs for decomposing vibrational spectra.

Calculated vibrational spectra support the interpretation of measured spectra and allow predictions to be made about the sensitivity of IR spectroscopy in catalytic reactions. The vibrational properties can be correlated with those from NMR spectroscopy and cast light on interesting relationships between structure and properties.

Moreover the "Physical and Theoretical Chemistry" research group investigates clusters, liquids and interfaces. Using appropriate methods, we combine experiment and theory. On the one hand we use IR, Raman and NMR spectroscopy, on the other hand we calculate properties by using density-functional calculations and classical molecular dynamics simulations as well as CPMD simulations for smaller systems. Step by step we are endeavoring to apply these methods to understand processes in catalysis.

Fig. 1: The Bruker VERTEX 80 FTIR spectrometer + stopped-flow-unit can be used to perform rapid-scan experiments. A gas scanner with speeds up to 320 kHz enables IR spectra to be recorded at intervals of 100 ms at a resolution of 2 cm<sup>-1</sup>. In Important topics are: combination with a stopped-flow unit, studies of Anomalies, structure and dynamics of water and the kinetics of homogeneous reactions can thus be aqueous solutions, properties of ionic liquids, carried out. (R. Ludwig)

[1] a) T. Gläsel, M. Hapke, in Cobalt in Catalysis and Synthesis [Eds.: M. Hapke, G. Hilt], Chapter 9, Wiley-VCH, Weinheim, 2020, pp. 287-335. Cobalt-Catalysed [2+2+2] Cycloadditions. b) T. Gläsel, B. N. Baumann, M. Hapke, Chem. Rec. 2021, 21, 3727-3745. Cobalt Catalysts for [2+2+2] Cycloaddition Reactions: Isolated Precatalysts and in situ Generated Catalysts. [2] P. Jungk, F. Fischer, M. Hapke, ACS Catal. 2016, 6, 3025-3029. In Situ-Generated Chiral Co(I)-Catalyst for Asymmetric [2+2+2] Cycloadditions of Triynes. [3] F. Fischer, M. Eder, M. Hapke, Catalysts 2021, 11, 596. CpCo(III) Precatalysts for [2+2+2] Cycloadditions. [4] T. Gläsel, H. Jiao, M. Hapke, ACS Catal. 2021, 11,13434-13444. Synthesis of Phosphinines from Co<sup>II</sup>-Catalyzed [2+2+2] Cycloaddition Reactions. [5] Overview: K. Faust, P. Denifl, M. Hapke, ChemCatChem, 2023, 15, e202300625. Recent Advances in Catalytic Chemical Recycling of Polyolefins.

high thermodynamic stability and enhanced electronic properties; A detailed quantum chemical study.

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hydrogen-bonded networks, hydration of ions, organic and bio molecules, hydrophobic effects, and also influence of temperature, pressure and additives on the aggregation behavior of organic molecules and on the structure of bio molecules. Our main goal is to predict macroscopic properties based on molecular interactions.

Our partner in the industrial area Bayer Pharmaceuticals.



[1] B. Golub, K. Fumino, P. Stange, V. Fossog, R, Hempelmann, D. Ondo, D. Paschek, R. Ludwig, J. Phys. Chem. B, 2021, 125, 4476-4488. Balance Between Contact and Solvent-Separated Ion Pairs in Mixtures of the Protic Ionic Liquid [Et,NH][MeSO,] with Water Controlled by Water Content and Temperature. [2] E. Shelepova, R. Ludwig, D. Dietmar; N. N. Medvedev, J. Mol. Liq. 2021, 329, 115589. Structural similarity of an ionic liquid and the mixture of the neutral molecules. [3] F. Ullah, S. Irshad, S. Khan, M. A. Hashmi, R. Ludwig, T. Mahmood, K. Ayub, J. Phys. Chem. Solids, 2021, 151, 109914. Nonlinear optical response of first-row transition metal doped Al12P12 nanoclusters; a first-principles study. [4] S. Irshad, F. Ullah, S. Khan, R. Ludwig, T. Mahmood, K. Ayub, Opt. & Laser Technol. 2021, 134, 106570. First row transition metals decorated boron phosphide nanoclusters as nonlinear optical materials with

### **Numerical Analysis**

Prof. Dr. Klaus Neymeyr University of Rostock Institute for Mathematics klaus.neymeyr@uni-rostock.de









The "Numerical Analysis" group develops chemometric tools for the extraction of pure component information from high-dimensional spectroscopic data and uses mathematical methods such as optimization, numerical linear algebra and modeling for this purpose.

The starting point is high-resolution series of spectra of chemical reaction systems. From these data, the number of chemical components involved, their spectra and the corresponding concentration profiles are to be deduced. Lambert-Beer's law gives the decomposition task the form of a nonnegative matrix factorization problem, which usually has many and also very different solutions.

The group develops tools for handling and visualizing these solution sets with the aim of extracting the chemically relevant solutions. In this way, we provide chemists with analytical tools that enable a deeper understanding of, in particular, catalytic reaction systems of homogeneous catalysis. The numerical process devel-opment is accompanied by corresponding computer program implementations. At

Likat, there are cooperations primarily with the groups of Prof. Brückner (Börner/Kubis) as well as Profs. Francke and Ludwig.

One current issue is the development of methods for subsystem identification and analysis in collaboration with the Francke group for spectroelectrochemical data.<sup>[1]</sup> The identification of "essential spectral information" for perturbed/noisy data is to be emphasized. These analyses determine such parts of a measurement series that have an influence on the uniqueness of the solutions.

In addition, the group analyzes data with a rank deficiency, which occurs in connection with certain reaction kinetics such as Michaelis-Menten kinetics. Such deficiencies complicate pure component extraction and pose a particular challenge.<sup>[2,5]</sup> For NMR data, we are developing spline-based peak tracking techniques for time series analyses.<sup>[3]</sup> Currently, we are pursuing a neural network approach in which the network estimates the parameters of a sum of functions in terms of optimal modeling.

[1] M. Sawall, C. Ruckebusch, M. Beese, R. Francke. A. Prudlik, K. Neymeyr, Anal. Chim. Acta 2022, 1233, 340448. An active constraint approach to identify essential spectral information in noisy data. [2] T. Andersons, M. Sawall, K. Neymeyr, J. Math. Chem. 2022, 60, 1750-1780. Analytical enclosure of the set of solutions of the three-species multivariate curve resolution problem. [3] D. Meinhardt, H. Schröder, J. Hellwig, E. Steimers, A. Friebel, T. Beweries, M. Sawall, E. von Harbou, K. Neymeyr, J. Magn. Reson. 2022, 339, 107212. Model-based signal tracking in the quantitative analysis of time series of NMR spectra. [4] K. Neymeyr, M. Sawall, A. C. Olivieri, J. Chemom. 2021, 35, e3363. On the signal contribution function with respect to different norms. [5] M. Sawall, K. Neymeyr, J. Chemom. 2021, 35(3), e3316. On the Area of Feasible Solutions for rank-deficient problems: I. Introduction of a generalized concept.

### **Material Design**

Prof. Dr. Axel Schulz University of Rostock Inorganic Chemistry axel.schulz@uni-rostock.de

The research group deals with inorganic and

The experimental work focuses on the synthesis elemental non-metal molecular chemistry from and complete characterization of novel main the fields of CN, EN (E = P, As, Sb, Bi) and SN group molecular compounds from the substansynthetic chemistry. ce classes described above. Many of the com-The Schulz research group is located at both the pounds we present are small and "manageable" university of rostock and the Leibniz Institute for and are therefore very well suited for complete Catalysis. The research area at the Leibniz Insticharacterization (gas phase: ir, mass spectrometute is divided into two thematic areas: try; solution: multinuclear NMR spectroscopy; innovative ligand and material syntheses solid, X-ray diffraction, Raman, IR spectroscopy, • functional materials (CN, PN, SN) solid-state NMrR spectroscopy). A comprehenwhere the linkage of major group element comsive characterization of a new substance inclupounds-minor group element compounds-catades the in-depth study of correlations between: lysis is the main focus. structure  $\leftrightarrow$  bonding  $\leftrightarrow$  properties.

Further topics can be found on our university homepage.

[1] J. Bresien, D. Michalik, A. Schulz, A. Villinger, E. Zander Angew. Chem. 2021, 133, 1530 – 1535; Angew. Chem Int. Ed. 2021, 60, 1507 - 1512. Aza-diphospha-indane-1,3-diyls: A class of resonance-stabilized biradicals. [2] T. Völzer, H. Beer, A. Schulz, S. Lochbrunner, J. Bresien Phys. Chem. Chem. Phys. 2021, 23, 7434 – 7441. Photoisomerization of a P-based diradical: Ultrafast dynamics through a conical intersection. [3] K. Bläsing, R. Labbow, A. Schulz, A. Villinger Angew. Chem. Int. Ed. 2021, 60, 13798 – 13802. Silylated Sulfuric Acid: Preparation of a Tris(trimethylsilyl)oxosulfonium [(Me<sub>3</sub>Si-O)<sub>3</sub>SO]<sup>+</sup> Salt. [4] L. Szych, Y. Pilopp, J. Bresien, A. Villinger, J. Rabeah, A. Schulz Angew. Chem. Int. Ed. 2022, e202114792. A Persistent Phosphanyl-Substituted Thioketyl Radical Anion. [5] L. Eickhoff, L. Ohms, J. Bresien, A. Villinger, D. Michalik, A. Schulz Chem. Eur. J. 2022, 28, e202103983. A Phosphorus Based Pacman Dication Generated by Cooperative Self-Activation of a Pacman Phosphane. [6] J. Surkau, K. Bläsing, J. Bresien, D. Michalik, A. Villinger, A. Schulz Chem. Eur. J. 2022, e202201905. A Lewis Acid Stabilized Ketenimine in an Unusual Variant of the Electrophilic Aromatic Substitution.



### Intermetallic Cooperativity in Supramolecular **Coordination Compounds**

Prof. Dr. Wolfram Seidel University of Rostock Inorganic Chemistry wolfram.seidel@uni-rostock.de

The group's research focus is on coordination chemistry and organometallic issues, with core competencies in classical synthetic chemistry. The focus of interest is on cooperative effects between different types of metal centers, which are mediated with the greatest possible effectiveness via specific ligands. Cooperative interactions not only form the basis for modern, intelligent materials such as single-molecule magnets or substances for the conversion of light into storable forms of energy, but also the mode of action of a large number of metalloproteins is based on bimetallic reaction patterns. In such systems with several metal centers acting cooperatively, inert substrates can be activated or light-driven charge separations can be forced as The work on the subject of light-induced charge a central process of every photocatalysis.

Our research work can be divided into the following two subject areas:

#### 1. Studies on the coordination-chemical potential of alkyne ligands that bear heteroatoms in both $\alpha$ -positions

In addition to terminal oxygen -O- and nitrogen -NR-, classical third-period donors such as sulfur -S- and phosphorus as -PR, come into consideration as donor centers for alkyne ligands. Our work focuses on the development of new coordination motifs or connectivities as well as comprehensive investigations into the electronic structure and the cooperative behavior of the connected metal centers.

Basically, it is important to explore the electronic interactions of the linked metals. A potential application of our approach lies in the development of redox-active metalloligands for catalysis.

#### 2. Development of novel dithiolene ligands as functional bridging ligands

separation and energy transfer in polynuclear complexes is based on investigations with phenanthroline-5,6-dithiolate (phendt2-). Phenanthrolines with donor substitution in the 5,6-position are particularly rigid bridging ligands that fulfill an advantageous condition for very fast electron transfer processes between connected metals.



#### (now: Resource Efficient Catalysis)

Prof. Dr. Thomas Werner University of Paderborn Organic Chemistry th.werner@uni-paderborn.de

We are engaged in the development and application of sustainable catalytic processes. One aspect of our work is the development and implementation of phosphorus based organocatalysts and synthetic methods such as halogenations, olefinations and reductions using PIII/PV redox cycling catalysis. This allows to reduce the amount of phosphorus needed for important organic transformations.

Moreover, we are interested in the use of earth abundant metals such as Fe, Ca, Mn in catalysis. Our methodological work is complemented by the focus on the transformation of renewable resources. In this regard we are working on the utilization of CO<sub>2</sub> as a C1 building, e.g. for the preparation of bio-based carbonates.



N.P P N.O P.O N,S  $E = S^{-}, OR, RN^{-}, PR_{2}$ 0.0 0.5

Fig. 1: Coordination of alkyne ligands that bear heteroatoms in both  $\alpha$ -positions

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Furthermore, we use the obtained products as synthesis building blocks, solvents, and monomers e.g. for isocyanate-free polyurethanes or linkers for hybrid materials. Beside CO<sub>2</sub> other renewable raw materials, such as fats and their derivatives, as well as sugars and terpenes are used.

Another aspect of our research is the evaluation of recycling concepts for homogenous catalysts, such as their immobilization onto inorganic supports using novel immobilization methods, such as plasma techniques. Our work is supported by mechanistic investigations (experimental, spectroscopic and theoretical), which is carried out in cooperation with colleagues at LIKAT and the University of Rostock.

<sup>[1]</sup> C. Timmermann, P. Thiem, D. Wanitschke, M. Hüttenschmidt, J. Romischke, A. Villinger, W. W. Seidel, Chem. Sci. 2021, 10.1039/ D1SC06149F. Migratory insertion of isocyanide into a ketenyl-tungsten bond as key step in cyclization reactions. [2] S. Ludwig, K. Helmdach, M. Hüttenschmidt, E. Oberem, J. Rabeah, A. Villinger, R. Ludwig, W. W. Seidel, Chem. Eur. J. 2020, 26, 16811-16817. Metal/Metal Redox Isomerism Governed by Configuration. [3] H. Lange, H. Schröder, E. Oberem, A. Villinger, J. Rabeah, R. Ludwig, K. Neymeyr, W. W. Seidel, Chem. Eur. J. 2020, 26, 11492-11502. Facile Synthesis of a stable side-on Phosphinyne Complex by Redox Driven Intramolecular Cyclisation.

PD Dr. habil. Wolfgang Baumann wolfgang.baumann@catalysis.de

Analytical Services provides all analytical work that is indispensable for successful chemical investigation to the research groups within LIKAT. In close cooperation with our clients, we develop the necessary methods and care for their adaption to special requirements. All analytical methods are supervised by experienced scientists. Close cooperation with the University of Rostock is an important feature, for some of the expensive analytical instruments are operated jointly, and staff is exchanged between the institutions. In spite of several Corona-pandemic-related measures that had to be followed, work was not restricted severely.

Since the research groups of LIKAT deal with rather different topics, the scope of analytical

problems, techniques, and tools is broad; we have to meet the requirements of synthetic laboratories performing molecular synthesis as well as of those doing solid-state and surface chemistry. We are trying to keep pace with technical progress (and sometimes have to use creative and unconventional approaches). Within the period covered by this report, several instruments (gas-liquid chromatography/mass spectrometry coupling, titrators) have been replaced by up-to-date devices. The newly built "Transfer Technical Center" now hosts all laboratories for elemental analysis in close neighbourhood which will improve workflow and working conditions.

In surface and solids' analytics, we again have access to new possibilities: During the last reporting period, the University of Rostock and LIKAT had jointly managed to acquire a highend electron microscope, and a "Near Ambient Pressure" photoelectron spectrometer (NAP-

Fig.1 : NMR tubes.



XPS) had been purchased for LIKAT from funds of the European Union.

Now we managed to get an scanning electron microscope (Environmental SEM) which will start its operation in 2023.

Common feature of these three instruments is that they are not restricted to inspection of samples in a high vacuum, as it is standard practice. Catalysts may become observed under a gas atmosphere, where reactions take place, "at work" (investigation of samples under varying temperatures and gas compositions). Further information on this subject may be found in the section describing Topic Field 01 "Structure-Reactivity Relationships". Especially considering the start of work in the Transfer Technical Center, the Environmental SEM will be a valuable addition to the existing transmission electron microscope (TEM) as it will be possible to characterize surfaces and coatings of catalyst carriers like monoliths without destructive preparation methods, unlike in the TEM.

The Analytical Services Department furthermore has a perceptible impact on the publication activity of LIKAT. From time to time, we publish own results, but most of the scientific output results from intensive collaboration with researchers from all LIKAT's departments. Some methods are made available as a service to external customers, among them the University, but also other institutions and companies, provided there are free capacities.

#### Electron Microscopy:

In a Scanning Electron Microscope (SEM), the surface of a specimen is scanned with a focused beam of electrons which causes emission of radiation, the latter being collected and analyzed. This provides insight both in structure and elemental composition of the surface with nanometer scale resolution, at objects of considerable size (several centimeter). Resolution is somewhat restricted in comparison to Transmission Electron Microscopy (TEM) where very thin layers are transmitted by the electron beam. Atomic resolution is achievable for layers of a few dozen nanometer thickness. Despite that, a SEM is an important device in structural characterization as it closes the gap between classical (light) microscopy and TEM.



Fig. 2: The NAP-XPS (Near Ambient Pressure X-ray Photoelectron Spectroscopy) commissioned in 2020.

### At present, Analytical Services operate the following methods:

- Chromatography (GC and HPLC)
- Mass Spectrometry and Hyphenated Techniques (GC-MS and HPLC-MS)
- High-Resolution Nuclear Magnetic Resonance (NMR)
- X-Ray Diffraction of powders and single crystals (XRD)
- Optical Spectroscopy (IR, UV-Vis and CD/ORD)
- Elemental Analysis (AAS, ICP-OES, RFA, combustion analysis, titration and photometry, sample pre-treatment/digestion)
- Photoelectron Spectroscopy (ESCA, XPS)
- Analytical Transmission Electron Microscopy (Cs-corrected STEM) with EELS and EDX, in the future also Scanning EM
- Capillary Electrophoresis (CE)

#### **Robert Francke**

Sustainable Chemistry through Reactions under Electricity

With Robert Francke and his expertise in preparative electrochemistry, LIKAT has secured an edge in a research field that is currently one of the most sought-after scientific disciplines. Among other things, it is about using electricity to produce valuable basic and fine chemicals in a sustainable and climate-friendly way. In 2021 Robert Francke joined the institute, where he heads the department of "Electrochemistry & Catalysis" and has been held a Heisenberg professorship since 2022.

His team is researching the production of both complex chemical compounds as well as simple molecules, such as hydrogen, a protagonist of the energy transition, which is also produced under voltage: by electrolysis of water. Robert Francke studied and obtained his doctorate



at the University of Bonn, then worked at the University of California and habilitated at the University of Rostock in 2020.

His research work was supported early, he was awarded the Liebig fellowship from the FCI (the Fonds of chemical industry), and was a Feodor Lynen fellow of the Alexander von Humboldt Foundation.

#### Mirko Kirschkowski Consolidation and Planed Optimization

Since august 2021, Mirko Kirschkowski has been the Commercial Director of LIKAT, whose course in terms of finances he described at the time as "consolidation and planned optimization". After all, for a research institute like LIKAT it will be more difficult than before to grow and develop due to the heavy burden on federal and state budgets in times of crisis. And of course he feels the same as the Scientific Director, Matthias Beller, a strong obligation to the taxpayer. Mirko Kirschkowski has worked, among other positions, as Managing Director of the German "that people's personalities have always been Center for Heart Failure at the University of shaped by a wide variety of facets, including Würzburg and as Administrative Director of the contradictory ones". And that these people, for all their differences, cooperate with each other Sigmund Freud Institute in Frankfurt am Main. and can produce great things together. And as a historian with a doctorate he knows

#### Eszter Baráth Harmony of Multiple Effects

She wanted to be a goldsmith when she was ten, but then Eszter Baráth studied chemistry fortunately for LIKAT, where she has been head of the research department "Catalysis & Renewable Raw Materials" since November 2021. She feels the pressure of the public to "protect the environment and also to assume social responsibility", as she once said in an interview. And she is convinced that chemistry and catalysis can meet this requirement.

Also because they come up with new sustainable synthesis routes for the broad use of renewables and materials. Among her insights, that a "convincing reaction is not necessarily rooted in one well-defined dominant effect, but rather a beautiful harmony of multiple effects." In her education, Eszter Baráth completed in-



ternships in Ludwigshafen and Kyoto, she completed her doctorate in Veszprem, did research in Rennes and Heidelberg, and habilitated in Munich in 2020. Since the end of 2022, she has also been funded by the "Leibniz Programme for Women Professors".

#### Milica Feldt Theory of Catalyis

She studied physics and says that her knowledge of chemistry is "sometimes a bit poor". This is something to be doubted, as the LIKAT has appointed Milicia Feldt as a junior research group leader. Since the fall of 2021, she and her group have been investigating non-heme iron complexes.

Milicia Feldt uses a metaphor from chemistry in an intranet presentation on the occasion of her start at LIKAT: Different transition metals behave guite differently in one and the same environment, "just like people behave quite differently in the same environment".

Milicia Feldt did her doctorate in Göttingen. As a postdoc she joined physical chemistry (Göttingen and Belgrade), organic chemistry (Münster) and in the group "Theoretical and





Computational Chemistry" of Jeremy Harvey at the at the KU Leuven, Belgium. Her achievements have been honored many times with travel grants and with a poster award at the congress of the International Society for Theoretical Chemical Physics 2019 in Tromsø.

#### **Osama El-Sepelgy**

Combination of Photocatalysis and Light-excited Biocatalysis

Osama El-Sepelgy has been conducting research at LIKAT since May 2021. He heads the junior research group "Modern Organic Chemistry". The goal is to explore novel strategies to tap those raw materials that, like carbon dioxide, are abundant but not very reactive. This involves the sustainable, and above all climate-friendly, production of fine and bulk chemicals - one of the challenges of the 21st century. Osama El-Sepelgy and his group are concentrating on the combination of photocatalysis of non-precious metals with photoexcited biocatalysis. Osama El-Sepelgy studied chemistry at the Mansoura University in Damietta, Egypt, com-



pleted his internship at the University of Leipzig and received his doctorate from the Jagiellonian University in Krakow in 2014. As a postdoc, he went to the RWTH Aachen,

from where he moved to Rostock and the LIKAT.

#### Johannes Gerardus de Vries Renewable Raw Materials for Chemistry

Research work on so-called platform chemicals at LIKAT is closely linked to the expertise of Johannes de Vries, who retired at the end of 2021. This topic involves a turnaround in chemistry, namely the replacement of crude oil and natural natural gas with renewable raw materials. 2014 Johannes de Vries, born in Amsterdam, came to LIKAT, where he built up the department of "Catalysis with Renewable Raw Materials".

A short time later several research groups at LIthat can be used in the laboratory to produce a KAT researched the potential of wood waste, for monomer for nylon from wood. example, for the chemical production of basic He had studied and obtained his doctorate in materials. Research on the platform chemical le-Groningen and researched and taught in the vulinic acid, for example was funded within the USA, Great Britain, Austria and the Netherlands. framework of the Leibniz competition, He initiiated research programs and projects, SAW. Already 20 years ago in the Netherlands and is still a member of important committees Johannes de Vries developed a catalytic process of scientific societies worldwide.

#### Barbara Heller Doing Good and Making it Public

In the summer of 2021 Barbara Heller, most recently the Commercial Director of the LIKAT, retired. She studied chemistry at the University of Rostock, where she received her doctorate. A quarter century she did research in the field of organic chemistry and catalysis, finally as group leader at IfOK, which became the Leibniz Institute for Catalysis in 2006. There Barbara Heller was responsible for public relations, which meant educating people and the media about catalysis and chemistry, i.e. about a subject that is commonly regarded as "difficult" and and unpopular. With charm, the right amount of persistence and the principle of "do good and talk about it," she established contacts with editorial offices and succeeded in getting journalists interested in the excellent research results of



LIKAT. Later, Barbara Heller took over the institute's staff and, at first on a temporary basis, the institute's administration.

In all these functions she ensured that the LIKAT with its scientific standing and its worldwide reputation is a name even to the uninitiated.



## Public FROM THE PRESS

## Hurdle race to hydrogen - PhD student discovers a new type of H<sub>2</sub>O splitting at LIKAT

#### August 2021

It sounds simple, and nature shows us how: Green plants store solar energy by splitting water into hydrogen and oxygen - using light and chloroplasts. Researchers are excited to arrive at hydrogen gas (H<sub>2</sub>) in a similar way, because produced "green" it is considered a protagonist of a sustainable energy and basic materials economy. Jacob Schneidewind from the Leibniz Institute for Catalysis in Rostock has shown a way to achieve this with his dissertation. He uncovered the mechanism of a new type of water splitting that can make photolysis possible at low cost. The report on this appeared in the specialist journal ENERGY & ENVIRONMENTAL SCIENCE.

Green hydrogen can be produced in different ways. Electrolysis using a catalyst and electricity from the wind or sun is currently being used technically. More elegant and possibly more cost-effective, however, is photolysis, in which sunlight directly causes the splitting of water with the help of a catalyst - without a diversion via electricity from wind or solar plants. Under the keyword "artificial photosynthesis", chemistry is currently intensively exploring this photocatalytic path.

#### What it Needs: Water, Light Source, Catalyst

12 years ago, a team from the Weizmann Institute, Israel, reported in SCIENCE magazine on a chemical reaction in which a novel catalyst used light to split water. "But no one understood in what way this happened," says Dr Jacob Schneidewind. "The only thing that was clear was that no one had ever seen or described this type of water splitting. It is also completely different from natural photosynthesis."

Here was something fundamentally new to learn about water splitting. And to explore a new way to use these processes technically. For three years, Jacob Schneidewind studied the original reaction of his Israeli colleagues using water, a light source and a ruthenium catalyst for his doctorate at LIKAT. The goal was to elucidate the processes at the molecular level and to simulate the processes on the computer.

#### Four Hurdles for Photons

A short reminiscence of secondary school biology lessons: during photolysis in green plants, an oxygen molecule ( $O_2$ ) is created from every two  $H_2O$  molecules, as well as exactly four protons of hydrogen ( $H^+$ ) and four electrons (e<sup>-</sup>). Jacob



Laboratory scal Photoreactor: The combination of light irradation and the right catalyst enables the splitting of water into its components (symbolic picture).

Schneidewind explains: "The energy for the release of the four electrons also comes from four absorbed light particles, the photons. To obtain enough photons, nature uses several absorbing centres."

You can think of the reaction as an energetic hurdle race, says Jacob Schneidewind. "There are then four hurdles to overcome before reaching the goal, i.e. the splitting of water. If even one of them is broken, photolysis fails - at least for this molecular bond." So much for the process in nature.

#### **Original Leaves Questions Unanswered**

In the laboratory at the Weizmann Institute, however, photolysis did not occur at several

absorbing centres, but only at a single point. "That seemed strange," says Dr Schneidewind. "That one catalytic centre alone would absorb four photons is extremely unlikely." Nor would the energy of a single photon be sufficient to jump all four hurdles. There was no meaningful explanation for this.

As a PhD student, Jacob Schneidewind worked his way into quantum chemistry and the kinetics of chemical reactions, which he used to model reactions on the computer. In the lab, he recreated the Israeli experiment with changing light sources, from short-wave, high-energy blue light to the low-energy red range. Colleagues at the University of Rostock took over the analyses using high-speed spectroscopy.

#### The Solution: Two Hurdles are Enough

"It surprised us all to see what was happening in the system," says Jacob Schneidewind. In fact, the photocatalytic pathway to hydrogen gets by with two photons instead of the usual four. And both the absorption of the photons and the actual fission reaction take place at a single centre, which consists of a pair of ruthenium atoms. "Once the first photon has cleared its hurdle, a new compound is formed that absorbs the second photon. And this requires even less energy for the second hurdle than was needed for the first hurdle." Thus, a wider bandwidth of light can be used, which can significantly impro-



Dr. Jacob Schneidewind in Aachen (Photo: Martin Grolms)

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ve efficiency.

Structurally, everything seems to be cleared up. What follows technically from this? "You could, for example, fill transparent plastic tubes with a suspension or solution of water and catalyst and expose them to the sun over a large area," says Dr Schneidewind. With the right catalyst, this approach would be three to four times cheaper than combining solar cells and an electrolyser. Starting in autumn, Jacob Schneidewind plans to develop a suitable catalyst for this with his own junior research group at RWTH Aachen University, where he moved after completing his doctorate.

Sustainable energy concepts assume, among other things, that in future green hydrogen will be produced in sunny regions and imported to Europe. The knowledge from LIKAT will help to develop appropriate technologies.

#### Dr. Jacob Schneidewind

2012 - 2014 Junior Studies at the University of Cologne (Chemistry)
2014 - 2015 Studies at Yale-NUS College, Singapur (Liberal Arts)
2015 - 2016 Research Stays with Prof. Dr. Robert H. Morris (University of Toronto) and Prof. Dr. Matthias Beller (LIKAT, Rostock)
2016 - 2016 B. Sc. (Chemistry, 2016), M. Sc. (Chemistry 2017) Universität Rostock
2017 - 2021 PhD with Prof. Dr. Matthias Beller (LI-KAT, Rostock)
since 2022 Junior Research Group Leader at the RTWH Aachen

schneidewind@itmc.rtwh-aachen.de Original Publication DOI: 10.1039/d1ee01053k

#### June 2022

Chemists at the Leibniz Institute for Catalysis, LI-KAT, together with the company APEX, developed a catalytic system that can chemically store hydrogen and release it in a highly pure form at will. On this basis, systems based on the principle of a battery could in the future donate hydrogen anytime and anywhere, e.g. to power fuel cells. Dr. Henrik Junge's research group published its findings in the specialist journal NATURE ENER-GY, which also had a commentator rate the work as a highlight. Among other things, the paper reports about the "remarkable activity" of the catalyst and the "extraordinary" efficiency of the chemical reactions.

In fact, this work can take a good step forward in the global effort to replace oil and gas as energy raw materials and to use CO<sub>2</sub>-neutral processes. After all, hydrogen is now accepted as the future basis for the energy sector, as Dr. Henrik Junge explains, but its storage is still problematic. Hydrogen is explosive in the presence of oxygen and, as a gas, is volatile and of low density under normal conditions, which is why leading research laboratories are primarily exploring chemical ways of storing it.

#### Formic Acid as a Storage Medium

Dr. Duo Wei, a postdoctoral researcher at LIKAT in Rostock, used formic acid and its salts, so-called formiates, as a storage medium for hydrogen. A year ago, the Rostock chemists described in the journal CHEMICAL SCIENCE how they catalytically store hydrogen in formiates using carbon dioxide from the air and the amino acid L-lysine . Dr. Junge: "Of course, it would be elegant if we could release the hydrogen again in the same system as needed to use it." That's exactly what the current work has accomplished. The chemists developed the catalyst that enables all the necessary chemical reactions on the basis of a manganese complex, so it does not require a precious metal, unlike most hydrogenation processes to date. There are other advantages, as LIKAT director Prof. Dr. Matthias Beller explains. Normally, when hydrogen is recovered from formiates, the carbon dioxide used for storage is released again. "We, on the other hand, permanently retain the CO<sub>2</sub> in our reaction system." The trick is for the researchers to bind the CO<sub>2</sub> to a common amino acid that occurs in nature and in ourselves.





#### High Yields of 90 and 80 Percent Respectively

The newly developed reaction system follows the principle of an electric battery, with the difference that hydrogen is used instead of electric current. Such a battery is thus filled once at the beginning with  $CO_2$  from the air. It can then go through the cycle of hydrogenation (H<sub>2</sub> storage) and dehydrogenation (H<sub>2</sub> release) several times, with new hydrogen always being loaded into the storage.

Among other things, the high yields of this process - more than 90 percent for H<sub>2</sub> storage and 80 percent H, release - highlighted a commentary with which the journal NATURE ENERGY, usually has such groundbreaking developments evaluated. Commentator Sheri Lense was impressed by the "remarkable activity" of the catalyst and an "exceptionally high total TON" (turnover number) even after ten charge cycles. In the future, a process on this basis will develop its full charm above all when the hydrogen to be stored comes from renewable sources in the region, such as wind power or photovoltaics. Henrik Junge: "Such sources do not gush forth continuously. That's why the green-based hydrogen economy needs large storage capacities, preferably of a chemical nature, also locally on site."

#### Patent Application with APEX Group

All of this is basic research, as Dr. Junge emphasizes, but it is highly suitable for helping to transform the economy and the energy sector with climate-neutral processes. In addition, chemistry is increasingly recognizing carbon dioxide in the atmosphere as a source of raw materials, starting material for a wide range of useful products, as Henrik Junge says.

LIKAT's cooperation with the APEX Group will ensure that their findings are put to practical use. Dr. Peter Sponholz, head of research and development at APEX is one of the five-member team of authors of the NATURE ENERGY paper. The application for a joint patent filed by APEX is currently underway.



Fig. 2.: As in this assembly, we can imagine the hydrogen battery for the future: The sun supplies the electricity for the electrolytic production (right in the picture) of hydrogen ( $H_2$ , white balls) from water. The  $H_2$  is stored in the battery storage (box in the middle) where it is mixed with CO<sub>2</sub> (combination of black and red balls) by means of a catalystand an amino acid to formate (combination of red, black and white balls) released again when needed (discharge of  $H_2$  through the tubes) and used, for example, in a fuel cell (left in the picture). (Picture montage: LIKAT)

#### Scientific Contact:

Dr. Henrik Junge (Group Leader "Catalysis for Energy") Phone: +49 (0) 381 12 81 – 174 E-Mail: henrik.junge@catalysis.de

Original Publication: https://doi.org/10.1038/s41560-022-01019-4

### Leibniz Science Campus ComBioCat: Enzyme and Metal Combined for Future Catalysts

#### August 2022

As biocatalysts, enzymes manage the metabolism of all living things. They do this extremely precisely, because even a single incorrectly converted substance could have fatal consequences for the organism. Young researchers from the Leibniz Science Campus ComBioCat are using this selective approach of enzymes and proteins in general to develop catalysts of the future: so-called artificial metalloenzymes. In the future, combinations of bio- and chemical catalysts will be used to design complex molecules, e.g. for pharmaceuticals, in a targeted and reliable manner.

#### The Best of Two Worlds

At the Leibniz Institute for Catalysis in Rostock, LIKAT, doctoral student Paul Hünemörder is currently in the process of linking a copper catalyst with an enzyme or protein as part of the ScienceCampus ComBioCat. The new catalyst is intended to combine "the best of both worlds," so to speak, he explains. "Chemical catalysts work quickly and produce high yields, but unfortunately they also produce undesirable byproducts in the process." That doesn't happen to biomolecules, he says, because they are "highly selective."

The development of metalloenzymes is a new field of research in chemistry. At LIKAT, work is underway in the research group of Esteban Mejìa, doctoral supervisor of Paul Hünemörder. "The trick is to find connection points at the molecular level where protein and metal can be linked," explains Esteban Mejìa. No artificial metalloenzymes are yet in industrial use. According to Mejìa and Hünemörder, they have so far also failed because "the proteins have to be modified, i.e. genetically modified, for this purpose." This makes them too expensive for widespread use

#### **Enzymes from Nature**

On the chemical side, Paul Hünemörder opted for copper as the reactive center. The search for a suitable enzyme was the responsibility of biochemists at the University of Greifswald. They chose a protein called Lactococcus Multid-



Fig. 1.: The copper catalyst, the chemical part of the future metalloenzyme, is tested, in a solution of cyclic alkenes. The reaction starts under UV light. (Photo: LIKAT/P. Hünemörder)

rug Resistance Regulator, or LmrR for short. As a protein, it causes antibiotic resistance in lactic acid bacteria. Its advantage is that it can be used as it occurs in nature and does not need to be genetically modified.

Proteins achieve their effect primarily through their complex folding, their protein structure. In the case of LmrR, this creates a flat pocket, "a kind of slit," as Paul Hünemörder says. This gave him the idea of sinking the synthetic part of the catalyst, each with a copper atom in the center, into this slot like a coin and connecting it to the protein in this way

#### Corset for the Copper Atom

The prerequisite is a kind of corset for the copper atom, a catalyst framework, or ligand in technical jargon. According to Paul Hünemörder, the search for a suitable substance proved to be quite difficult. The only suitable substance was terpyridine, a so-called pincer ligand, which is so called because its shape allows it to pincer the catalyst.

"But the most important thing is that this ligand gives the copper system a very flat structure," says Paul Hünemörder. "Which makes the catalyst fit perfectly into the ,slot' of the enzyme." Based on initial tests, it seems to work, too. In the future, the metalloenzyme, which in this case is strictly speaking a "metalloprotein," will convert so-called cyclic alkenes into precursors and intermediates for pharmaceuticals. What advantage does it bring there?

#### Image and Reflection

In terms of structure, cyclic alkenes often exist left-handed and right-handed, imaginable as image and mirror image. In nature, enzymes with their highly precise catalytic action ensure that only one variant, the "true" one, is produced. In a chemical synthesis, on the other hand, both variants can be produced. Chemically, they are completely identical, but in their physiological effects they sometimes differ dramatically.

In the 1950s, the painkiller thalidomide caused severe malformations in unborn children because it caused the formation of a mirror-image molecular variant in the organism of the pregnant woman. Industrially, therefore, such end products sometimes have to be separated at great expense so that the desired molecular variant can be used.

This is precisely what the use of an artificial metalloenzyme would eliminate. The aim of the work in Rostock and Greifswald is to ensure that



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the selective mode of operation of the protein LmrR produces only the desired form of intermediate products. Chemists therefore refer to this reaction as asymmetric.

#### Mechanism Research

The copper center in the catalyst now does its job "quickly and reliably," as Paul Hünemörder and his student research group were able to demonstrate in the laboratory. Now the challenge is to prove that the protein part of the new catalyst also works, i.e. that it recognizes the "handedness" of the starting materials and only allows the "correct" variant to react. Paul Hünemörder expects a result in the fall. The researchers are convinced that artificial metalloenzymes will give the chemical industry a decisive advantage in the future. And the work

a decisive advantage in the future. And the work is also a theoretical gain. In analyses of the reaction mechanism, the young chemists identified an intermediate that turned out to be essential for the chemical process but had not previously played a role in the technical literature. The findings may help to transfer the reaction principle to other substance classes.

Scientific Contact: Paul Hünemörder (PhD Student at reseach group "Catalysis & Polymer Chemistry") Phone: +49 (0) 381 12 81 – 416 E-Mail: paul.huenemoerder@catalysis.de

Fig. 2: Paul Hünemörder (Photo: LIKAT/Maslack)

### Sniffer Dog for Drug Degradation Products - LIKAT Simplifies Molecular Labeling Process Using Deuterium

January 2022

Drugs that we take are chemically altered as they are degraded in the body. In the case of newly developed active ingredients, and not only there, it is important to know which degradation products (metabolites) are formed in the process, because these can be incompatible or even harmful. To detect such metabolites, chemists label the substances under investigation with the hydrogen isotope deuterium. This deuteration makes it possible to precisely track active substances as they are broken down and metabolized. At LIKAT in Rostock, Kathrin Junge's research group in the department of Matthias Beller succeeded in considerably simplifying the labeling of chemical compounds by means of a new catalyst.

"In a process known as deuteration, a certain number of hydrogen atoms in the drug are replaced by deuterium," explains Dr. Kathrin Junge. The difference between the two: While hydrogen has only a single proton in its atomic nucleus, the deuterium nucleus contains a neutron in addition to its proton.

Deuterium and hydrogen are, so to speak, siblings: isotopes of hydrogen. Chemically, both behave completely identically. Only physically do they differ due to the higher molecular weight of deuterium. This makes it possible to detect and analyze a deuterated drug at any stage of its degradation.

The research team reports on this in the renowned journal NATURE CHEMISTRY.

Cheaper and More Sustainable than Before Chemists around the world usually use deuterium gas for deuteration. For this, they need catalysts that contain a precious metal, such as platinum. The team at LIKAT, on the other hand, uses deuterated water, D<sub>2</sub>O. This is cheaper and also more readily available than deuterium gas, as Dr. Junge says.

Her research group developed a catalyst specifically for this purpose. And it is also cheaper and more sustainable than has been the case in the past. "We use iron instead of the usual precious metals and use cellulose as a carrier material, which is waste from the wood industry." The catalyst works, and this is another difference, "very selectively," as Kathrin Junge explains. That means, it ensures that not all hydrogen atoms in the molecule are replaced by deuterium, but only at certain positions in the molecule.

#### **Deuteriation: Hot Topic in Chemical Research**

Molecular labeling using deuterium not only helps to elucidate the degradation mechanisms of active ingredients. As pharmacists have discovered, deuterium can significantly enhance the effect of drugs. In 2017, the U.S. Food and Drug Administration (FDA) released the first deuterated drug. Since then, the field has become a hot topic in chemistry research, says Kathrin Junge.

At LIKAT, Dr. Wu Li was mainly involved in the project. He was supported in the laboratory by Florian Bourriquen, a PhD student at LIKAT. Both have been able to demonstrate that their method works not only for a selected model substance, but for a wide range of substances. They tested around 90 compounds, including natural substances such as amino acids and DNA nucleotides, hormones such as melatonin and estradiol, and pharmaceutical agents such as thyrosol for hyperthyroidism and the antiseptic thymol.

The reaction mechanism for deuteration by means of  $D_2O$  as well as the structure of the deuterated substances were elucidated by analysis groups at LIKAT.

#### Method for Improved Effect of Drugs

Assessing the medical effect of such deuterated substances is a matter for pharmaceutical research, says Dr. Kathrin Junge. With the results from LIKAT, a method is now available that is much easier to implement than the previous procedure. In the future, such aspects (including sustainability) would play a much greater role in drug approval procedures than they have in the past. The new findings on deuteration will, among other things, be incorporated into a current EU-funded research project in which several European pharmaceutical companies are also collaborating.

#### Scientific Contact:

Dr. Kathrin Junge (Group Leader "Sustainable Redox Reactions") Phone: +49 (0) 381 12 81 – 138 E-Mail: kathrin.junge@catalysis.de

#### **Original Publication:**

,Scalable and selective deuteration of (hetero)arenes' https://www.nature.com/articles/s41557-021-00846-4



## TRANSFER

### **"THEORIA CUM PRAXI" - RESEARCH FOR PRACTICE**

Knowledge and technology transfer (KTT) is now vement of industrial partners as future users in considered the third pillar of science alongside teaching and research. For members of the Leibniz Association's sense, transfer means the "exchange between science and the non-academic world", which always takes place in two directions: on the one hand, the provision of scientific findings for societal needs or decision-making processes, and on the other hand, the integration of society-generated queries and issues into into current research questions. Both require an intensive dialogue on a target group-specific level.

#### Transfer as a Central Task

As a publicly funded institute, we are obliged to transfer our research results to society in a target group-specific manner.

LIKAT is located at the interface between basic research and applied research. It is thus a link between academic research institutions (universities, institutes of the Max Planck Society) and industrial research departments (companies in the chemical, petrochemical and pharmaceutical industries).

LIKAT understands knowledge & technology transfer to mean all activities that serve the purpose of scientific findings and technologies and transfer them to the non-academic world. There- dialogue with society, politics and industry enables the adaptation of research questions to social debates and and problems.

Technology transfer in particular, as technical utilization and commercial exploitation, has long been a constant feature of LIKAT profile. This is reflected by noumerous industrial cooperations, transfers and patenting. The close invol-

the research process is an example of successful two-way transfer.

Cooperation with industry is a basic prerequisite for t the transfer of technology (technical utilization and commercial exploitation). In this respect the Catalysis2Scale transfer technical center will play an important role (right picture).

The transfer of knowledge at LIKAT is becoming increasingly important: As a "target-group-specific and quality-assured translation of scientific findings" and, conversly, as "translation of problem descriptions and needs from business, politics and society into research questions that can be dealt with scientifically". Predestined for such successful knowledge transfer are Leibniz formats such as Leibniz fragt (Leibniz asks), Leibniz im Bundestag (Leibniz in the Bundestag) or Book a Scientist, in which LIKAT regularly participates In 2021 and 2022, scientists from the institute were involved in a total of 55 patent applications as well as ten transfers.

Knowledge transfer takes also place, among other things, through scientific training, events such as the the summer workshop Rostock's Eleven and the Long Night of Science, press relations, social media, visits by schoolchildren, the implementation of internships and participation in various high-profile events (Wissenskarawane, Girlsday, Day of Science, etc.).

All employees of the LIKAT are supported by a transfer officer who is available to all LiKat employees.

There are clear definitions, rules and recommendations for transfer activities in the *Strategy* 2023.



### THE CATALYSIS2SCALE TRANSFER TECHNICAL CENTER

Start of Work	Autumn 2019	Total Area	> 1000
Opening	July 4, 2022	Laboratory Area	appro
		Office Space	appro
Total Cost	approx. 12.5 Mio. €	Test Hall	appro

With the institute's own transfer pilot plant, which is unique in northeastern Germany, for testing and transferring chemical research results from the laboratory to practice (pilot scale), the Leibniz Institute is creating another unique selling point.

The topic Circular Economy will set the strategic direction for investigations in the pilot plant: The main focus will be on processes that convert  $CO_2$  into valuable and sustainable substances, such as synthetic fuels and basic chemicals. The technical center has a functional building and a building hall for the infrastructure area. In the 750 m<sup>2</sup> hall, several pilots can be carried out simultaneously. The respective projects/apparatus can be separated from each other by flexible room separation systems.

m<sup>2</sup>

200 m<sup>2</sup>

150 m<sup>2</sup>

650 m<sup>2</sup>

A separate storage area for technical gases or gas bundles (hydrogen; synthesis gas,  $CO_{2'}$ methane; approx. 30 m<sup>2</sup>) is provided for applications with these substrates. Generated products are temporarily stored in a fenced outdoor storage area (roofed; 50-75 m<sup>2</sup>).

\_Main Research Topics \_

**CO**<sub>2</sub>**-capture** from the atmosphere and point sources (green carbon)

Generation of **green hydrogen** and its conversion to (carbon-based) e-fuels and sustainable chemicals

Establishment of the Hydrogen Research Factory MV

Production and further development of **innovative high-performance materials** and catalysts (multi-kg scale)

#### \_\_\_Building \_\_

**Functional Building:** 5 laboratories, 7 offices, control room and storage area for raw materials and products

**Test Hall:** area of 750 m<sup>2</sup> for pilot plants with flexible room partitioning systems, walk-in fume hoods, autoclave rooms (for work under high pressure, explosion protection integrated)

**Infrastructure:** photovoltaics & electricity storage, electrolyser & hydrogen storage,  $CO_2$  capture plant & storage, exhaust air purification



#### Transfer of knowledge from the laboratory to practice - Technical center opened at LIKAT in Rostock

Chemists at the Leibniz Institute for Catalysis in Rostock can now test the application readiness of their laboratory findings themselves on a pilot scale. The institute's new pilot plant, which was officially opened on July 4, serves this purpose. Among other things, it provides space for test rigs for chemical reactions in the kilogram range, bringing basic research in particular closer to practical applications. The pilot plant was built in a construction period of about three and a half years and was funded by the federal government and the state of Mecklenburg-Western Pomerania to the tune of about 12 million euros.

With the possibilities of the pilot plant, LIKAT will in future also be able to participate in those tenders for funding projects that require proof of the functioning of laboratory chemistry in the kilogram range. In the opinion of its director, Prof. Dr. Matthias Beller, this will enable the Leibniz Institute to fulfill its mission, as laid down in its statutes, even more clearly than before: to conduct cutting-edge basic research and to apply the findings to practical applications.

The main focus of LIKAT's research is on new catalysts and reactions that enable sustainable chemistry based on renewable raw materials and energy. Hydrogen plays a special role here as an energy carrier and raw material, provided it is obtained from renewable sources. At the pilot plant, for example, ways of CO<sub>2</sub>-neutral production and storage of green power and raw materials from hydrogen are being tested. In addition, the Rostock researchers want to make their specially developed catalysts available for semi-industrial uses. There is no research facility in Germany that can do this on this scale. According to Matthias Beller, the pilot plant will thus also develop its international appeal. With the help of a grant from the state's Ministry of Economics, the pilot plant supplies itself with electrical energy via a photovoltaic system. Green hydrogen is produced there via electrolysis and CO<sub>2</sub> from the air. Both raw materials are to be processed at the pilot plant in innovative processes to produce e-fuels as well as energy storage media and basic chemicals such as kerosene and methanol. All chemical pro-

Transfer - Catalysis2Scale Transfer Technical Center

cesses require new catalysts, which are being developed at LIKAT. For example, there are no market-ready solutions yet for  $CO_2$  capture from the atmosphere.

In addition to LIKAT researchers, start-ups and established companies will be able to work hand in hand at the Technikum and benefit from each other. Among the first projects now starting there is the development of a demonstrator for so-called hydrogen batteries , which LIKAT is developing together with the APEX Group.

## Start for the "Research Factory Hydrogen MV - Northeast as Pioneer for Technologies of the Energy Transition

The award of the first grants to the Leibniz Institute for Catalysis, marks the start of the joint project "Research Factory Hydrogen MV". Together with two other research institutes, LIKAT will develop processes and technologies based on renewable energies for  $CO_2$ -neutral production cycles, and develop them to the point where they are ready for application.

In addition to LIKAT, the other partners are the Rostock-based Fraunhofer Institute for Large-scale Structures in Production Engineering (IGP) and the Leibniz Institute for Plasma Research and Technology (INP Greifswald.)

The research work is carried out in LIKAT's own *Catalysis2Scale* technical center.



Fig.: Pleased with the funding decision for the PtX transfer project at LIKAT: Reinhard Meyer, Mecklenburg-Western Pomerania's Minister of Economics and funding provider (right), Bettina Martin, Minister of Science, and Prof. Dr. Matthias Beller, Director of LIKAT. The decision was made on July 4, 2022, for the opening of the of the new technical center at LIKAT. (Photo: LIKAT)

### DEGREES

LIKAT explicitly acknowledges its responsibility to actively promote equal opportunities and gender equality and anchored this in its statutes in 2012. Equality in this context means not only enabling equal opportunities for the sexes, but also bringing about gender balance through binding measures. In addition, the diversity of people and ideas is respected, appreciated and promoted. We actively promote equality and oppose all forms of discrimination. Equal opportunities, equality and diversity are laid down as overarching goals in the Leibniz Association's statutes, which are binding for us. We want to offer all employees resilient career prospects and the best possible conditions for individual life and career planning, taking into account the compatibility of work and caring responsibilities. Measures to reconcile work and caring responsibilities, such as the company agreement on flexitime, temporary part-time work or dual-career measures are clearly defined and documented and an integral part of everyday working life at LIKAT. We would like to highlight the LIKAT Community Fund. It was established in 2016 as a come-back fund to provide financial support for employees before, during and after a family break. Since then, it has been steadily expanded and is now an

established financial instrument anchored in the budget to cover our employees in temporary employment during pregnancy, parental or care leave, or in cases of particular social hardship. In addition, childcare costs during an external conference or event are now covered for all LI-KAT employees. The fund offers employees and scholarship holders alike planning security and binds them more closely to the institute than before.

In 2021, after a long break, we established an employee survey that asked about various aspects of employee satisfaction and also posed questions with regard to equality work. Among other things, these included support for childcare, the equality body itself, and sexual harassment and violence.

In the same year, ICESCO and LIKAT, among others, organized the virtual workshop International Day of Women and Girls in Science, which reached about 5000 participants from 350 universities.

With the beginning of 2022, we published our gender equality plan on our websites (catalysis. de) in both English and German. In addition, we made training materials on the topic of unconscious bias available to our employees on the institute's intranet.

### 2021

#### Doctorates

Budweg, Svenja (Beller), El-Hage, Firas (NG Pospech), Hauptmann, Richy (NG Pospech), Hervochon, Julien (extern) (Beller), Iffländer, Karl Friedrich (Strunk), Kunkel, Benny (Wohlrab), Leonard, David (Beller), Liu, Xin (de Vries), Marx, Maximilian (Beller), Meyer, Tim (Börner), Ngo, Anh Binh (Brückner), Perechodjuk, Anna (Linke), Schneider, Carolin (Beller), Schneidewind, Jacob (Beller), Stefanow, Vivian (de Vries), Täufer, Tobias (NG Pospech), Wang, Fan (Beller), Yuan, Yang (Börner), Zhang, Youcan (Börner)

#### Masters

Kraußer, Laura (Linke), Leidecker, Benedict Bossow, Dennis (Strunk), Staude, Josh (Strunk), (Börner), Löbner, Sebastian (Wohlrab), Lorenz, Rippke, Mirko (Beweries), Schönke, Eric (Fran-Felix (Strunk), Makhmutov, Denis (extern) (Lincke), Gräber, Leo (Kragl), Nguyen, Duc Manh (extern) (Kragl), Giap Van, Hung (Strunk), Brandt, ke), Mollaert, Guillaume (extern) (Beller), Mürdel, Felix (Strunk), Phong Dam, Le Quoc (extern) Sina (Beweries), Gudkova, Aija (Francke), Scherkus, Anton (Francke), Gutgesell, Merlin (Strunk), (Brückner), Schömig, Nadja (Strunk), Trang, Pham Minh (Francke), Wellnitz, Tim (NG He-Thaens, Jannik (Beller), Schlapp, Janina (Beweries), Hollack, Johannes (Strunk), Räsch, Erik ring-Junghans) (Strunk), Patel, Harvi (Strunk)

#### **Bachelors**

Albrecht, Ole (Francke), Hildebrandt, Laura (Francke), Zach, Luisa (NG Pospech)

### 2022

#### Doctorates

Ai, Han-Jun (Börner), Aydin, Zeynep (Linke), Chandrashekhar, Vishwas (Beller), Dell'Acqua, Andrea (de Vries), Dühren, Ricarda (Beller), Guo, Xuewen (Kragl), Kopf, Sara (Beller), Krake, Everaldo (Baumann), Kucmierczyk, Peter (extern) (Beller), Lang, Moritz (Strunk), Mosrati, Jawaher (Wohlrab), Naliwajko, Pawel (Strunk), Rothe, Julia (Beweries), Skrypnik, Andrey (Linke), Spiegelberg, Brian (de Vries), Sun, Kangkang (extern) (Beller), Wu, Fupeng (Börner), Yang, Qingxin (Linke), Zhao, Fengqian (Börner),

#### Masters

#### **Bachelors**

Hirte, Paula (extern) (Wohlrab), Lorenzen, Ludwig (Beweries) The Leibniz Institute for Catalysis (LIKAT Rostock) is a research institution of the Leibniz Association and has the legal form of a registered association (e.V.). As an affiliated institute of the University of Rostock, LIKAT is an organizationally and legally independent research institute with the organs of a general meeting, a board of curators and a scientific & industrial advisory board. Funding is provided on a parity basis by the federal and state governments. The Ministry of Education, Science and Culture of Mecklenburg-Western Pomerania and the Federal Ministry of Education and Research (BMBF) are responsible for the technical aspects.

#### General Meeting

### Board of Curators

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(until march 2023 Prof. Dr. Angelika Brückner and Prof. Dr. Jennifer Strunk)

#### **Topic Speakers**

- Topic 01 NN (until 03/2023 Prof. Angelika Brückner), PD Dr. habil. Wolfgang Baumann Topic 02 Prof. Dr. Evgenii Kondratenko & Prof. Dr. Haijun Jiao Topic 03 Dr. David Linke & Dr.-Ing. Udo Armbruster Topic 04 Dr. habil. Eszter Bárath & Dr. Ali Abdel-Mageed Topic 05 Prof. Dr. Robert Francke (until 05/2023 Prof. Dr. Jennifer Strunk) & Dr. Henrik Junge Topic 06 Dr. Sebastian Wohlrab & Dr. Bernd Müller
- Topic 07 Prof. Dr. Torsten Beweries & Dr. Christian Hering-Junghans

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PD Dr. habil. Wolfgang Baumann, Analytics Dr. Mirko Kirschkowski, Administration Andreas Schupp, Technics Dr. Sandra Hinze, Staff

### MATRIX STRUCTURE

Topics	Structure-Reactivity 01 Relationships	Kinetic, Theory & 02 Mechanisms	Reaction Engineering & <b>03</b> Implementation	Renewable Raw 04 Materials	Energy & 05 Environment	More efficient 06 processes	New Products & 07 Processes
Research Departments	NN Wolfgang Baumann	Evgenii Kondratenko Haijun Jiao	David Linke Udo Armbruster	Eszter Baráth Ali Abdel-Mageed	Robert Francke Henrik Junge	Sebastian Wohlrab Bernd Müller	Torsten Beweries Christian Hering-Junghans
Synergies in Catalysis Eszter Baráth	Selective Catalytic Synthesis Methods Eszter Baráth	Catalysis w. Phosph. Materiab Christian Hering-Junghans Catalysis for Sust. Syntheses Jagedeesh Rajenahally	Catalysis for Sust. Syntheses Jagedeesh Rajenahally	Sel. Cat. Synthesis Methods Eszter Baráth Catalysis w. Phosph. Materials Christian Hering-Junghans Catalysis for Sust. Syntheses Jagedeesh Rajenahally	Ĩ	Catalysis for Sust. Syntheses Jagedeesh Rajenahally	Sel. Catal. Synt. Methods Eszter Baráth Catalysis with Phosphorous Materials Christian Hering-Junghans
Applied Homo- geneous Catalysis Matthias Beller	Catalysis for Energy Henrik Junge Sustain. Redox Reactions Kathrin Junge	<b>Theory of Catalysis</b> Haijun Jiao	Catalysis for Life Sciences Helfried Neumann Applied Carbonylations Ralf Jackstell Catalysis for Energy Henrik Junge	Sustain. Redox Reactions Kathrin Junge	Catalysis for Energy Hen rik Junge	Sustain. Redox Reactions Kathrin Junge Catalysis for Life Sciences Helfried Neumann Applied Carbonylations Ralf Jackstel	Sustain. Redox Reactions Kathrin Junge Catalysis for Life Sciences Helfried Neumann
Modern Concepts in Molecular Catalysis Torsten Beweries	Cat. with Early Trans. Metals Fabian Reiß Cat. with Late Trans. Metals Torsten Beweries Cat. Functionalization Jola Pospech	Cat. with Early Transition Metals Fabian Reiß Mech. in homog. Catalysis Hans-Joachim Drexler					Cat. with Early Trans. Metals Fabian Reiß Cat. with Late Trans. Metals Torsten Beweries Cat. Functionalization Jola Pospech
Hydrogenations & Hydroformylations Armin Börner				Catalysis for Heterocycles Xiao-Feng Wu		Hydrogenations & Hydroformylations Jens Holz	Catalysis for Heterocycles Xiao-Feng Wu Hydrogen. & Hydroformyl. Jens Holz
Electrochemistry & Catalysis Robert Francke					Molecular Electrochemistry Robert Francke	Molecular Electrochemistry Robert Francke Cat.design f. Electrosynth. Bernd Müller	Molecular Electrochemistry Robert Francke Cat.design f. Electrosynth. Bernd Müller
Advanced Methods for Applied Catalysis Evgenii Kondratenko	Magn. Res. & X-Ray Meth. Jabor Rabeah Opt. Spectroscopy Christoph Kubis Reaction Mechanisms Evgenii Kondratenko	Magn. Res. & X-Ray Meth. Jabor Rabeah Opt. Spectroscopy Christoph Kubis Reaction Mechanisms Evgenii Kondratenko			Magn. Res. & X-Ray Meth. Jabor Rabeah Opt. Spectroscopy Christoph Kubis Reaction Mechanisms Evgenii Kondratenko	Reaction Mechanisms Evgenii Kondratenko	Reaction Mechanisms Evgenii Kon dratenko
Biocatalysis & Polymer Chemistry Udo Kragl			Polymer Chem. & Catalysis Esteban Mejia Biocatalysis Udo Kragl	Polymer Chem. & Catalysis Esteban Mejia Homog. Cat. w. Renewables Sergey Tin			Polymer Chem. & Catalysis Esteban Mejia Biocatalysis Udo Kragl
Catalyst Discovery & Reaction Engineering David Linke			High-Throughput Technol. Uwe Rodemerck Reaction Engineering David Linke		Reaction Engineering David Linke	High-Throughput Technol. Uwe Rodemerck Reaction Engineering David Linke	High-Throughput Technol. Uwe Rodemerck Reaction Engineering David Linke
Heterogeneous Photocatalysis Jennifer Strunk					CO <sub>2</sub> -Reduction Tim Peppel Micro Reaction Engineering Norbert Steinfeldt	Micro Reaction Engineering Norbert Steinfeldt	
Heterogeneous Catalytic Processes Sebastian Wohlrab	Surface Chemistry in Appl. Catalysis Ali Abdel-Mageed Inorg. Functional Materials Sebastian Wohlrab		Technol. Oriented Processes Udo Armbruster Surface Chem. in appl. Cat. Ali Abdel-Mageed Inorg. Functional Materials Sebastian Wohlrab	Surface Chem. in Appl. Cat. Ali Abdel-Mageed Inorg. Functional Materials Sebastian Wohlrab	Technology Oriented Processes Udo Armbruster	Technology Oriented Processes Udo Armbruster Inorg, Functional Materials Sebastian Wohlrab	
Young Research Groups	Modern org. Chemistry Osama El-Sepelgy Theory of Homog. & Biocat. Milica Feldt	Theory of Homog. & Biocat. Milica Feldt		Modern org. Chemistry Osama El-Sepelgy Theory of Homog. & Biocat. Milica Feldt			Theory of Homog. & Biocat. Milica Feldt
"Uni in Leibniz" Associated Groups	Björn Corzilius - Marko Hapke Axel Schulz	Ralf Ludwig · Klaus Neymeyr		Thomas Wemer	Malte Brasholz · Klaus Neymeyr Wolfram Seidel	Thomas Werner	Marko Hapke · Axel Schulz Thomas Wemer
Analytics Wolfgang Baumann	Analytics						

As a member of the Leibniz Association, answering socially relevant research questions is at the forefront of our research approach. This approach requires a holistic and interdisciplinary approach. Consequently, the operative research work at LIKAT is assigned to cross-divisional topics and specific competences of the entire institute are bundled.

The reorganization of the individual rersearch groups into cross-research-domain topics promotes transparency and intensive communication between all research departments and research groups. The goal is to develop an information culture that promotes effective information exchange at all levels: professional, organizational, joint projects and new joint proposal submissions.



# PUBLICATIONS

2021 | 2022

#### Publikationen 2021

[1] S. Abbas, F. Rashid, E. Ulker, S. Zaib, K. Ayub, S. Ullah, M. A. Nadeem, S. Yousuf, R. Ludwig, S. Ali, J. Iqbal, *Journal of Biomolecular Structure and Dynamics* **2021**, *39*, 1068-1081, Anticancer evaluation of a manganese complex on HeLa and MCF-7 cancer cells: design, deterministic solvothermal synthesis approach, Hirshfeld analysis, DNA binding, intracellular reactive oxygen species production, electrochemical characterization and density functional theory.

[2] A. M. AbdelMageed, K. Wiese, A. Hauble, J. Bansmann, J. Rabeah, M. Parlinska-Wojtan, A. Brueckner, R. J. Behm, J. Catal. **2021**, 401, 160-173, Steering the selectivity in  $CO_2$  reduction on highly active Ru/TiO<sub>2</sub> catalysts: Support particle size effects.

[3] S. Adak, J. Rabeah, R. Ranjan, T. S. Khan, M. K. Poddar, R. K. Gupta, T. Sasaki, S. Kumar, A. Bordoloi, C. S. Gopinath, A. Brueckner, R. Bal, *Applied Catalysis A: General* **2021**, *624*, 118305, *In-situ* experimental and computational approach to investigate the nature of active site in low-temperature CO-PROX over CuO<sub>x</sub>-CeO<sub>2</sub> catalyst.

[4] H.-J. Ai, W. Lu, X.-F. Wu, Angew. Chem. Int. Ed. **2021**, 60, 17178-17184, Ligand-Controlled Regiodivergent Thiocarbonylation of Alkynes toward Linear and Branched  $\alpha$ , $\beta$ -Unsaturated Thioesters.

[5] H.-J. Ai, X. Ma, Q. Song, X.-F. Wu, *Science China Chemistry* **2021**, *64*, 1630-1659, C-F bond activation under transition-metal-free conditions.

[6] H.-J. Ai, J. Rabeah, A. Brueckner, X.-F. Wu, *Chemical Communications* **2021**, *57*, 1466-1469, Rhodium-catalyzed carbonylative coupling of alkyl halides with thiols: a radical process faster than easier nucleophilic substitution.

[7] H.-J. Ai, F. Zhao, H.-Q. Geng, X.-F. Wu, *ACS Catalysis* **2021**, *11*, 3614-3619, Palladium-Catalyzed Thiocarbonylation of Alkenes toward Linear Thioesters.

[8] L. Al Sheakh, T. Niemann, A. Villinger, P. Stange, D. H. Zaitsau, A. Strate, R. Ludwig, *ChemPhysChem* **2021**, *22*, 1850-1856, Three in One: The Versatility of Hydrogen Bonding Interaction in Halide Salts with Hydroxy-Functionalized Pyridinium Cations. [9] E. Alberico, T. Leischner, H. Junge,
A. Kammer, R. Sang, J. Seifert, W.
Baumann, A. Spannenberg, K. Junge,
M. Beller, *Chem. Sci.* 2021, *12*, 13101-13119, HCOOH disproportionation to MeOH promoted by molybdenum PNP complexes.

[10] S. Arlt, K. Blaesing, J. Harloff, K. C. Laatz, D. Michalik, S. Nier, A. Schulz, P. Stoer, A. Stoffers, A. Villinger, *ChemistryOpen* **2021**, *10*, 62-71, Pseudohalogen Chemistry in Ionic Liquids with Non-innocent Cations and Anions.

[11] Z. Aydin, A. Zanina, V. A. Kondratenko, R. Eckelt, S. Bartling, H. Lund, N. Rockstroh, C. R. Kreyenschulte, D. Linke, E. V. Kondratenko, *Catalysis Science & Technology* **2021**, Elucidating the effects of individual components in  $K_xMnO_y/SiO_2$  and water on selectivity enhancement in the oxidative coupling of methane.

[12] S.-T. Bai, G. De Smet, Y. Liao, R. Sun, C. Zhou, M. Beller, B. U. W. Maes, B. F. Sels, *Chem. Soc. Rev.* **2021**, *50*, 4259-4298, Homogeneous and heterogeneous catalysts for hydrogenation of  $CO_2$  to methanol under mild conditions.

[13] Z.-P. Bao, R.-G. Miao, X. Qi, X.-F. Wu, *Chemical Communications* **2021**, *57*, 1955-1958, A novel construction of acetamides from rhodium-catalyzed aminocarbonylation of DMC with nitro compounds.

[14] A. Bara-Estaún, C. L. Lyall, J. P. Lowe, P. G. Pringle, P. C. J. Kamer, R. Franke, U. Hintermair, *Faraday Discussions* **2021**, *229*, 422-442, Multi-nuclear, high-pressure, operando FlowNMR spectroscopic study of Rh/ PPh<sub>3</sub> – catalysed hydroformylation of 1-hexene.

[15] S. Barroso, M. Joksch, P. Puylaert, S. Tin, S. J. Bell, L. Donnellan, S. Duguid, C. Muir, P. Zhao, V. Farina, D. N. Tran, J. G. de Vries, *J Org Chem* **2021**, *86*, 103-109, Improvement in the Palladium-Catalyzed Miyaura Borylation Reaction by Optimization of the Base: Scope and Mechanistic Study.

[16] R. Bassi, P. Baeza, C. Sepulveda, I. T. Ghampson, E. Camu, A. Brueckner, U. Bentrup, J. L. G. Fierro, N. Escalona, *Applied Catalysis A: General* **2021**, *625*, 118328, Conversion of levulinic acid over rhenium oxide catalysts: Effect of metal content.

[17] M. Beller, F. Fischer, A. Locher,

H. Neumann, C. Taeschler, F. Ye, S. Zhang, *CHIMIA International Journal for Chemistry* **2021**, *75*, 923-935, Recent Developments and Aspects of Industrial Fluoroalkylation.

[18] F. Bendrath, P. Langer, *Chemis-try of Heterocyclic Compounds* **2021**, 57, 1146-1148, Synthesis and permethylation of methyl 5-(2-chloropy-ridin-3-yl)pentanoates.

[19] U. Bentrup, C. Kubis, J. Weiß, *Wiley Analytical Science* **2021**, Monitoring of heterogeneous catalyst action by infrared spectroscopy.

[20] K. Blaesing, J. Bresien, S. Maurer, A. Schulz, A. Villinger, *Eur. J. Inorg. Chem.* **2021**, *2021*, 1913-1920, Trimethylsilyl Pseudohalide Adducts of  $GaCl_3$  and  $B(C_6F_5)_3$ .

[21] K. Blaesing, R. Labbow, A. Schulz, A. Villinger, Angewandte Chemie International Edition **2021**, 60, 13798-13802, Silylated Sulfuric Acid: Preparation of a Tris(trimethylsilyl)oxosulfonium  $[(Me_3Si-O)_3SO]^+$  Salt.

[22] S. A. Bonke, T. Risse, A. Schnegg, A. Brueckner, *Nature Reviews Methods Primers* **2021**, *1*, 33, *In situ* electron paramagnetic resonance spectroscopy for catalysis.

[23] J. Bresien, K. Faust, A. Schulz, *REVIEWS IN INORGANIC CHEMISTRY* **2021**, Bicyclic and tricyclic phosphanes with p-block substituents.

[24] J. Bresien, D. Michalik, A. Schulz, A. Villinger, E. Zander, Angewandte Chemie International Edition 2021, 60, 1507-1512, Azadiphosphaindane-1,3-diyls: A Class of Resonance-Stabilized Biradicals.

[25] J. Bresien, A. Schulz, L. S. Szych, A. Villinger, R. Wustrack, *Inorg. Chem.* **2021**, 60, 11591-11598, Insertion of  $CS_2$  into a Phosphorus–Arsenic Single Bond and Investigations on Phosphane Arsanyldithiocarboxylates.

[26] A. Britz, S. I. Bokarev, T. A. Assefa, È. G. Bajnóczi, Z. Németh, G. Vankó, N. Rockstroh, H. Junge, M. Beller, G. Doumy, A. M. March, S. H. Southworth, S. Lochbrunner, O. Kuehn, C. Bressler, W. Gawelda, *ChemPhysChem* **2021**, *22*, 693-700, Site-Selective Real-Time Observation of Bimolecular Electron Transfer in a Photocatalytic System Using L-Edge X-Ray Absorption Spectroscopy\*\*.

[27] S. Chakrabortty, A. A. Almasalma, J. G. de Vries, *Catalysis Science*  & Technology **2021**, *11*, 5388-5411, Recent developments in asymmetric hydroformylation.

[28] S. Chakrabortty, N. Rockstroh, S. Bartling, H. Lund, B. H. Mueller, P. C. J. Kamer, J. G. de Vries, *Catalysis Science & Technology* **2021**, *11*, 7608-7616, The solvent determines the product in the hydrogenation of aromatic ketones using unligated RhCl<sub>3</sub> as catalyst precursor.

[29] B. Chen, X.-F. Wu, *Org. Biomol. Chem.* **2021**, *19*, 9654-9658, Manganese(III)-promoted thiocarbonylation of alkylborates with disulfides: synthesis of aliphatic thioesters.

[30] S. Chen, A. M. AbdelMageed, M. Li, S. Cisneros, J. Bansmann, J. Rabeah, A. Brueckner, A. Groß, R. J. Behm, *J. Catal.* **2021**, *400*, 407-420, Electronic metal-support interactions and their promotional effect on CO<sub>2</sub> methanation on Ru/ZrO<sub>2</sub> catalysts.

[31] S. Chen, A. M. AbdelMageed, C. Mochizuki, T. Ishida, T. Murayama, J. Rabeah, M. Parlinska-Wojtan, A. Brueckner, R. J. Behm, *ACS Catal.* **2021**, *11*, 9022-9033, Controlling the O-Vacancy Formation and Performance of Au/ZnO Catalysts in CO<sub>2</sub> Reduction to Methanol by the ZnO Particle Size.

[32] L. Dai, C. Strelow, T. Kipp, A. Mews, I. Benkenstein, D. Eifler, T. H. Vuong, J. Rabeah, J. McGettrick, R. Lesyuk, C. Klinke, *Chemistry of Materials* **2021**, *33*, 275-284, Colloidal Manganese-Doped ZnS Nanoplatelets and Their Optical Properties.

[33] X. Dai, X. Wang, J. Rabeah, C. Kreyenschulte, A. Brueckner, F. Shi, *Chem. Europ. J.* **2021**, *27*, 16889-16895, Supported Cull Single-Ion Catalyst for Total Carbon Utilization of  $C_2$  and  $C_3$  Biomass-Based Platform Molecules in the N-Formylation of Amines.

[34]F. Dankert, C. von Hänisch, *Eur. J. Inorg. Chem.* **2021**, *2021*, 2907-2927, Siloxane Coordination Revisited: Si–O Bond Character, Reactivity and Magnificent Molecular Shapes.

[35] L. D. de Almeida, H. Wang, K. Junge, X. Cui, M. Beller, *Angew. Chem. Int. Ed.* **2021**, *60*, 550-565, Recent Advances in Catalytic Hydrosilylations: Developments beyond Traditional Platinum Catalysts.

[36] J. De Jesus Silva, N. Bartalucci, B. Jelier, S. Grosslight, T. Gensch, C. Schunemann, B. Muller, P. C. J. Kamer, C. Coperet, M. S. Sigman, A. Togni, *ChemRxiv* **2021**, 1-15, Development and molecular understanding of a Pd-catalyzed cyanation of aryl boronic acids enabled by high-throughput experimentation and data analysis.

[37] J. G. de Vries, in Organophosphorus Chemistry: Vol. 50, The Royal Society of Chemistry, **2021**, pp. 243-270.

[38] A. Dell'Acqua, L. Wille, B. M. Stadler, S. Tin, J. G. de Vries, *Chem. Commun.* **2021**, *57*, 10524-10527, Ozonolysis of  $\alpha$ -angelica lactone: a renewable route to malonates.

[39] F. G. Delolo, J. Yang, H. Neumann, E. N. dos Santos, E. V. Gusevskaya, M. Beller, *ACS Sust. Chem. Eng.* **2021**, *9*, 5148-5154, Cobalt-Catalyzed Hydroformylation under Mild Conditions in the Presence of Phosphine Oxides.

[40] H. N. Do, N. M. Quan, B. Van Phuc, D. Van Tinh, N. Q. Tien, T. T. T. Nga, V. T. Nguyen, T. Q. Hung, T. T. Dang, P. Langer, *Synlett* **2021**, *32*, 611-615, Efficient Copper-Catalysed Synthesis of Carbazoles by Double N-Arylation of Primary Amines with 2,2'-Dibromobiphenyl in the Presence of Air.

[41] T. Doan, A. Dang, D. Nguyen, T. Tran, T. H. Vuong, M. T. Le, T. H. Pham, *Viet. J. Chem.* **2021**, *59*, 935-942, The promotion effect of iron to Cu/ZSM-5 catalyst for NO<sub>x</sub> removal by NH<sub>3</sub>-SCR.

[42] M. V. Doble, L. Obrecht, H.-J. Joosten, M. Lee, H. J. Rozeboom, E. Branigan, J. H. Naismith, D. B. Janssen, A. G. Jarvis, P. C. J. Kamer, ACS *Catal.* **2021**, *11*, 3620-3627, Engineering Thermostability in Artificial Metalloenzymes to Increase Catalytic Activity.

[43] N. Dropka, K. Boettcher, M. Holena, *Crystals* **2021**, *11*, 1218, Development and Optimization of VGF-GaAs Crystal Growth Process Using Data Mining and Machine Learning Techniques.

[44] N. Dropka, S. Ecklebe, M. Holena, *Crystals* **2021**, *11*, 138, Real Time Predictions of VGF-GaAs Growth Dynamics by LSTM Neural Networks.

[45] S. Du, W.-F. Wang, Y. Song, Z. Chen, X.-F. Wu, *Org. Lett.* **2021**, *23*, 974-978, Palladium-Catalyzed Cascade Carbonylative Synthesis of 1,2,4-Triazol-3-ones from Hydrazonoyl Chlorides and NaN<sub>3</sub>.

[46] S. Du, Z. Yang, J. Tang, Z. Chen, X.-F. Wu, *Org. Lett.* **2021**, *23*, 2359-2363, Synthesis of 3H-1,2,4-Triazol-3-ones via NiCl<sub>2</sub>-Promoted Cascade Annulation of Hydrazonoyl Chlorides and Sodium Cyanate.

[47] L. Duarte de Almeida, F. Bourriquen, K. Junge, M. Beller, *Adv. Synth. Catal.* **2021**, *363*, 4177-4181, Catalytic Formal Hydroamination of Allylic Alcohols Using Manganese PNP-Pincer Complexes.

[48] R. Duehren, P. Kucmierczyk, R. Jackstell, R. Franke, M. Beller, *Catal. Sci. Technol.* **2021**, *11*, 2026-2030, Ruthenium-catalysed hydroxycarbonylation of olefins.

[49] R. Dühren, P. Kucmierczyk, C. Schneider, R. Jackstell, R. Franke, M. Beller, *Catal. Sci Technol.* **2021**, I, 5777-5780, Ruthenium-catalysed domino hydroformylation–hydrogenation–esterification of olefins.

[50] P. Enders, R. Francke, in Electrochemistry in Organic Synthesis, Vol. 2021/5, 1st edition ed. (Ed.: L. Ackermann), Georg Thieme Verlag KG, Stuttgart, **2021**.

[51] S. Espinoza, D. Linke, C. Wulf, S. Schimmler, S. A. Schunk, P. Benner, R. Kraehnert, U. Kragl, R. Palkovits, S. Palkovits, M. Oezaslan, R. Gläser, T. Bönisch, N. Bohmer, M. Resch, M. Beller, O. Deutschmann, U. Bornscheuer, M. Greiner, W. Leitner, W. Kurt, Bausteine Forschungsdatenmanagement **2021**, 57-71, NFDI for Catalysis-Related Sciences: NFDI4Cat.

[52] C. Eyovge, C. S. Deenen, F. Ruiz-Zepeda, S. Bartling, Y. Smirnov, M. Morales-Masis, A. Susarrey-Arce, H. Gardeniers, *ACS Appl. Nano Mat.* **2021**, *4*, 8600-8610, Color Tuning of Electrochromic TiO<sub>2</sub> Nanofibrous Layers Loaded with Metal and Metal Oxide Nanoparticles for Smart Colored Windows.

[53] M. J. G. Fait, A. Spannenberg, E. V. K. D. Linke, *IUCrData* **2021**, *6*, x211332, 1,3-Thiazole-4-carbonitrile.

[54] A. Farhat, A. Yaqoob, R. A. Khera, M. U. Riaz, F. A. Anjum, P. Langer, J. Iqbal, *Optik* **2021**, *242*, 167098, Designing and theoretical characterization of benzodithiophene dione based donor molecules for small molecule organic solar cells. [55] F. Fischer, M. Eder, M. Hapke, Ca- X.-F. Wu, Chem. Sci. 2021, 12, 14937talysts 2021, 11, 596, CpCo(III) Precatalysts for [2+2+2] Cycloadditions.

[56] M. Fischer, C. Hering-Junghans, Chem. Sci. 2021, 12, 10279-10289, On 1,3-phosphaazaallenes and their diverse reactivity.

[57] M. Fischer, S. Nees, T. Kupfer, J. T. Goettel, H. Braunschweig, C. Hering-Junghans, J. Am. Chem. Soc. 2021, 143, 4106-4111, Isolable Phospha- and Arsaalumenes.

[58] M. Fischer, F. Reiß, C. Hering-Junghans, Chem. Commun. 2021, 57, 5626-5629, Titanocene pnictinidene complexes.

[59] P. A. Forero Cortés, M. Marx, M. Trose, M. Beller, Chem Catalysis 2021, 1, 298-338, Heteroleptic copper complexes with nitrogen and phosphorus ligands in photocatalysis: Overview and perspectives.

[60] R. Francke, Current Opinion in Electrochemistry 2021, 28, 100719, Recent progress in the electrochemistry of hypervalent iodine compounds.

[61] R. Francke, A. Prudlik, R. D. Little, in Electrochemistry in Organic Synthesis, Vol. 2021/5, 1st edition ed. (Ed.: L. Ackermann), Georg Thieme Verlag KG, Stuttgart, 2021.

[62] J. Gao, R. Ma, L. Feng, Y. Liu, R. Jackstell, R. V. Jagadeesh, M. Beller, Angew. Chem. Int. Ed. 2021, 60, 18591-18598, Ambient Hydrogenation and Deuteration of Alkenes Using a Nanostructured Ni-Core-Shell Catalyst.

[63] Q. Gao, J.-M. Lu, L. Yao, S. Wang, J. Ying, X.-F. Wu, Org. Lett. 2021, 23, 178-182, Cobalt-Catalyzed Direct C–H Carbonylative Synthesis of Free (NH)-Indolo[1,2-a]quinoxalin-6(5H)ones.

[64] Y. Ge, F. Ye, J. Yang, A. Spannenberg, R. Jackstell, M. Beller, JACS Au 2021, 1, 1257-1265, Palladium-Catalyzed Domino Aminocarbonylation of Alkynols: Direct and Selective Synthesis of Itaconimides.

Y. Ge, F. Ye, J. Yang, A. [65] Spannenberg, H. Jiao, R. Jackstell, M. Beller, Angew. Chem. Int. Ed. 2021, 60, 22393-22400, Palladium-Catalyzed Cascade Carbonylation to  $\alpha,\beta$ -Unsaturated Piperidones via Selective Cleavage of Carbon–Carbon Triple Bonds.

[66] H.-Q. Geng, T. Meyer, R. Franke,

14943, Copper-catalyzed hydroformylation and hydroxymethylation of styrenes.

[67] H.-Q. Geng, W. Wang, X.-F. Wu, Catal. Commun. 2021, 148, 106170, Nickel-catalyzed carbonylative synthesis of dihydrobenzofurans.

[68] H.-Q. Geng, X.-F. Wu, Org. Lett. 2021, 23, 8062-8066, Copper-Catalyzed Alkoxycarbonylation of Alkyl lodides for the Synthesis of Aliphatic Esters: Hydrogen Makes the Differen-

[69] S. H. Gilbert, S. Tin, J. A. Fuentes, T. Fanjul, M. L. Clarke, Tetrahedron 2021, 80, 131863, Rhodium catalysts derived from a fluorinated phanephos ligand are highly active catalysts for direct asymmetric reductive amination of secondary amines.

[70] T. Gläsel, B. N. Baumann, M. Hapke, Chem. Record 2021, 21, 3727-3745, Cobalt Catalysts for [2+2+2] Cycloaddition Reactions: Isolated Precatalysts and in situ Generated Catalysts.

[71] T. Gläsel, H. Jiao, M. Hapke, ACS Catal. 2021, 11, 13434-13444, Synthesis of Phosphinines from Coll-Catalyzed [2+2+2] Cycloaddition Reactions.

[72] B. Golub, K. Fumino, P. Stange, V. Fossog, R. Hempelmann, D. Ondo, D. Paschek, R. Ludwig, J. Phys. Chem. B 2021, 125, 4476-4488, Balance Between Contact and Solvent-Separated Ion Pairs in Mixtures of the Protic Ionic Liquid [Et,NH][MeSO,] with Water Controlled by Water Content and Temperature.

[73] V. Goyal, G. Naik, A. Narani, K. Natte, R. V. Jagadeesh, Tetrahedron 2021, 98, 132414, Recent developments in reductive N-methylation with base-metal catalysts. [74] L. Grefe, E. Mejía, Tetrahedron 2021, 98, 132433, Earth-abundant bimetallic and multimetallic catalysts for Epoxide/CO<sub>2</sub> ring-opening copolymerization.

[75] L. M. Gronbach, A. Voss, M. Frahm, A. Villinger, J. Bresien, D. Michalik, M. Brasholz, Org. Lett. 2021, 23, 7834-7838, Lewis Acid-Catalyzed Carbofunctionalization of Uncommon C,N-Diacyliminium Ions: Controlling Regio- and Enantioselectivity.

[76] J.-P. Guetlein, M. Lubbe, H. Feist, A. Villinger, P. Langer, Zeitschr. f. Naturforschung B 2021, 76,

1-26, Regioselective synthesis of salicylates and acetophenones by formal [3+3]-cyclocondensations of 3-oxoorthoesters with 1,3-bis(trimethylsilyloxy)-1,3-butadienes.

[77] S. G. Guillet, G. Pisanò, S. Chakrabortty, B. H. Müller, J. G. de Vries, P. C. J. Kamer, C. S. J. Cazin, S. P. Nolan, Eur. J. Inorg. Chem. 2021, I, 3506-3511, A Simple Synthetic Route to [Rh(acac)(CO)(NHC)] Complexes: Ligand Property Diagnostic Tools and Precatalysts.

[78] B. Guo, E. Otten, J. G. de Vries, in Metal-Ligand Co-operativity: Catalysis and the Pincer-Metal Platform (Eds.: G. van Koten, K. Kirchner, M.-E. Moret), Springer International Publishing, Cham, 2021, pp. 321-377.

[79] C.-H. Guo, M. Liang, H. Jiao, Catal. Sci. Technol. 2021, 11, 2529-2539, Cycloaddition mechanisms of CO<sub>2</sub> and epoxide catalyzed by salophen - an organocatalyst free from metals and halides.

[80] X. Guo, J. Rabeah, R. Sun, D. Wang, E. Mejía, ACS Appl. Mater. Interf. 2021, 13, 42889-42897, Fluorescent Hybrid Porous Polymers as Sustainable Heterogeneous Photocatalysts for Cross-Dehydrogenative Coupling Reactions.

[81] P. Gupta, J.-E. Siewert, T. Wellnitz, M. Fischer, W. Baumann, T. Beweries, C. Hering-Junghans, Dalton Trans. 2021, 50, 1838-1844, Reactivity of phospha-Wittig reagents towards NHCs and NHOs.

[82] B. Han, J. Zhang, H. Jiao, L. Wu, Chinese J. Catal. 2021, 42, 2059-2067, Zirconium-hydride- catalyzed site-selective hydroboration of amides for the synthesis of amines: Mechanism, scope, and application.

[83] P. Hasche, J. Haak, F. Anke, C. Kubis, W. Baumann, H.-J. Drexler, H. Jiao, T. Beweries, Catal. Sci. Technol. 2021, 11, 3514-3526, Dehydropolymerisation of methylamine borane using highly active rhodium(III) bis(thiophosphinite) pincer complexes: catalytic and mechanistic insights.

[84] D. He, T. Wang, T. Li, X. Wang, H. Wang, X. Dai, F. Shi, J. Catal. 2021, 400, 397-406, Efficient hydrogenation catalyst designing via preferential adsorption sites construction towards active copper.

[85] Y. He, X. Qin, X. He, X.-F. Wu, Z.

Yin, Eur. J. Org. Chem. 2021, 2021, 5831-5834, Practical Synthesis of Halogenated N-Heterocycles via Electrochemical Anodic Oxidation of Unactivated Alkenes.

[86] Y. Himeda, M. Beller, in CO. Hvdrogenation Catalysis (Ed.: Y. Himeda), WILEY-VCH GmbH, 2021, pp. 1-12.

[87] M. T. Hoang, T. D. Pham, T. T. Pham, M. K. Nguyen, D. T. T. Nu, T. H. Nguyen, S. Bartling, B. Van der Bruggen, Environ. Sci. Poll. Research 2021, 28, 11869-11881, Esterification of sugarcane bagasse by citric acid for Pb2+ adsorption: effect of different chemical pretreatment methods.

[88] Y. Hu, Z. Wei, A. Frey, C. Kubis, C.-Y. Ren, A. Spannenberg, H. Jiao, T. Werner, ChemSusChem 2021, 14, 363-372, Catalytic, Kinetic, and Mechanistic Insights into the Fixation of CO<sub>2</sub> with Epoxides Catalyzed by Phenol-Functionalized Phosphonium Salts.

[89] Y.-W. Huo, X. Qi, T. Xu, W. Lu, X.-F. Wu, ChemistrySelect 2021, 6, 7037-7039, Heterogeneous Carbonylative Sonogashira Reaction Based on Pd/g-C<sub>2</sub>N<sub>4</sub> Catalyst by Using Formic Acid as the CO Source.

[90] Y.-W. Huo, L. Yao, X. Qi, X.-F. Wu, Org. Chem. Front. 2021, 8, 6974-6978, Nickel-catalyzed reductive aminocarbonylation of vinyl triflates with nitro compounds for the synthesis of  $\alpha$ , $\beta$ -unsaturated amides.

[91] A. Indra, R. Beltrán-Suito, M. Mueller, R. P. Sivasankaran, M. Schwarze, A. Acharjya, B. Pradhan, J. Hofkens, A. Brueckner, A. Thomas, P. W. Menezes, M. Driess, ChemSusChem 2021, 14, 306-312, Promoting Photocatalytic Hydrogen Evolution Activity of Graphitic Carbon Nitride with Hole-Transfer Agents.

[92] S. Iqbal, M. Sharif, P. Langer, SYNLETT 2021, Suzuki-Miyaura Coupling Reactions of Fluorohalobenzenes.

[93] S. Irshad, F. Ullah, S. Khan, R. Ludwig, T. Mahmood, K. Ayub, Optics & Laser Technol. 2021, 134, 106570, First row transition metals decorated boron phosphide nanoclusters as nonlinear optical materials with high thermodynamic stability and enhanced electronic properties; A detailed quantum chemical study.

[94] C. Jacquot, V. Middelkoop, A.

Koeckritz, A. Pohar, R. Bienert, S. Kellici, I.-A. Bărăgău, B. Venezia, A. Gavriilidis, B. Likozar, A. M. Beale, Sustainable Mater. Technol. 2021, 30, e00329, 3D printed catalytic reactors for aerobic selective oxidation of benzyl alcohol into benzaldehyde in continuous multiphase flow.

[95] Y. Jiao, H. Ma, H. Wang, Y.-W. Li, X.-D. Wen, H. Jiao, Catal. Sci. Technol. 2021, 11, 191-210, Interactive network of the dehydrogenation of alkanes, alkenes and alkynes - surface carbon hydrogenative coupling on Ru(111).

[96] R. P. Kaiser, E. F. Krake, L. Backer, J. Urlaub, W. Baumann, N. Handler, H. Buschmann, T. Beweries, U. Holzgrabe, C. Bolm, Chem. Commun. 2021, 57, 11956-11959, Ball milling - a new concept for predicting degradation profiles in active pharmaceutical ingredients.

[97] M. Kanai, M. Beller, Org. Biomol. Chem. 2021, 19, 702-704, Introduction to hybrid catalysis.

[98] T. Kaper, M. Fischer, H. Thye, D. Geik, M. Schmidtmann, R. Beckhaus, S. Doye, Chem. Eur. J. 2021, 27, 6899-6903, Intermolecular Hydroaminoalkylation of Alkynes.

[99] S. Keller, U. Bentrup, J. Rabeah, A. Brueckner, J. Catal. 2021, Impact of dopants on catalysts containing Ce1 $xM_vO_{2-\delta}$  (M = Fe, Sb or Bi) in NH<sub>3</sub>-SCR of NO\_ – A multiple spectroscopic approach.

[100] F. Khamespanah, M. Marx, D. B. Crochet, U. R. Pokharel, F. R. Fronczek, A. W. Maverick, M. Beller, Nat. Commun. 2021, 12, 1997, Oxalate production via oxidation of ascorbate rather than reduction of carbon dioxide.

[101] S. Khan, M. A. Gilani, S. Munsif, S. Muhammad, R. Ludwig, K. Ayub, J. Mol. Graph. Modelling 2021, 106, 107935, Inorganic electrides of alkali metal doped Zn,,O,, nanocage with excellent nonlinear optical response.

[102] S. Kirchhecker, A. Dell'Acqua, A. Angenvoort, A. Spannenberg, K. Ito, S. Tin, A. Taden, J. G. de Vries, Green Chem. 2021, 23, 957-965, HMF-glycerol acetals as additives for the debonding of polyurethane adhesives.

[103] S. Kirchhecker, B. Spiegelberg, J. G. de Vries, in Iridium Catalysts for Organic Reactions (Eds.: L. A. Oro, C. Claver), Springer International Publishing, Cham, 2021, pp. 341-395.

[104] V. A. Kondratenko, U. Karimova, A. A. Kasimov, E. V. Kondratenko, Appl. Catal. A 2021, 619, 118143, Methane conversion into synthesis gas over supported well-defined Pt, Rh or Ru nanoparticles: Effects of metal and support.

[105] S. Kopf, H. Neumann, M. Beller, Chem. Commun. 2021, 57, 1137-1140, Manganese-catalyzed selective C-H activation and deuteration by means of a catalytic transient directing group strategy.

[106] S. Kopf, F. Ye, H. Neumann, M. Beller, Chem. Eur. J. 2021, 27, 9768-9773, Ruthenium-Catalyzed Deuteration of Aromatic Carbonyl Compounds with a Catalytic Transient Directing Group.

[107] B. Kortewille, A. Springer, J. Strunk, Catal. Commun. 2021, 152, 106286, Verification of impurity-related photocatalytic activity of insulating oxide supports.

[108] H. Kosslick, Y. Wang, M. F. Ibad, X. Guo, M. Luetgens, S. Lochbrunner, M. Frank, N. Q. Liem, A. Schulz, Adv. Chem. Eng. Sci. 2021, 11, 290-315, High-performance room-light-driven  $\beta$ -AgVO<sub>3</sub>/mpg-C<sub>3</sub>N<sub>4</sub> core/shell photocatalyst prepared by mechanochemical method.

[109] E. F. Krake, W. Baumann, Molecules 2021, 26, Selective Oxidation of Clopidogrel by Peroxymonosulfate (PMS) and Sodium Halide (NaX) System: An NMR Study.

[110] B. Kunkel, S. Wohlrab, Catal. Commun. 2021, 155, 106317, Enhancement and limits of the selective oxidation of methane to formaldehyde over V-SBA-15: Influence of water cofeed and product decomposition.

[111] A. Kutuzova, T. Dontsova, W. Kwapinski, Catalysts 2021, 11, 728, Application of TiO<sub>2</sub>-based Photocatalysts to Antibiotics Degradation: Cases of Sulfamethoxazole, Trimethoprim and Ciprofloxacin.

[112] T. Lange, S. Reichenberger, M. Rohe, M. Bartsch, L. Kampermann, J. Klein, J. Strunk, G. Bacher, R. Schloegl, S. Barcikowski, Adv. Funct. Mater. 2021, 31, 2009323, Alumina-Protected, Durable and Photostable Zinc Sulfide Particles from Scalable Atomic Layer Deposition.

[113] P. Langer, Synlett 2021, Synthe-

sis and Reactions of 1,3,5-Tri- and 1,3,5,7-Tetracarbonyl Compounds.

[114] P. Langer, *Synlett* **2021**, Domino Reactions of Chromones with Heterocyclic Enamines.

[115] P. Langer, *Synlett* **2021**, Synthesis of Purines and Related Molecules by Cyclization Reactions of Heterocyclic Enamines.

[116] P. Langer, *Synlett* **2021**, Adventures in 1,3-Selenazole Chemistry.

[117] M. T. Le, S. Singh, M. Nguyen-Quang, A. B. Ngo, A. Brueckner, U. Armbruster, *Sci. Total Environ.* **2021**, 784, 147394, Insight into the properties of  $MnO_2$ - $Co_3O_4$ - $CeO_2$  catalyst series for the selective catalytic reduction of  $NO_x$  by  $C_3H_6$  and  $NH_3$ .

[118] Z. Le, Y. Zhu, Z.-P. Bao, J. Ying, X.-F. Wu, *Adv. Synth. Catal.* **2021**, *363*, 1878-1881, Palladium-Catalyzed Carbonylative Synthesis of 1,5-Dihydro-2H-pyrrol-2-ones from Propargyl Amines and Benzyl Chlorides.

[119] D. K. Leonard, W. Li, N. Rockstroh, K. Junge, M. Beller, *Catal. Commun.* **2021**, *157*, 106333, Aerobic iron-catalyzed site-selective C(sp<sup>3</sup>)– C(sp<sup>3</sup>) bond cleavage in N-heterocycles.

[120] C. Li, C. F. R. Mackenzie, S. A. Said, A. K. Pal, M. A. Haghighatbin, A. Babaei, M. Sessolo, D. B. Cordes, A. M. Z. Slawin, P. C. J. Kamer, H. J. Bolink, C. F. Hogan, E. Zysman-Colman, *Inorg. Chem.* **2021**, *60*, 10323-10339, Wide-Bite-Angle Diphosphine Ligands in Thermally Activated Delayed Fluorescent Copper(I) Complexes: Impact on the Performance of Electroluminescence Applications.

[121] C.-L. Li, H. Wang, X.-F. Wu, in Carbon Monoxide in Organic Synthesis (Ed.: B. Gabriele), Wiley VCH, **2021**, pp. 83-112.

[122] W. Li, R. Qu, W. Liu, F. Bourriquen, S. Bartling, N. Rockstroh, K. Junge, M. Beller, *Chem. Sci.* **2021**, *12*, 14033-14038, Copper-catalysed low-temperature water–gas shift reaction for selective deuteration of aryl halides.

[123] Y. Li, C.-L. Zhang, W.-H. Huang, N. Sun, M. Hao, H. Neumann, M. Beller, *Chem. Sci.* **2021**, *12*, 10467-10473, A general strategy for the synthesis of  $\alpha$ -trifluoromethyl- and  $\alpha$ -perfluoroalkyl- $\beta$ -lactams via palladium-catalyzed carbonylation. [124] K. Lindenau, N. Jannsen, M. Rippke, H. Al Hamwi, C. Selle, H.-J. Drexler, A. Spannenberg, M. Sawall, K. Neymeyr, D. Heller, F. Reiß, T. Beweries, *Catal. Sci. Technol.* **2021**, *11*, 4034-4050, Mechanistic insights into dehydrocoupling of amine boranes using dinuclear zirconocene complexes.

[125] K. Lindenau, E. Zander, C. Schuenemann, A. Spannenberg, M. V. Andreev, V. V. Burlakov, F. Reiß, T. Beweries, *Organometallics* **2021**, *40*, 3177-3184, Synthesis and Characterization of Dinuclear Allenediide Bridged Hafnocene(IV) Complexes.

[126] C. Liu, X. Wen, Y. Yang, Y.-W. Li, H. Jiao, *J. Phys. Chem. C* **2021**, *125*, 5602-5615, Nonoxidative Conversion of Methane, Ethane, and Ethylene on Flat Ir(111) and Stepped Ir(211) Surfaces.

[127] J. Liu, C. Schneider, J. Yang, Z. Wei, H. Jiao, R. Franke, R. Jackstell, M. Beller, *Angew. Chem. Int. Ed.* **2021**, *60*, 371-379, A General and Highly Selective Palladium-Catalyzed Hydroamidation of 1,3-Diynes.

[128] J. Liu, Z. Wei, H. Jiao, ACS Catal. 2021, 11, 4593-4605, Catalytic Activity of Aliphatic PNP Ligated Colll/I Amine and Amido Complexes in Hydrogenation Reaction—Structure, Stability, and Substrate Dependence.

[129] J.-L. Liu, C.-Y. Hou, X. Qi, X.-F. Wu, *Mol. Catal.* **2021**, *514*, 111842, Palladium-catalyzed carbonylative synthesis of 3-arylquinolin-2(1H)-ones from benzyl chlorides and o-nitrobenzaldehydes.

[130] J.-L. Liu, R.-R. Xu, W. Wang, X. Qi, X.-F. Wu, *Org. Biomol. Chem.* **2021**, *19*, 3584-3588, Palladium-catalyzed carbonylative cyclization of benzyl chlorides with anthranils for the synthesis of 3-arylguinolin-2(1H)-ones.

[131] X. Liu, T. Werner, *Adv. Synth. Catal.* **2021**, *363*, 1096-1104, Selective Construction of C–C and C=C Bonds by Manganese Catalyzed Coupling of Alcohols with Phosphorus Ylides.

[132] X. Liu, T. Werner, *Chem. Sci.* **2021**, *12*, 10590-10597, Indirect reduction of  $CO_2$  and recycling of polymers by manganese-catalyzed transfer hydrogenation of amides, carbamates, urea derivatives, and polyurethanes.

[133] Y. Liu, X. Qi, X.-F. Wu, J. Org. Chem. **2021**, 86, 13824-13832, Palladium-Catalyzed Reductive Aminocarbonylation of Benzylammonium Triflates with o-Nitrobenzaldehydes for the Synthesis of 3-Arylquinolin-2(1H)-ones.

[134] J.-M. Lu, Y.-W. Huo, X. Qi, X.-F. Wu, *Mol. Catal.* **2021**, *509*, 111627, Palladium-catalyzed carbonylative synthesis of quinazolines: Silane act as better nucleophile than amidine.

[135] S.-N. Lu, H. Yang, J. Zhang, Z. Chen, X.-F. Wu, *Adv. Synth. Catal.* **2021**, *363*, 4982-4987, Oxidative Cyclization of Trifluoroacetimidohydrazides with D-Glucose for the Metal-Free Synthesis of 3-Trifluoromethyl-1,2,4-Triazoles.

[136] R. Ludwig, *J. Mol. Liq.* **2021**, *340*, 116882, Towards thermodynamically stable anionic dimers with "anti-electrostatic" hydrogen bonds overcoming like-charge repulsion.

[137] D. Luo, Y. He, X. Yu, F. Wang, J. Zhao, W. Zheng, H. Jiao, Y. Yang, Y. Li, X. Wen, *J. Catal.* **2021**, *395*, 293-301, Intrinsic mechanism of active metal dependent primary amine selectivity in the reductive amination of carbonyl compounds.

[138] C. Medwed, A. Holzinger, S. Hofer, A. Hartmann, D. Michalik, K. Glaser, U. Karsten, Protoplasma **2021**, Ecophysiological, morphological, and biochemical traits of free-living Diplosphaera chodatii (Trebouxiophyceae) reveal adaptation to harsh environmental conditions.

[139] T. Meyer, R. Konrath, P. C. J. Kamer, X.-F. Wu, *Asian J. Org. Chem.* **2021**, *10*, 245-250, Pincer Ligand Enhanced Rhodium-Catalyzed Carbonylation of Formaldehyde: Direct Ethylene Glycol Production.

[140] T. Meyer, J. Rabeah, A. Brueckner, X.-F. Wu, *Chem. Eur. J.* **2021**, *27*, 5642-5647, Visible-Light-Induced Palladium-Catalyzed Dehydrogenative Carbonylation of Amines to Oxalamides.

[141] R.-G. Miao, X. Qi, X.-F. Wu, Eur. J. Org. Chem. 2021, 2021, 5219-5221, Synthesis of Aryl Methyl Sulfides from Arysulfonyl Chlorides with Dimethyl Carbonate as the Solvent and C1 Source.

[142] M. Miola, S. Li, X.-M. Hu, M. Ceccato, A.-E. Surkus, E. Welter, S. U. Pedersen, H. Junge, T. Skrydstrup, M. Beller, K. Daasbjerg, *Adv. Mater. Interf. B*, 8, 2100067, Highly Scalable Conversion of Blood Protoporphyrin to Efficient Electrocatalyst for CO<sub>2</sub>-to-CO Conversion.

[143] N. Mohebbati, A. Prudlik, A. Scherkus, A. Gudkova, R. Francke, *ChemElectroChem* **2021**, *8*, 3837-3843, TEMPO-Modified Polymethacrylates as Mediators in Electrosynthesis – Redox Behavior and Electrocatalytic Activity toward Alcohol Substrates.

[144] S. Möller, N. Jannsen, J. Rüger, H.-J. Drexler, M. Horstmann, F. Bauer, B. Breit, D. Heller, *Chem. Eur. J.* **2021**, *27*, 14034-14041, Catalyst Deactivation During Rhodium Complex-Catalyzed Propargylic C–H Activation.

[145] J. Mosrati, A. M. AbdelMageed, T. H. Vuong, R. Grauke, S. Bartling, N. Rockstroh, H. Atia, U. Armbruster, S. Wohlrab, J. Rabeah, A. Brueckner, ACS *Catal.* **2021**, *11*, 10933-10949, Tiny Species with Big Impact: High Activity of Cu Single Atoms on  $CeO_2$ -TiO<sub>2</sub> Deciphered by Operando Spectroscopy.

[146] J. Mosrati, H. Atia, R. Eckelt, T. Huyen Vuong, J. Rabeah, M. Mhamdi, U. Armbruster, J. Catal. 2021, 395, 325-339, Ta and Mo oxides supported on  $CeO_2$ -TiO<sub>2</sub> for the selective catalytic reduction of NO<sub>x</sub> with NH<sub>3</sub> at low temperature.

[147] S. Mostafapour, H. Schroeder, C. Kubis, M. Sawall, B. Hemmateenejad, K. Neymeyr, *Chemom. Intell. Lab. Sys.* **2021**, *210*, 104228, A comparative study of MCR-based kinetic analyses for chemical reaction systems with rate constant ambiguities.

[148] N. G. Moustakas, in Materials Science in Photocatalysis (Eds.: E. I. García-López, L. Palmisano), *Elsevier*, **2021**, pp. 255-265.

[149] N. G. Moustakas, F. Lorenz, M. Dilla, T. Peppel, J. Strunk, *Chem. Eur. J.* **2021**, *27*, 17213-17219, Pivotal Role of Holes in Photocatalytic  $CO_2$  Reduction on TiO<sub>2</sub>.

[150] A. Mueller, T. Krahl, J. Radnik, A. Wagner, C. Kreyenschulte, W. S. M. Werner, B. Ritter, E. Kemnitz, W. E. S. Unger, *Surf. Interf. Anal.* **2021**, *53*, 494-508, Chemical in-depth analysis of  $(Ca/Sr)F_2$  core–shell like nanoparticles by X-ray photoelectron spectroscopy with tunable excitation energy.

[151] R. Muhammad, Y. Ali, Y. Messaddeq, H. ur Rashid, M. Antonio Utrera Martines, M. Naveed Umar, S. W. Khan, A. Riaz, *Catalysts* **2021**, *11*, 357, Conditions Optimization and Physiochemical Analysis of Oil Obtained by Catalytic Pyrolysis of Scrap Tube Rubber Using MgO as Catalyst.

[152] K. Murugesan, A. M. Alenad, A. S. Alshammari, M. Sohail, R. V. Jagadeesh, *Tetrahedron* **2021**, *102*, 132526, Reductive N-alkylation of primary amides using nickel-nanoparticles.

[153] F. Nadolny, U. Bentrup, N. Rockstroh, F. Alscher, W. Reschetilowski, S. Peitz, R. Franke, A. Brueckner, *Catal. Sci. Technol.* **2021**, *11*, 4732-4740, Oligomerization of n-butenes over Ni/SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>: influence of support modification by steam-treating.

[154] P. Naliwajko, J. Strunk, in Heterogeneous Photocatalysis (Ed.: J. Strunk), **2021**, pp. 101-126.

[155] M. Namayandeh Jorabchi, R. Ludwig, D. Paschek, *J. Phys. Chem. B* **2021**, *125*, 1647-1659, Quasi-Universal Solubility Behavior of Light Gases in Imidazolium-Based Ionic Liquids with Varying Anions: A Molecular Dynamics Simulation Study.

[156] E. G. Narváez O, P. M. Bonilla V, D. A. Zurita, C. D. Alcívar L, J. Heredia-Moya, S. E. Ulic, J. L. Jios, O. E. Piro, G. A. Echeverría, P. Langer, *J. Fluorine Chem.* **2021**, *242*, 109717, Synthesis, experimental and theoretical study of novel 2-haloalkyl (-CF<sub>2</sub>H, -CCl<sub>2</sub>H, -CF<sub>2</sub>CF<sub>3</sub>)-, 3-bromo and bromomethyl substituted chromones.

[157] K. Natte, R. V. Jagadeesh, in Kirk-Othmer Encyclopedia of Chemical Technology, **2021**, pp. 1-34.

[158] S. Nees, F. Fantuzzi, T. Wellnitz, M. Fischer, J.-E. Siewert, J. T. Goettel, A. Hofmann, M. Härterich, H. Braunschweig, C. Hering-Junghans, *Angew. Chem. Int. Ed.* **2021**, *60*, 24318-24325, Cyclo-Dipnictadialanes.

[159] H. Neumann, R. V. Jagadeesh, in Carbon Monoxide in Organic Synthesis (Ed.: B. Gabriele), Wiley VCH, **2021**, pp. 113-148.

[160] J. Neumann, R. Ludwig, D. Paschek, J. Phys. Chem. B 2021, 125, 5132-5144, Hydrogen Bonds between lons of Opposite and Like Charge in Hydroxyl-Functionalized Ionic Liquids: an Exhaustive Examination of the Interplay between Global and Local Motions and Intermolecular Hydrogen Bond Lifetimes and Kinetics. [161] J. Neumann, D. Paschek, A. Strate, R. Ludwig, *J. Phys. Chem. B* **2021**, *125*, 281-286, Kinetics of Hydrogen Bonding between Ions with Opposite and Like Charges in Hydroxyl-Functionalized Ionic Liquids.

[162] K. Neymeyr, M. Beese, M. Sawall, *J. Chemom.* **2021**, *35*, e3381, On properties of EFA plots.

[163] K. Neymeyr, M. Sawall, A. C. Olivieri, *J. Chemom.* **2021**, *35*, e3363, On the signal contribution function with respect to different norms.

[164] N.-K. Nguyen, D. L. Tran, T. Q. Hung, T. M. Le, N. T. Son, Q. T. Trinh, T. T. Dang, P. Langer, *Tetrahedron Lett.* **2021**, *68*, 152936, Facile access to bis(indolyl)methanes by copper-catalysed alkylation of indoles using alcohols under air.

[165] N. Ortner, H. Lund, U. Armbruster, S. Wohlrab, E. V. Kondratenko, *Catal. Today* **2021**, Factors affecting primary and secondary pathways in  $CO_2$  hydrogenation to methanol over CuZnln/MZrO<sub>x</sub> (La, Ti or Y).

[166] T. Otroshchenko, G. Jiang, V. A. Kondratenko, U. Rodemerck, E. V. Kondratenko, *Chem. Soc. Rev.* **2021**, *50*, 473-527, Current status and perspectives in oxidative, non-oxidative and  $CO_2$ -mediated dehydrogenation of propane and isobutane over metal oxide catalysts.

[167] T. Otroshchenko, Q. Zhang, E. V. Kondratenko, *ACS Catal.* **2021**, *11*, 14159-14167, Enhancing Propene Formation in the Metathesis of Ethylene with 2-Butene at Close to Room Temperature over MoO<sub>x</sub>/SiO<sub>2</sub> through Support Promotion with P, Cl, or S.

[168] T. Otroshchenko, Q. Zhang, E. V. Kondratenko, *Catal. Lett.* **2021**, Room-Temperature Metathesis of Ethylene with 2-Butene to Propene Over  $MoO_x$ -Based Catalysts: Mixed Oxides as Perspective Support Materials.

[169] V. Overbeck, A. Appelhagen, R. Roeßler, T. Niemann, R. Ludwig, J. Mol. Liq. 2021, 322, 114983, Rotational correlation times, diffusion coefficients and quadrupolar peaks of the protic ionic liquid ethylammonium nitrate by means of <sup>1</sup>H fast field cycling NMR relaxometry.

[170] V. Overbeck, H. Schroeder, A.-M. Bonsa, K. Neymeyr, R. Ludwig, *Phys. Chem. Chem. Phys.* **2021**, *23*, 2663-2675, Insights into the translational and rotational dynamics of cations and anions in protic ionic liquids by means of NMR fast-fieldcycling relaxometry.

[171] R. Paul, S. Chandra Shit, H. Mandal, J. Rabeah, S. S. Kashyap, Y. Nailwal, D. B. Shinde, Z. Lai, J. Mondal, ACS Appl. Nano Mater. 2021, 4, 11732-11742, Benzothiazole-Linked Metal-Free Covalent Organic Framework Nanostructures for Visible-Light-Driven Photocatalytic Conversion of Phenylboronic Acids to Phenols.

[172] G. B. Peddakasu, V. K. Velisoju, N. Gutta, S. Medak, M. Dumpalapally, V. Akula, Catal. Today 2021, 375, 112-119, Elucidation of surface active sites by formic acid adsorbed IR studies in the hydrogenation of levulinic acid to valeric acid over rare earth metal doped titania supported nickel catalysts.

[173] T. Peppel, M. Köckerling, Materials 2021, 14, 2676, New Low-Melting Triply Charged Homoleptic Cr(III)-Based Ionic Liquids in Comparison to Their Singly Charged Heteroleptic Analogues.

[174] T. Peppel, M. Koeckerling, IUCrData 2021, 6, x210818, 1-Butyl-3-methylimidazolium tribromido(triphenylphosphane-kP)nickelate(II) butan-1-ol hemisolvate.

[175] T. Peppel, M. Koeckerling, IUCrData 2021, 6, x210562, (S)-Alanine ethyl ester tetracyanidoborate,  $(C_5H_{12}NO)[B(CN)_4].$ 

[176] P. Piehl, R. Amuso, A. Spannenberg, B. Gabriele, H. Neumann, M. Beller, Catal. Sci. Technol. 2021, 11, 2512-2517, Efficient methylation of anilines with methanol catalysed by cyclometalated ruthenium complexes.

[177] I. S. Pieta, A. Michalik, E. Kraleva, D. Mrdenovic, A. Sek, E. Wahaczyk, A. Lewalska-Graczyk, M. Krysa, A. Sroka-Bartnicka, P. Pieta, R. Nowakowski, A. Lew, E. M. Serwicka, Catalysts 2021, 11, 660, Bio-DEE Synthesis and Dehydrogenation Coupling of Bio-Ethanol to Bio-Butanol over Multicomponent Mixed Metal Oxide Catalysts.

[178] M. B. Ponce, S. Parpart, A. Villinger, E. T. Rodríguez, P. Ehlers, P. Langer, Synthesis 2021, 53, 1237-1246, Synthesis of Pyrrolo[1,2-a][1,6]- and [1,8]naphthyridines by Alkyne-Carbonyl Metathesis.

[179] L. Pudnika, I. Domraceva, T. Werner, R. Zalubovskis, A. Grandane, Synthesis 2021, Base-Free Catalytic Wittig-/Cross-Coupling Reaction Sequence as Short Synthetic Strategy for the Preparation of Highly Functionalized Arylbenzoxepinones.

[180] F. A. Qaraah, S. A. Mahyoub, A. Hezam, Q. A. Drmosh, J. Munyaneza, Q. Yu, G. Xiu, J. Environm. Chem. Eng. 2021, 9, 106587, One step-polymerization for constructing 1D/2D oxygen doped g-C<sub>2</sub>N<sub>4</sub> isotype heterojunctions with highly improved visible-light-driven photocatalytic activity.

[181] J. Radolko, P. Ehlers, P. Langer, Adv. Svnth. Catal. 2021, 363, 3616-3654, Recent Advances in Transition-Metal-Catalyzed Reactions of N-Tosylhydrazones.

[182] S. U. Rahman, H. S. Ali, B. Jafari, S. Zaib, A. Hameed, Y. M. S. A. Al-Kahraman, P. Langer, J. Igbal, Computational Biol. Chem. 2021, 91, 107326, Structure-based virtual screening of dipeptidyl peptidase 4 inhibitors and their in vitro analysis.

[183] T. Rahn, P. Langer, Vietnam J. Chem. 2021, 59, 87-89, Synthesis and Reactions of 1-cyclopropyl-1,3-bis(trimethylsilyloxy)-1,3-buatdiene.

[184] Y. Ren, T. Dong, S. Ding, X. Liu, H. Zheng, L. Gao, J. Hu, ACS Appl. Nano Mater. 2021, 4, 9274-9282, AgBr Nanoparticles Anchored on CdS Nanorods as Photocatalysts for H<sub>2</sub> Evolution.

[185] N. U. D. Reshi, V. B. Saptal, M. Beller, J. K. Bera, ACS Catal. 2021, 11, 13809-13837, Recent Progress in Transition-Metal-Catalyzed Asymmetric Reductive Amination.

[186] V. Ritleng, J. G. de Vries, Molecules 2021, 26, 4076, Ruthenacycles and Iridacycles as Transfer Hydrogenation Catalysts.

[187] U. Rosenthal, Zeitschr. f. anorg. Allgem. Chem. 2021, 647, 1246-1249, Influence of Impurities on the Productivity in Homogeneous Catalytic Reactions: Trimerization of 1,4-Dimethoxy-but-2-yne and Tetramerization of Propargyl Alcohol.

[188] U. Rosenthal, ChemistryOpen 2021, 10, 1234-1243, Latest News: Reactions of Group 4 Bis(trimethylsilyl)acetylene Metallocene Complexes and Applications of the Obtained Products.

[189] U. Rosenthal, Chem. Eur. J. 2021, 27. 17751-17760. Take a "Snapshot" of New Syntheses, Reactions, and Characterizations from Unusual Unsaturated Ring Strained Group 4 Metallacycles.

[190] P. Ryabchuk, M. Anwar, S. Dastgir, K. Junge, M. Beller, ACS Sustainable Chem. Eng. 2021, 9, 10062-10072, From Mobile Phones to Catalysts: E-Waste-Derived Heterogeneous Copper Catalysts for Hydrogenation Reactions.

[191] R. Saleem, A. Farhat, R. A. Khera, P. Langer, J. Igbal, Computational Theoret. Chem. 2021, 1197, 113154, Designing of small molecule non-fullerene acceptors with cyanobenzene core for photovoltaic application.

[192] R. Sang, Y. Hu, R. Razzag, R. Jackstell, R. Franke, M. Beller, Org. Chem. Front. 2021, 8, 799-811, State-of-the-art palladium-catalyzed alkoxycarbonylations.

[193] N. Sarki, V. Goyal, K. Natte, R. V. Jagadeesh, Adv. Synth. Catal. 2021, 363, 5028-5046, Base Metal-Catalyzed C-Methylation Reactions Using Methanol.

[194] M. Sawall, C. Fischer, B. J. Elvers, S. Pätsch, K. Neymeyr, Anal. Chim. Acta 2021, 1185, 339065, A multi-method chemometric analysis in spectroelectrochemistry: Case study on molybdenum mono-dithiolene complexes.

[195] M. Sawall, K. Neymeyr, J. Chemom. 2021, 35, e3316, On the area of feasible solutions for rank-deficient problems: I. Introduction of a generalized concept.

[196] J. T. Schille, I. Nolte, J. Beck, D. Jilani, C. Roolf, A. Pews-Davtyan, A. Rolfs, L. Henze, M. Beller, B. Brenig, C. Junghanss, E. Schuetz, H. Murua Escobar, Front. Veterinary Sci. 2021, 7, PDA IndolyImaleimides Induce Anti-Tumor Effects in Prostate Carcinoma Cell Lines Through Mitotic Death.

[197] C. Schneider, R. Franke, R. Jackstell, M. Beller, Catal. Sci. Technol. 2021, 11, 2703-2707, A direct synthesis of carboxylic acids via platinum-catalysed hydroxycarbonylation of olefins.

[198] C. Schneider, T. Leischner, P. Ryabchuk, R. Jackstell, K. Junge, M. Beller, CCS Chem. 2021, 3, 512-530, Development of bulk organic chemical processes-history, status, and opportunities for academic research.

[199] J. Schneidewind, M. A. Araüello Cordero, H. Junge, S. Lochbrunner, M. Beller, Energy & Environm. Sci. 2021, 14, 4427-4436, Two-photon, visible light water splitting at a molecular ruthenium complex.

[200] J. Schneidewind, H. Olickel, Chem.-Methods 2021, 1, 87-88, Improving Data Analysis in Chemistry and Biology Through Versatile Baseline Correction.

[201] G. Schnell, H. Lund, S. Bartling, C. Polley, A. Riaz, V. Senz, A. Springer, H. Seitz, Appl. Surf. Sci. 2021, 570, 151115, Heat accumulation during femtosecond laser treatment at high repetition rate – A morphological, chemical and crystallographic characterization of self-organized structures on Ti<sub>c</sub>Al<sub>4</sub>V.

[202] M. Schröder, D. Rauber, C. Matt, C. W. M. Kay, Appl. Mag. Reason. 2021, Pentacene in 1,3,5-Tri(1-naphtyl)benzene: A Novel Standard for Transient EPR Spectroscopy at Room Temperature.

[203] A. Schulz, A. Hinz, A. Roelke, A. Villinger, R. Wustrack, Zeitschr. f. anorg. Allgem. Chem. 2021, 647, 245-257, On New Staudinger Type **Reactions of Phosphorus Centered** Biradicaloids,  $[P(\mu-NR)]_{2}$  (R = Ter, Hyp), with Ionic and Covalent Azides.

[204] A. Schumann, J. Bresien, M. Fischer, C. Hering-Junghans, Chem. Commun. 2021, 57, 1014-1017, Aryl-substituted triarsiranes: synthesis and reactivity.

[205] C. H. Schwarz, D. Kraus, E. Alberico, H. Junge, M. Haumann, Eur. J. Inorg. Chem. 2021, 2021, 1745-1751, Immobilized Ru-Pincer Complexes for Continuous Gas-Phase Low-Temperature Methanol Reforming-Improving the Activity by a Second Ru-Complex and Variation of Hydroxide Additives.

[206] M. Sebek, H. Atia, N. Steinfeldt, J. Flow Chem. 2021, Synthesis of flowcompatible Ru-Me/Al<sub>2</sub>O<sub>2</sub> catalysts and their application in hydrogenation of 1-iodo-4-nitrobenzene.

[207] M. Sebek, T. Peppel, H. Lund, I. Medic, A. Springer, P. Mazierski, A. Zaleska-Medynska, J. Strunk, N. Steinfeldt, Chem. Eng. J. 2021, 425, 130619, Thermal annealing of ordered TiO<sub>2</sub> nanotube arrays with water vapor-assisted crystallization under a continuous gas flow for superior

photocatalytic performance.

[208] P. Seefeldt, R. Dasi, A. Villinger, M. Brasholz, ChemPhotoChem 2021, 5, 979-983, Photoredox-Induced Deaminative Radical-Cationic Three-Component Couplings with N-Alkylpyridinium Salts and Alkenes.

[209] Y. Shang, J.-S. Wang, J. Ying, X.-F. Wu, ChemistrySelect 2021, 6, 12220-12223, Palladium-Catalyzed Carbonylative Synthesis of 1-Acyl-1,5-dihydro-2H-pyrrol-2-ones from Propargyl Amines and Acid Chlorides.

[210] E. A. Shelepova, R. Ludwig, D. Paschek, N. N. Medvedev, J. Mol. Liq. 2021, 329, 115589, Structural similarity of an ionic liquid and the mixture of the neutral molecules.

[211] H. Shen, M. Yang, L. Hao, J. Wang, J. Strunk, Z. Sun, Nano Research 2021, Photocatalytic nitrogen reduction to ammonia: Insights into the role of defect engineering in photocatalysts.

[212] X. Shi, S. Li, M. Reiß, A. Spannenberg, T. Holtrichter-Roeßmann, F. Reiß, T. Beweries, Chem. Sci. 2021, 12, 16074-16084, 1-Zirconacyclobuta-2,3-dienes: synthesis of organometallic analogs of elusive 1,2-cyclobutadiene, unprecedented intramolecular C-H activation, and reactivity studies.

[213] J.-E. Siewert, A. Schumann, C. Hering-Junghans, Dalton Trans. 2021, 15111-15117, Phosphine-catalysed reductive coupling of dihalophosphanes.

[214] R. Siewert, R. Ludwig, S. P. Verevkin, Phys. Chem. Chem. Phys. 2021, 23, 25226-25238, Non-covalent interactions in molecular systems: thermodynamic evaluation of the hydrogen bond strength in aminoalcohols.

[215] R. Sikandar, A. Farhat, R. A. Khera, S. Jabeen, A. R. Ayub, P. Langer, J. Iqbal, J. Mol. Graph. Model. 2021, 106, 107918, Tuning the optoelectronic properties of oligothienyl silane derivatives and their photovoltaic properties.

[216] C. Sindlinger, C. Hering-Junghans, Nachr. Chem. 2021, 69, 52-66, Trend report inorganic chemistry: main groups.

[217] B. Singh, M. B. Gawande, A. D. Kute, R. S. Varma, P. Fornasiero, P. McNeice, R. V. Jagadeesh, M. Bel-

ler, R. Zbořil, Chem. Rev. 2021, 121, 13620-13697, Single-Atom (Iron-Based) Catalysts: Synthesis and Applications.

[218] A. S. Skrypnik, Q. Yang, A. A. Matvienko, V. Y. Bychkov, Y. P. Tulenin, H. Lund, S. A. Petrov, R. Kraehnert, A. Arinchtein, J. Weiss, A. Brueckner, E. V. Kondratenko, Appl. Catal. B 2021, 291, 120121, Understanding reaction-induced restructuring of well-defined Fe O C compositions and its effect on  $\hat{CO}_{2}$ hydrogenation.

[219] M. Sobhani, A. Frey, A. Rettmann, R. Thom, A. Villinger, P. Ehlers, P. Langer, J. Org. Chem. 2021, 86, 14420-14432, Synthesis of Dibenzotropones by Alkyne-Carbonyl Metathesis.

[220] I. Sokolovs, N. Mohebbati, R. Francke, E. Suna, Angew. Chem. Int. Ed. 2021, 60, 15832-15837, Electrochemical Generation of Hypervalent Bromine(III) Compounds.

[221] Y. Song, L.-C. Wang, S. Du, Z. Chen, X.-F. Wu, Org. Biomol. Chem. 2021, 19, 6115-6119. The cascade coupling/iodoaminocyclization reaction of trifluoroacetimidoyl chlorides and allylamines: metal-free access to 2-trifluoromethyl-imidazolines.

[222] P. Sprenger, M. Stehle, A. Gaur, J. Weiß, D. Brueckner, Y. Zhang, J. Garrevoet, J.-P. Suuronen, M. Thomann, A. Fischer, J.-D. Grunwaldt, T. L. Sheppard, ChemCatChem 2021, 13, 2483-2493, Chemical Imaging of Mixed Metal Oxide Catalysts for Propylene Oxidation: From Model Binary Systems to Complex Multicomponent Systems.

[223] B. M. Stadler, J. G. de Vries, Philo. Trans. Royal Soc. A 2021, 379, 20200341, Chemical upcycling ofpolymers.

[224] A.-E. Stamate, O. D. Pavel, R. Zăvoianu, I. Brezeștean, A. Ciorîță, R. Bîrjega, K. Neubauer, A. Koeckritz, I.-C. Marcu, Materials 2021, 14, 7457, Ce-Containing MgAl-Layered Double Hydroxide-Graphene Oxide Hybrid Materials as Multifunctional Catalysts for Organic Transformations.

[225] V. Stefanow, A. Grandane, M. Eh, J. Panten, A. Spannenberg, T. Werner, Org. Process Res. Dev. 2021, 25, 89-97, Stereoselective Synthesis of a cis-Cedrane-8,9-diol as a Key Intermediate for an Amber Odorant.

[226] J. Strunk, Heterogeneous Photocatalysis: From Fundamentals to Applications in Energy Conversion and Depollution, Royal Society of Chemistry, 2021.

[227] J. Strunk, *Bunsenmagazin* **2021**, 235-237, Saving the world with CO<sub>2</sub>!

[228] P. Sudarsanam, A. Koeckritz, H. Atia, M. H. Amin, A. Brueckner, *ChemCatChem* **2021**, *13*, 1990-1997, Synergistic Nanostructured MnO<sub>2</sub>/ TiO<sub>2</sub> Catalyst for Highly Selective Synthesis of Aromatic Imines.

[229] K. Sun, H. Shan, G.-P. Lu, C. Cai, M. Beller, *Angew. Chem. Int. Ed.* **2021**, I, 25188-25202, Synthesis of N-Heterocycles via Oxidant-Free Dehydrocyclization of Alcohols Using Heterogeneous Catalysts.

[230] Y. Sun, Y. Chen, X. Zhang, Y. He, Z. Qiu, W. Zheng, F. Wang, H. Jiao, Y. Yang, Y. Li, X. Wen, *Angew. Chem. Int. Ed.* **2021**, *60*, 25538-25545, The Facile Dissociation of Carbon–Oxygen Bonds in  $CO_2$  and CO on the Surface of LaCoSiHx Intermetallic Compound.

[231] L. S. Szych, K. P. Lüdtke, Y. Pilopp, J. Bresien, A. Villinger, A. Schulz, *Dalton Trans.* **2021**, *50*, 16568-16577, Reaction of potassium phosphide KP(iPr)Ter with chalcogens, heteroallenes and an acyl chloride.

[232] T. Taeufer, M. A. Argüello Cordero, A. Petrosyan, A.-E. Surkus, S. Lochbrunner, J. Pospech, *ChemPhoto-Chem* **2021**, *5*, 999-1003, Photophysical and Electrochemical Properties of Pyrimidopteridine-Based Organic Photoredox Catalysts.

[233] T. Taeufer, R. Hauptmann, F. El-Hage, T. S. Mayer, H. Jiao, J. Rabeah, J. Pospech, *ACS Catal.* **2021**, *11*, 4862-4869, Pyrimidopteridine-Catalyzed Hydroamination of Stilbenes with Primary Amines: A Dual Photoredox and Hydrogen Atom Transfer Catalyst.

[234] T. Taeufer, A. Spannenberg, J. Pospech, *IUCrData* **2021**, *6*, x211026, 1-[(Methylsulfonyl)oxy]pyridin-1-ium methanesulfonate.

[235] J. Tang, J. Zhang, Y. Zhang, Z. Chen, X.-F. Wu, *Org. Chem. Front.* **2021**, Palladium-catalyzed carbonylative synthesis of 5-trifluoromethyl-1,2,4-triazoles from trifluoroacetimidohydrazides and aryl iodides.

[236] N. Tka, M. A. H. Ayed, M. B. Braiek, M. Jabli, N. Chaaben, K.

Alimi, S. Jopp, P. Langer, *Beilstein J. Org. Chem.* **2021**, *17*, 1629-1640, 2,4-Bis(arylethynyl)-9-chloro-5,6,7,8-tetrahydroacridines: synthesis and photophysical properties.

[237] N. Tka, M. A. H. Ayed, M. B. Braiek, M. Jabli, P. Langer, *Beilstein J. Org. Chem.* **2021**, *17*, 2450–2461, Synthesis and investigation on optical and electrochemical properties of 2,4-diaryl-9-chloro-5,6,7,8-tetrahy-droacridines.

[238] J. Tönjes, L. Longwitz, T. Werner, *Green Chem.* **2021**, *23*, 4852-4857, Poly(methylhydrosiloxane) as a reductant in the catalytic base-free Wittig reaction.

[239] D. Tuan, A. Dang, D. Nguyen, K. Dinh, P. Dam, T. H. Vuong, M. T. Le, P. T. Huyen, *Catal. Industry* **2021**, *13*, 27-37, Influence of Aluminum Sources on Synthesis of SAPO-34 and NH<sub>3</sub>-SCR of NO<sub>x</sub> by as-Prepared Cu/ SAPO-34 Catalysts.

[240] F. Ullah, S. Irshad, S. Khan, M. A. Hashmi, R. Ludwig, T. Mahmood, K. Ayub, *J. Phys. Chem. Solids* **2021**, *151*, 109914, Nonlinear optical response of first-row transition metal doped Al<sub>12</sub>P<sub>12</sub> nanoclusters; a first-principles study.

[241] F. Unglaube, C. R. Kreyenschulte, E. Mejía, *ChemCatChem* **2021**, *13*, 2583-2591, Development and Application of Efficient Ag-based Hydrogenation Catalysts Prepared from Rice Husk Waste.

[242] F. Unglaube, A. Lammers, C. R. Kreyenschulte, M. Lalk, E. Mejía, *ChemistryOpen* **2021**, *10*, 1244-1250, Preparation, Characterization and Antimicrobial Properties of Nanosized Silver-Containing Carbon/Silica Composites from Rice Husk Waste.

[243] S. Vali Zade, K. Neymeyr, H. Abdollahi, M. Sawall, *Microchem. J.* 2021, *160*, 105615, Characterization of the unimodality constraint as an effective chemistry-based condition in resolving of chemical processes data.

[244] B. Van Phuc, H. N. Do, N. M. Quan, N. N. Tuan, N. Q. An, N. Van Tuyen, H. L. T. Anh, T. Q. Hung, T. T. Dang, P. Langer, *Synlett* **2021**, *32*, 1004-1008, Copper-Catalyzed Synthesis of  $\beta$ - and  $\delta$ -Carbolines by Double N-Arylation of Primary Amines.

[245] S. P. Verevkin, S. O. Kondratev, D. H. Zaitsau, K. V. Zherikova, R. Ludwig, *J. Mol. Lig.* **2021**, *343*, 117547, Quantification and understanding of non-covalent interactions in molecular and ionic systems: Dispersion interactions and hydrogen bonding analysed by thermodynamic methods.

[246] X. H. Vu, U. Armbruster, *Biomass Conv. Biorefinery* 2021, Engineering of zeolite crystals for catalytic cracking of triglycerides to renewable hydrocarbon fuels and chemicals: a review.

[247] X. H. Vu, S. Nguyen, T. T. Dang, U. Armbruster, *Biomass Conv. Biorefinery* 2021, *11*, 755-766, Improved biofuel quality in catalytic cracking of triglyceride-rich biomass over nanocrystalline and hierarchical ZSM-5 catalysts.

[248] T. H. Vuong, N. Rockstroh, U. Bentrup, J. Rabeah, J. Knossalla, S. Peitz, R. Franke, A. Brueckner, ACS Catal. 2021, 11, 3541-3552, Role of Surface Acidity in Formation and Performance of Active Ni Single Sites in Supported Catalysts for Butene Dimerization: A View inside by Operando EPR and In Situ FTIR Spectroscopy.

[249] C. Wang, O. El-Sepelgy, *Curr. Opinion Green and Sustainable Chem.* **2021**, *32*, 100547, Reductive depolymerization of plastics catalyzed with transition metal complexes.

[250] F. Wang, X. Tian, H. Jiao, *J. Phys. Chem. C* **2021**, *125*, 11419-11431, Adsorption of CO,  $H_2$ ,  $H_2O$ , and  $CO_2$  on Fe-, Co-, Ni-, Cu-, Pd-, and Pt-Doped Mo<sub>2</sub>C(101) Surfaces.

[251] J. Wang, X. Dai, H. Wang, H. Liu, J. Rabeah, A. Brueckner, F. Shi, M. Gong, X. Yang, *Nat. Commun.* **2021**, *12*, 6840, Dihydroxyacetone valorization with high atom efficiency via controlling radical oxidation pathways over natural mineral-inspired catalyst.

[252] J.-S. Wang, Y. Na, J. Ying, X.-F. Wu, *Org. Chem. Front.* **2021**, *8*, 2429-2433, Palladium-catalyzed 1,2-amino carbonylation of 1,3-dienes with (N-SO<sub>2</sub>Py)-2-iodoanilines: 2,3-dihydroquinolin-4(1H)-ones synthesis.

[253] J.-S. Wang, Y. Na, J. Ying, X.-F. Wu, *Mol. Catal.* **2021**, *516*, 111989, Cobalt-catalyzed regiodivergent synthesis of 5- and 6-substituted 1,3-dihydroisobenzofurans via cy-cloaddition of diynes and alkynes.

[254] J.-S. Wang, Q. Wang, Y. Zhu, Q. Gao, J. Ying, X.-F. Wu, *Org. Chem.*  *Front.* **2021**, *8*, 4188-4191, Cobalt-catalyzed carbonylative cycloaddition of substituted diynes to access complexed polycyclic compounds.

[255] J.-S. Wang, J. Ying, X.-F. Wu, *Mol. Catal.* **2021**, *516*, 111956, Cobalt-catalyzed regioselective cycloaddition of unsymmetric diynes and nitriles to form substituted pyridines.

[256] J. S. Wang, L. Y. Yao, J. Ying, X. L. Luo, X. F. Wu, *Org. Chem. Front.* **2021**, *8*, 792-798, Palladium-catalyzed directing group assisted and regioselectivity reversed cyclocarbonylation of arylallenes with 2-iodoanilines.

[257] L.-C. Wang, Y. Zhang, Z. Chen, X.-F. Wu, *Adv. Synth. Catal.* **2021**, *363*, 1417-1426, Palladium-Catalyzed Carbonylative Synthesis of 2-(Trifluoromethyl)quinazolin-4(3H)-ones from Trifluoroacetimidoyl Chlorides and Nitro Compounds.

[258] S. Wang, J.-S. Wang, Z. Le, J. Ying, X.-F. Wu, *Org. Biomol. Chem.* **2021**, *19*, 7353-7356, Palladium-catalyzed carbonylative synthesis of aryl esters from p-benzoquinones and aryl triflates.

[259] S. Wang, L. Yao, J. Ying, X.-F. Wu, *Org. Biomol. Chem.* **2021**, *19*, 8246-8249, Palladium-catalyzed carbonylation of iminoquinones and aryl iodides to access aryl p-amino benzoates.

[260] W. Wang, Z.-P. Bao, X. Qi, X.-F. Wu, Org. Lett. **2021**, 23, 6589-6593, Nickel-Catalyzed One-Pot Carbonylative Synthesis of 2-Mono- and 2,3-Disubstituted Thiochromenones from 2-Bromobenzenesulfonyl Chlorides and Alkynes.

[261] W. Wang, X. Qi, X.-F. Wu, *Adv. Synth. Catal.* **2021**, *363*, 2541-2545, Palladium-Catalyzed Thiocarbonylation of Benzyl Chlorides with Sulfonyl Chlorides for the Synthesis of Arylacetyl Thioesters.

[262] S. Weber, S. Schäfer, M. Saccoccio, N. Ortner, M. Bertmer, K. Seidel, S. Berendts, M. Lerch, R. Gläser, H. Kohlmann, S. A. Schunk, *Catalysts* **2021**, *11*, 334, Mayenite-Based Electride  $C_{12}A_{7e-}$ : A Reactivity and Stability Study.

[263] D. Wei, H. Junge, M. Beller, *Chem. Sci.* **2021**, *12*, 6020-6024, An amino acid based system for  $CO_2$ capture and catalytic utilization to produce formates. [264] Z. Wei, X. Tian, M. Bender, M. Beller, H. Jiao, ACS Catal. 2021, 11, 6908-6919, Mechanisms of Coll and Acid Jointly Catalyzed Domino Conversion of  $CO_2$ ,  $H_2$ , and  $CH_3OH$  to Dialkoxymethane: A DFT Study.

[265] F. Weiner, J. T. Schille, J. I. Hein, X. F. Wu, M. Beller, C. Junghanß, H. Murua Escobar, I. Nolte, *PLoS One* **2021**, *16*, e0256468, Evaluation of combination protocols of the chemotherapeutic agent FX-9 with azacitidine, dichloroacetic acid, doxorubicin or carboplatin on prostate carcinoma cell lines.

[266] F. Weiner, J. T. Schille, D. Koczan, X. F. Wu, M. Beller, C. Junghanss, M. Hewicker-Trautwein, H. Murua Escobar, I. Nolte, *BMC Cancer* **2021**, *21*, 1088, Novel chemotherapeutic agent FX-9 activates NF-κB signaling and induces G1 phase arrest by activating CDKN1A in a human prostate cancer cell line.

[267] J. Weiß, C. Rautenberg, T. Rall, C. Kubis, E. Kondratenko, U. Bentrup, A. Brueckner, *Chem. Methods* **2021**, *1*, 307-307, A Versatile Ambient-to-High-Pressure Reaction Transmission Cell for in situ/operando Infrared Spectroscopic Investigations.

[268] T. Wellnitz, C. Hering-Junghans, *Eur. J. Inorg. Chem.* **2021**, *2021*, 8-21, Synthesis and Reactivity of Monocyclic Homoleptic Oligophosphanes.

[269] M. A. Wirth, L. Longwitz, M. Kanwischer, P. Gros, P. Leinweber, T. Werner, *Ecotoxicol. Environm. Safety* **2021**, *225*, 112768, AMPA-<sup>15</sup>N – Synthesis and application as standard compound in traceable degradation studies of glyphosate.

[270] S. Woellner, T. Nowak, G.-R. Zhang, N. Rockstroh, H. Ghanem, S. Rosiwal, A. Brueckner, B. J. M. Etzold, *ChemistryOpen* **2021**, *10*, 600-606, Avoiding Pitfalls in Comparison of Activity and Selectivity of Solid Catalysts for Electrochemical HMF Oxidation.

[271] S. Wohlrab, E. V. Kondratenko, *Catalysts* **2021**, *11*, 475, Catalytic Concepts for Methane Combustion.

[272] A. Wotzka, M. Namayandeh Jorabchi, S. Wohlrab, *Membranes* **2021**, *11*, 439, Separation of H<sub>2</sub>O/CO<sub>2</sub> Mixtures by MFI Membranes: Experiment and Monte Carlo Study.

[273] F.-P. Wu, J. Holz, Y. Yuan, X.-F. Wu, CCS Chem. **2021**, *3*, 2643-2654, Copper-Catalyzed Carbonylative Synthesis of  $\beta$ -Boryl Amides via Boroamidation of Alkenes.

[274] F.-P. Wu, X.-F. Wu, Angew. Chem. Int. Ed. **2021**, 60, 695-700, Ligand-Controlled Copper-Catalyzed Regiodivergent Carbonylative Synthesis of  $\alpha$ -Amino Ketones and  $\alpha$ -Boryl Amides from Imines and Alkyl Iodides.

[275] F.-P. Wu, X.-F. Wu, *Angew. Chem. Int. Ed.* **2021**, *60*, 11730-11734, Copper-Catalyzed Borylative Methylation of Alkyl lodides with CO as the C1 Source: Advantaged by Faster Reaction of CuH over CuBpin.

[276] F.-P. Wu, X.-F. Wu, *Chem. Sci.* **2021**, *12*, 10341-10346, Pd/Cu-Catalyzed amide-enabled selectivity-reversed borocarbonylation of unactivated alkenes.

[277] F.-P. Wu, Y. Yuan, J. Liu, X.-F. Wu, Angew. Chem. Int. Ed. **2021**, 60, 8818-8822, Pd/Cu-Catalyzed Defluorinative Carbonylative Coupling of Aryl lodides and gem-Difluoroalkenes: Efficient Synthesis of  $\alpha$ -Fluorochalcones.

[278] F.-P. Wu, Y. Yuan, X.-F. Wu, Angew. Chem. Int. Ed. 2021, 60, 25787-25792, Copper-Catalyzed 1,2-Trifluoromethylation Carbonylation of Unactivated Alkenes: Efficient Access to  $\beta$ -Trifluoromethylated Aliphatic Carboxylic Acid Derivatives.

[279] C. Wulf, M. Beller, T. Boenisch, O. Deutschmann, S. Hanf, N. Kockmann, R. Kraehnert, M. Oezaslan, S. Palkovits, S. Schimmler, S. A. Schunk, K. Wagemann, D. Linke, *Chem-CatChem* **2021**, *13*, 3223-3236, A Unified Research Data Infrastructure for Catalysis Research – Challenges and Concepts.

[280] J. Xiao, J. J. M. Vequizo, T. Hisatomi, J. Rabeah, M. Nakabayashi, Z. Wang, Q. Xiao, H. Li, Z. Pan, M. Krause, N. Yin, G. Smith, N. Shibata, A. Brueckner, A. Yamakata, T. Takata, K. Domen, J. Am. Chem. Soc. **2021**, *143*, 10059-10064, Simultaneously Tuning the Defects and Surface Properties of Ta<sub>3</sub>N<sub>5</sub> Nanoparticles by Mg–Zr Codoping for Significantly Accelerated Photocatalytic H<sub>2</sub> Evolution.

[281] J.-X. Xu, F.-P. Wu, X.-F. Wu, *Catal. Commun.* **2021**, *149*, 106205, Rhodium-catalyzed borylative carbon monoxide reduction to gem-diborylmethane. [282] T. Xu, P. Lu, S. Wohlrab, W. Chen, A. Springer, X.-F. Wu, W. Lu, *Catal. Commun.* **2021**, *157*, 106328, In situ grown palladium nanoparticles on polyester fabric as easy-separable and recyclable catalyst for Suzuki-Miyaura reaction.

[283] T. Xu, Q. Wang, Z. Yang, L. Yi, J.-S. Wang, W. Lu, J. Ying, X.-F. Wu, *Chem. Asian J.* **2021**, *16*, 2027-2030, Supported Palladium-Catalyzed Carbonylative Synthesis of Diaryl Ketones from Aryl Bromides and Arylboronic Acids.

[284] T. Xu, Y. Zhang, L. Yi, W. Lu, Z. Chen, X.-F. Wu, *Mol. Catal.* **2021**, *513*, 111767, Efficient synthesis of 2-trifluoromethyl-benzimidazoles via cascade annulation of trifluoroacetimidoyl chlorides and amines based on a heterogeneous copper doped  $g-C_3N_4$  catalyst.

[285] H. Yang, S.-N. Lu, Z. Chen, X.-F. Wu, *J. Org. Chem.* **2021**, *86*, 4361-4370, Silver-Mediated [3 + 2] Cycloaddition of Azomethine Ylides with Trifluoroacetimidoyl Chlorides for the Synthesis of 5-(Trifluoromethyl)imidazoles.

[286] H. Yang, S.-N. Lu, Y. Song, Z. Chen, X.-F. Wu, *Org. Chem. Front.* **2021**, Copper-mediated [3 + 2] cycloaddition of trifluoroacetimidoyl chlorides and N-isocyanoiminotriphenylphosphorane for the synthesis of 3-trifluoromethyl-1,2,4-triazoles.

[287] H. Yang, H. Wang, L. Wei, Y. Yang, Y.-W. Li, X.-d. Wen, H. Jiao, *Phys. Chem. Chem. Phys.* **2021**, *23*, 26392-26400, Simple mechanisms of  $CH_4$  reforming with  $CO_2$  and  $H_2O$  on a supported Ni/ZrO<sub>2</sub> catalyst.

[288] H. Yang, T.-H. Xu, S.-N. Lu, Z. Chen, X.-F. Wu, *Org. Chem. Front.* **2021**, *8*, 3440-3445, Synthesis of 5-trifluoromethyl-1,2,3-triazoles via base-mediated cascade annulation of diazo compounds with trifluoroacetimidoyl chlorides.

[289] J. Yang, A. Acharjya, M.-Y. Ye, J. Rabeah, S. Li, Z. Kochovski, S. Youk, J. Roeser, J. Grüneberg, C. Penschke, M. Schwarze, T. Wang, Y. Lu, R. van de Krol, M. Oschatz, R. Schomäcker, P. Saalfrank, A. Thomas, *Angew. Chem. Int. Ed.* **2021**, *60*, 19797-19803, Protonated Imine-Linked Covalent Organic Frameworks for Photocatalytic Hydrogen Evolution.

[290] J. Yang, J. Liu, Y. Ge, W. Huang,

F. Ferretti, H. Neumann, H. Jiao, R. Franke, R. Jackstell, M. Beller, *Angew. Chem. Int. Ed.* **2021**, *60*, 9527-9533, Efficient Palladium-Catalyzed Carbonylation of 1,3-Dienes: Selective Synthesis of Adipates and Other Aliphatic Diesters.

[291] J. Yang, S. Ren, B. Su, Y. zhou, G. Hu, L. Jiang, J. Cao, W. Liu, L. Yao, M. Kong, J. Yang, Q. Liu, *Catal. Lett.* **2021**, *151*, 2964-2971, Insight into  $N_2O$  Formation Over Different Crystal Phases of MnO<sub>2</sub> During Low-Temperature  $NH_3$ -SCR of NO.

[292] Q. Yang, A. Skrypnik, A. Matvienko, H. Lund, M. Holena, E. V. Kondratenko, *Appl. Catal. B* **2021**, *282*, 119554, Revealing property-performance relationships for efficient CO<sub>2</sub> hydrogenation to higher hydrocarbons over Fe-based catalysts: Statistical analysis of literature data and its experimental validation.

[293] L. Yao, Y. Shang, J.-S. Wang, A. Pan, J. Ying, X.-F. Wu, *Org. Chem. Front.* **2021**, *8*, 1926-1929, Palladium-catalyzed carbonylative cyclization of 2-alkynylanilines and aryl iodides to access N-acyl indoles.

[294] L. Yao, J. Ying, X.-F. Wu, *Org. Chem. Front.* **2021**, *8*, 6541-6545, Nickel-catalyzed cascade carbonylative synthesis of N-benzoyl indoles from 2-nitroalkynes and aryl iodides.

[295] F. Ye, Y. Ge, A. Spannenberg, H. Neumann, L.-W. Xu, M. Beller, *Nat. Commun.* **2021**, *12*, 3257, 3,3-Difluoroallyl ammonium salts: highly versatile, stable and selective gem-difluoroallylation reagents.

[296] Y. Yuan, F.-P. Wu, A. Spannenberg, X.-F. Wu, *Sci. China Chem.* **2021**, *64*, 2142-2153, Cu/Pd-catalyzed borocarbonylative trifunctionalization of alkynes and allenes: synthesis of β-geminal-diboryl ketones.

[297] Y. Yuan, F.-P. Wu, X.-F. Wu, *Chem. Sci.* **2021**, *12*, 13777-13781, Copper-catalyzed borofunctionalization of styrenes with B<sub>2</sub>pin, and CO.

[298] Y. Yuan, F. Zhao, X.-F. Wu, *Chem. Sci.* **2021**, *12*, 12676-12681, Copper-catalyzed enantioselective carbonylation toward  $\alpha$ -chiral secondary amides.

[299] D. H. Zaitsau, R. Ludwig, S. P. Verevkin, *Phys. Chem. Chem. Phys.* **2021**, *23*, 7398-7406, Determination of the dispersion forces in the gas phase structures of ionic liquids using

exclusively thermodynamic methods.

[300] B. Zhang, D. Peña Fuentes, A. Boerner, *ChemTexts* **2021**, *8*, 2, Hydroformylation.

[301] G. Zhang, Y. Cheng, M. Beller, F. Chen, *Adv. Synth. Catal.* **2021**, **363**, 1583-1596, Direct Carboxylation with Carbon Dioxide via Cooperative Photoredox and Transition-Metal Dual Catalysis.

[302] J. Zhang, J. Tang, Z. Chen, X.-F. Wu, *Adv. Synth. Catal.* **2021**, *363*, 3060-3069, Synthesis of 5-Trifluoromethyl-1,2,4-Triazoles via Metal-Free Annulation of Trifluoroacetimidohydrazides and Methyl Ketones.

[303] J. Zhang, J. Tang, Z. Chen, X.-F. Wu, *Chinese J. Chem.* **2021**, *39*, 3443-3447, Elemental Sulfur and Dimethyl Sulfoxide-Promoted Oxidative Cyclization of Trifluoroacetimidohydrazides with Methylhetarenes for the Synthesis of 3-Hetaryl-5-trifluoromethyl-1,2,4-triazoles.

[304] J. Zhang, T.-H. Xu, Z. Chen, X.-F. Wu, *Org. Chem. Front.* **2021**, *8*, 4490-4495, Metal-free oxidative cyclization of trifluoroacetimidohydrazides with methylhetarenes: a facile access to 3-hetaryl-5-trifluoromethyl-1,2,4-triazoles.

[305] Y. Zhang, H.-Q. Geng, X.-F. Wu, Angew. Chem. Int. Ed. **2021**, 60, 24292-24298, Palladium-Catalyzed Perfluoroalkylative Carbonylation of Unactivated Alkenes: Access to  $\beta$ -Perfluoroalkyl Esters.

[306] Y. Zhang, H.-Q. Geng, X.-F. Wu, *Chem. Eur. J.* **2021**, *27*, 17682-17687, Palladium-Catalyzed Carbonylative Four-Component Synthesis of  $\beta$ -Perfluoroalkyl Amides.

[307] D. Zhao, H. Lund, U. Rodemerck, D. Linke, G. Jiang, E. V. Kondratenko, *Catal. Sci. Technol.* **2021**, *11*, 1386-1394, Revealing fundamentals affecting activity and product selectivity in non-oxidative propane dehydrogenation over bare Al<sub>2</sub>O<sub>3</sub>.

[308] D. Zhao, X. Tian, D. E. Doronkin, S. Han, V. A. Kondratenko, J.-D. Grunwaldt, A. Perechodjuk, T. H. Vuong, J. Rabeah, R. Eckelt, U. Rodemerck, D. Linke, G. Jiang, H. Jiao, E. V. Kondratenko, *Nature* **2021**, *599*, 234-238, In situ formation of ZnO<sub>x</sub> species for efficient propane dehydrogenation.

[309] F. Zhao, H.-J. Ai, X.-F. Wu, Chinese J. Chem. **2021**, 39, 927-932, Radical Carbonylation under Low CO Pressure: Synthesis of Esters from Activated Alkylamines at Transition Metal-Free Conditions.

[310] F. Zhao, X.-F. Wu, *Org. Chem. Front.* **2021**, *8*, 670-675, Deaminative carbonylative thioesterification of activated alkylamines with thiophenols under transition-metal-free conditions.

[311] F. Zhao, X.-F. Wu, J. Catal. 2021, 397, 201-204, The first bismuth self-mediated oxidative carbonylative coupling reaction via BillI/BiV redox intermediates.

[312] F. Zhao, X.-F. Wu, Organometallics 2021, 40, 2400-2404, Sulfonylation of Bismuth Reagents with Sulfinates or  $SO_2$  through BillI/BiV Intermediates.

[313] J. Zhao, Y. He, F. Wang, Y. Yang, W. Zheng, C. Huo, H. Jiao, Y. Yang, Y. Li, X. Wen, *J. Catal.* **2021**, *404*, 244-249, A recyclable CoGa intermetallic compound catalyst for the hydroformylation reaction.

[314] Y. Zheng, M. Dong, E. Qu, J. Bai, X.-F. Wu, W. Li, *Chem. Eur. J.* **2021**, *27*, 16219-16224, Pd-Catalyzed Carbonylative Synthesis of 4H-Benzo[d] [1,3]Oxazin-4-Ones Using Benzene-1,3,5-Triyl Triformate as the CO Source.

[315] V. V. Zhivonitko, H. Beer, D. O. Zakharov, J. Bresien, A. Schulz, *ChemPhysChem* **2021**, *22*, 813-817, Hyperpolarization Effects in Parahydrogen Activation with Pnictogen Biradicaloids: Metal-free PHIP and SABRE.

[316] J. Zhu, F. Cannizzaro, L. Liu, H. Zhang, N. Kosinov, I. A. W. Filot, J. Rabeah, A. Brueckner, E. J. M. Hensen, ACS Catal. 2021, 11, 11371-11384, Ni–In Synergy in  $CO_2$  Hydrogenation to Methanol.

[317] J. Zhu, P. Langer, C. Ulrich, J. Eberle, *Antioxidants* **2021**, *10*, 1514, Crucial Role of Reactive Oxygen Species (ROS) for the Proapoptotic Effects of Indirubin Derivatives in Cutaneous SCC Cells.

[318] Y. Zhu, Z. Le, J. Ying, X.-F. Wu, J. Organomet. Chem. 2021, 956, 122115, Palladium-catalyzed carbonylation of propargyl diols with primary amines for the synthesis of functionalized acids.

#### Publikationen 2022

[1] S. Abbas, S. Afzal, H. Nadeem, D. Hussain, P. Langer, J. Sévigny, Z. Ashraf, J. Iqbal, *Bioorg. Chem.* **2022**, *118*, 105456, Synthesis, characterization and biological evaluation of thiadiazole amide derivatives as nucleoside triphosphate diphosphohydrolases (NTPDases) inhibitors.

[2] A. M. Abdel-Mageed, S. Wohlrab, *Catalysts* **2022**, *12*, 16, Review of CO<sub>2</sub> Reduction on Supported Metals (Alloys) and Single-Atom Catalysts (SACs) for the Use of Green Hydrogen in Power-to-Gas Concepts.

[3] H. Abed, J. Mosrati, A. M. Abdel-Mageed, S. Cisneros, T. Huyen Vuong, N. Rockstroh, S. Bartling, S. Wohlrab, A. Brueckner, J. Rabeah, *ChemCatChem* **2022**, *14*, e202200923, Preferential CO Oxidation on a Highly Active Cu Single Atom Catalyst Supported by Ce-TiO<sub>x</sub>.

[4] H.-J. Ai, M. Beller, X.-F. Wu, *Nat. Sci. Rev.* **2022**, *9*, Palladium-catalysed efficient synthesis of primary alkyl halides from terminal and internal alkenes.

[5] H.-J. Ai, B. N. Leidecker, P. Dam, C. Kubis, J. Rabeah, X.-F. Wu, *Angew. Chem. Int. Ed.* **2022**, *61*, e202211939, Iron-Catalyzed Alkoxycarbonylation of Alkyl Bromides via a Two-Electron Transfer Process.

[6] H.-J. Ai, Y. Yuan, X.-F. Wu, *Chem. Sci.* **2022**, *13*, 2481-2486, Ruthenium pincer complex-catalyzed heterocycle compatible alkoxycarbonylation of alkyl iodides: substrate keeps the catalyst active.

[7] A. S. H. Kumar, S. K. Al-Dawery, D. S. M. Vishnu, V. N. Kalevaru, P. S. S. Prasad, *Eng. Sci.* **2022**, *20*, 209-217, Low Temperature Conversion of Ethane to Ethylene Using Zirconia Supported Molybdenum Oxide Catalysts.

[8] A. S. Al-Fatesh, S. O. Kasim, A. A. Ibrahim, A. I. Osman, A. E. Abasaeed, H. Atia, U. Armbruster, L. Frusteri, A. bin Jumah, Y. Mohammed Alanazi, A. H. Fakeeha, *Fuel* **2022**, *330*, 125523, Greenhouse gases utilization via catalytic reforming with Sc promoted Ni/ SBA-15.

[9] A. S. Al-Fatesh, R. Kumar, S. O.
Kasim, A. A. Ibrahim, A. H. Fakeeha, A.
E. Abasaeed, H. Atia, U. Armbruster,
C. Kreyenschulte, H. Lund, S. Bartling,
Y. Ahmed Mohammed, Y. A. Albaqmaa, M. S. Lanre, M. L. Chaudhary, F. Almubaddel, B. Chowdhury, *Ind. Eng. Chem. Res.* **2022**, *61*, 164-174, Effect of Cerium Promoters on an MCM-41-Supported Nickel Catalyst in Dry Reforming of Methane.

[10] L. Al-Sheakh, S. Fritsch, A. Appelhagen, A. Villinger, R. Ludwig, *Molecules* **2022**, *27*, 366, Thermodynamically Stable Cationic Dimers in Carboxyl-Functionalized Ionic Liquids: The Paradoxical Case of "Anti-Electrostatic" Hydrogen Bonding.

[11] M. Al-Yusufi, N. Steinfeldt, R. Eckelt, H. Atia, H. Lund, S. Bartling, N. Rockstroh, A. Koeckritz, *ACS Sustainable Chem. Eng.* **2022**, *10*, 4954-4968, Efficient Base Nickel-Catalyzed Hydrogenolysis of Furfural-Derived Tetrahydrofurfuryl Alcohol to 1,5-Pentanediol.

[12] K. Alkanad, A. Hezam, N. Al-Zaqri, M. A. Bajiri, G. Alnaggar, Q. A. Drmosh, H. A. Almukhlifi, L. Neratur Krishnappagowda, *ACS Omega* **2022**, 7, 38686-38699, One-Step Hydrothermal Synthesis of Anatase TiO<sub>2</sub> Nanotubes for Efficient Photocatalytic  $CO_2$ Reduction.

[13] G. Alnaggar, A. Hezam, M. A. Bajiri, Q. A. Drmosh, S. Ananda, *Chemosphere* **2022**, *303*, 134562, Sulfate radicals induced from peroxymonosulfate on electrochemically synthesized  $TiO_2$ -MoO<sub>3</sub> heterostructure with Ti-O-Mo bond charge transfer pathway for potential organic pollutant removal under solar light irradiation.

[14] E. Ammon, A. Villinger, P. Ehlers, P. Langer, *Synlett* **2022**, *33*, 1633-1636, Synthesis of Spirocyclic Diindeno[1,2-b:2',1'-d]thiophenes.

[15] T. An, C. Liu, Y. Yin, X.-F. Wu, Z. Yin, *Organometallics* **2022**, *41*, 1731-1737, Palladium-Catalyzed Denitrogenative Carbonylation of Benzotriazoles with Cr(CO)6 as the Carbonyl Source.

[16] T. Andersons, M. Sawall, K. Neymeyr, *J. Mathematical Chem.* **2022**, *60*, 1750-1780, Analytical enclosure of the set of solutions of the three-species multivariate curve resolution problem.

[17] A. Arinchtein, M.-Y. Ye, Q. Yang, C. Kreyenschulte, A. Wagner, M. Frisch, A. Brueckner, E. Kondratenko, R. Kraehnert, *ChemCatChem* **2022**, *14*, e202200240, Dynamics of Reaction-Induced Changes of Model-Type Iron Oxide Phases in the CO<sub>2</sub>-Fischer-Tropsch-Synthesis.

[18] Z. Aydin, A. Zanina, V. A. Kondratenko, J. Rabeah, J. Li, J. Chen, Y. Li, G. Jiang, H. Lund, S. Bartling, D. Linke, E. V. Kondratenko, ACS Catal. 2022, 12, 1298-1309, Effects of N<sub>2</sub>O and Water on Activity and Selectivity in the Oxidative Coupling of Methane over  $Mn-Na_2WO_4/SiO_2$ : Role of Oxygen Species.

[19] Z.-P. Bao, Y. Zhang, X.-F. Wu, J. Catal. 2022, 413, 163-167, Palladium-catalyzed four-component difluoroalkylative carbonylation of aryl olefins and ethylene.

[20] Z.-P. Bao, Y. Zhang, X.-F. Wu, *Chem. Sci.* **2022**, *13*, 9387-9391, Palladium-catalyzed difluoroalkylative carbonylation of styrenes toward difluoropentanedioates.

[21] A. Bara-Estaún, C. L. Lyall, J. P. Lowe, P. G. Pringle, P. C. J. Kamer, R. Franke, U. Hintermair, *Catal. Sci. Technol.* **2022**, *12*, 5501-5516, Mapping catalyst activation, turnover speciation and deactivation in Rh/PPh<sub>3</sub>-catalysed olefin hydroformylation.

[22] H. Beer, A. Linke, J. Bresien, G. Mlostoń, M. Celeda, A. Villinger, A. Schulz, *Inorg. Chem.* **2022**, *61*, 2031-2038, Synthesis of Bicyclic P,S-Heterocycles via the Addition of Thioketones to a Phosphorus-Centered Open-Shell Singlet Biradical.

[23] H. Beer, A. Linke, J. Bresien, A. Villinger, A. Schulz, *Inorg. Chem. Front.* **2022**, *9*, 2659-2667, A cyclic thioketone as biradical heterocy-clopentane-1,3-diyl: synthesis, structure and activation chemistry.

[24] M. Beller, M. Bender, U. T. Bornscheuer, S. Schunk, *Chem. Ing. Tech.* **2022**, *94*, 1559-1559, Catalysis – Far from Being a Mature Technology.

[25] A. Binh Ngo, T. Huyen Vuong, H. Atia, J. Weiß, J. Rabeah, U. Armbruster, A. Brueckner, *ChemCatChem* **2022**, n/a, e202200175, Role of V and W Sites in  $V_2O_5$ - $WO_3$ /TiO\_2 Catalysts and Effect of Formaldehyde during NH<sub>3</sub>-SCR of NO<sub>v</sub>.

[26] M. Blanco Ponce, M. I. Mangione, R. Hermosilla Espinosa, E. Torres Rodríguez, P. Ehlers, P. Langer, *Eur. J. Org. Chem.* **2022**, 2022, e202101306, Synthesis and Properties of Thieno[3,2-f]isoquinolines and Benzothieno[3,2-f]isoquinolines.

[27] G. Boeck, H. Christen, T. Peppel

in Genealogy and Social History: Understanding the Global Past through Family Case Studies (Ed.: E. Martone), Cambridge Scholars Publishing **2022**, pp. 289-320.

[28] A. Boerner, J. Zeidler, Chemie der Biologie, Springer Spektrum Berlin, Heidelberg, **2022**.

[29] B. Boga, N. Steinfeldt, N. G. Moustakas, T. Peppel, H. Lund, J. Rabeah, Z. Pap, V.-M. Cristea, J. Strunk, *Catalysts* **2022**, *12*, 978, Role of  $SrCO_3$ on Photocatalytic Performance of  $SrTiO_3$ -SrCO<sub>3</sub> Composites.

[30] N. F. Both, A. Spannenberg, K. Junge, M. Beller, *Organometallics* **2022**, *41*, 1797-1805, Low-Valent Molybdenum PNP Pincer Complexes as Catalysts for the Semihydrogenation of Alkynes.

[31] F. Bourriquen, J. Hervochon, R. Qu, S. Bartling, N. Rockstroh, K. Junge, C. Fischmeister, M. Beller, *Chem. Commun.* **2022**, *58*, 8842-8845, Diastereoselective hydrogenation of arenes and pyridines using supported ruthenium nanoparticles under mild conditions.

[32] F. Bourriquen, N. Rockstroh, S. Bartling, K. Junge, M. Beller, *Angew. Chem. Int. Ed.* **2022**, *61*, e202202423, Manganese-Catalysed Deuterium Labelling of Anilines and Electron-Rich (Hetero)Arenes.

[33] J. Bresien, K. Faust, A. Schulz, *Rev. Inorg. Chem.* **2022**, *42*, 1-20, Bicyclic and tricyclic phosphanes with p-block substituents.

[34] X. Cao, C. Liu, T. Zhang, Q. Xu, D. Zhang, X. Liu, H. Jiao, X. Wen, Y. Yang, Y. Li, J. W. Niemantsverdriet, J. Zhu, *J. Phys. Chem. C* **2022**, *126*, 10035-10044, Revisiting Oxygen Adsorption on Ir(100).

[35] J. H. Carter, A. M. Abdel-Mageed, D. Zhou, D. J. Morgan, X. Liu, J. Bansmann, S. Chen, R. J. Behm, G. J. Hutchings, *ACS Nano* **2022**, *16*, 15197-15205, Reversible Growth of Gold Nanoparticles in the Low-Temperature Water–Gas Shift Reaction.

[36] S. Chakrabortty, K. Konieczny, B. H. Mueller, A. Spannenberg, P. C. J. Kamer, J. G. de Vries, *Catal. Sci. Technol.* **2022**, *12*, 1392-1399, Betti base derived P-stereogenic phosphine-diamidophosphite ligands with a single atom spacer and their application in asymmetric catalysis. [37] V. G. Chandrashekhar, W. Baumann, M. Beller, R. V. Jagadeesh, *Science* **2022**, *376*, 1433-1441, Nickel-catalyzed hydrogenative coupling of nitriles and amines for general amine synthesis.

[38] V. G. Chandrashekhar, K. Natte, A. M. Alenad, A. S. Alshammari, C. Kreyenschulte, R. V. Jagadeesh, *ChemCatChem* **2022**, *14*, e202101234, Reductive Amination, Hydrogenation and Hydrodeoxygenation of 5-Hydroxymethylfurfural using Silica-supported Cobalt- Nanoparticles.

[39] V. G. Chandrashekhar, T. Senthamarai, R. G. Kadam, O. Malina, J. Kašlík, R. Zbořil, M. B. Gawande, R. V. Jagadeesh, M. Beller, *Nat. Catal.* **2022**, *5*, 20-29, Silica-supported Fe/ Fe–O nanoparticles for the catalytic hydrogenation of nitriles to amines in the presence of aluminium additives.

[40] B. Chen, C.-S. Kuai, J.-X. Xu, X.-F. Wu, *Adv. Synth. Catal.* **2022**, *364*, 487-492, Manganese(III)-Promoted Double Carbonylation of Anilines Toward  $\alpha$ -Ketoamides Synthesis.

[41] B. Chen, H. Yin, Z.-P. Bao, C.-S. Kuai, X.-F. Wu, *Org. Chem. Front.* **2022**, *9*, 5631-5636, Direct difunctional carbonylation of terminal alkynes with sodium sulfinates to access olefin sulfonyl methyl esters under metal-free conditions.

[42] B. Chen, K. Yu, X.-F. Wu, *Org. Biomol. Chem.* **2022**, *20*, 5264-5269, Visible-light-induced defluorinative carbonylative coupling of alkyl iodides with  $\alpha$ -trifluoromethyl substituted styrenes.

[43] Z. Chen, H. Junge, M. Beller, Front. Energy 2022, 16, 697-699, Amino acid promoted hydrogen battery system using Mn-pincer complex for reversible  $CO_2$  hydrogenation to formic acid.

[44] Z. Chen, X.-F. Wu, in The Chemical Transformations of C1 Compounds, **2022**, pp. 31-70.

[45] A. Cheruvathoor Poulose, G. Zoppellaro, I. Konidakis, E. Serpetzoglou, E. Stratakis, O. Tomanec, M. Beller, A. Bakandritsos, R. Zbořil, *Nat. Nanotechnol.* **2022**, *17*, 485-492, Fast and selective reduction of nitroarenes under visible light with an earth-abundant plasmonic photocatalyst.

[46] S. Cisneros, A. Abdel-Mageed, J. Mosrati, S. Bartling, N. Rockstroh, H.

Atia, H. Abed, J. Rabeah, A. Brueckner, *iScience* **2022**, *25*, 103886, Oxygen vacancies in  $Ru/TiO_2$  - drivers of low-temperature  $CO_2$  methanation assessed by multimodal operando spectroscopy.

[47] S. Cisneros, S. Chen, C. Fauth, A. M. Abdel-Mageed, S. Pollastri, J. Bansmann, L. Olivi, G. Aquilanti, H. Atia, J. Rabeah, M. Parlinska-Wojtan, A. Brueckner, R. J. Behm, *Appl. Catal. B* 2022, *317*, 121748, Controlling the selectivity of high-surface-area Ru/ TiO<sub>2</sub> catalysts in CO<sub>2</sub> reduction - modifying the reaction properties by Si doping of the support.

[48] L. Dai, A. Torche, C. Strelow, T. Kipp, T. H. Vuong, J. Rabeah, K. Oldenburg, G. Bester, A. Mews, C. Klinke, R. Lesyuk, *ACS Appl. Mater. Interf.* **2022**, *14*, 18806-18815, Role of Magnetic Coupling in Photoluminescence Kinetics of Mn<sup>2+</sup>-Doped ZnS Nanoplatelets.

[49] W. Dai, R.-G. Miao, R. Zhao, X. Qi, X.-F. Wu, Org. Chem. Front. 2022, 9, 6223-6228, Palladium-catalyzed desulfonylative aminocarbonylation of benzylsulfonyl chlorides with o-aminobenzaldehydes/o-aminoacetophenones for the synthesis of guinoin-2(1H)-ones.

[50] F. Dankert, M. Fischer, C. Hering-Junghans, *ChemRxiv* 2022, 1-25, On the ambiphilic character of phosphanylidenephosphoranes and manipulation of phosphinidenoid reactivity with Lewis acids.

[51] F. Dankert, M. Fischer, C. Hering-Junghans, *Dalton Trans.* 2022, *51*, 11267-11276, Modulating the reactivity of phosphanylidenephosphoranes towards water with Lewis acids.

[52] F. Dankert, P. Gupta, T. Wellnitz, W. Baumann, C. Hering-Junghans, *Dalton Trans.* **2022**, *51*, 18642-18651, Deoxygenation of chalcogen oxides  $EO_2$  (E = S, Se) with phospha-Wittig reagents.

[53] F. Dankert, C. Hering-Junghans, *Chem. Commun.* **2022**, *58*, 1242-1262, Heavier group 13/15 multiple bond systems: synthesis, structure and chemical bond activation.

[54] F. Dankert, J.-E. Siewert, P. Gupta, F. Weigend, C. Hering-Junghans, *Angew. Chem. Int. Ed.* **2022**, n/a, e202207064, Metal-Free N–H Bond Activation by Phospha-Wittig Reagents\*\*.

[55] R. Dasi, A. Villinger, M. Brasholz, *Org. Lett.* **2022**, *24*, 8041-8046, Photocatalytic Azetidine Synthesis by Aerobic Dehydrogenative [2 + 2] Cycloadditions of Amines with Alkenes.

[56] D. Decker, H.-J. Drexler, W. Baumann, F. Reiß, T. Beweries, *New J. Chem.* **2022**, *46*, 22314-22321, Catalytic dehydrocoupling of methylamine borane using Yamashita's [Ir(PBP)] boryl complex – characterisation of a novel highly fluxional Ir tetrahydride.

[57] D. Decker, Z. Wei, J. Rabeah, H.-J. Drexler, A. Brueckner, H. Jiao, T. Beweries, *Inorg. Chem. Front.* **2022**, *9*, 761-770, Catalytic and mechanistic studies of a highly active and E-selective Co(II) PNNH pincer catalyst system for transfer-semihydrogenation of internal alkynes.

[58] A. Dell'Acqua, C. Schünemann, E. Baráth, S. Tin, J. G. de Vries, *Chem. Commun.* **2022**, *58*, 13091-13094, New bifunctional monomers from methyl vinyl glycolate.

[59] F. G. Delolo, J. Fessler, H. Neumann, K. Junge, E. N. dos Santos, E. V. Gusevskaya, M. Beller, *Chem. Eur. J.* **2022**, *28*, e202103903, Cobalt-Catalysed Reductive Etherification Using Phosphine Oxide Promoters under Hydroformylation Conditions.

[60] F. G. Delolo, J. Fessler, H. Neumann, K. Junge, E. N. dos Santos, E. V. Gusevskaya, M. Beller, *Mol. Catal.* **2022**, *530*, 112621, Cobalt-catalyzed ring expansion/ring opening of oxetanes using phosphine oxides as promoters under hydroformylation conditions.

[61] K. Ding, X.-F. Wu, B. Han, Z. Liu, The Chemical Transformations of C1 Compounds, Volume 2, Wiley-VCH GmbH, **2022**.

[62] S. Ding, T. Dong, T. Peppel, N. Steinfeldt, J. Hu, J. Strunk, J. Colloid Interface Sci. 2022, 607, 1717-1729, Construction of amorphous SiO<sub>2</sub> modified  $\beta$ -Bi<sub>2</sub>O<sub>3</sub> porous hierarchical microspheres for photocatalytic antibiotics degradation.

[63] N. Dropka, X. Tang, G. K. Chappa, M. Holena, *Crystals* **2022**, *12*, 1764, Smart Design of Cz-Ge Crystal Growth Furnace and Process.

[64] R. Duehren, P. Kucmierczyk, R. Jackstell, R. Franke, M. Beller, *Chem. Ing. Tech.* **2022**, *94*, 1688-1694,

Palladium-Catalyzed Hydroxycarbonylation of Diisobutene: Systematic Optimization by Central Composite Design.

[65] A. Eichhorst, M. Gallhof, A. Voss, A. Sekora, L. Eggers, L. T. Huyen, C. Junghanss, H. Murua Escobar, M. Brasholz, *ChemMedChem* **2022**, *17*, e202200162, Spirooxindol-1,3-oxazine Alkaloids: Highly Potent and Selective Antitumor Agents Evolved from Iterative Structure Optimization.

[66] L. Eickhoff, L. Ohms, J. Bresien, A. Villinger, D. Michalik, A. Schulz, *Chem. Eur. J.* **2022**, *28*, e202103983, A Phosphorus-Based Pacman Dication Generated by Cooperative Self-Activation of a Pacman Phosphane.

[67] F. El Ouahabi, W. Smit, C. Angelici, M. Polyakov, U. Rodemerck, C. Fischer, V. N. Kalevaru, S. Wohlrab, S. Tin, G. P. M. van Klink, J. C. van der Waal, F. Orange, J. G. de Vries, ACS Sustainable Chem. Eng. 2022, 10, 766-775, Conversion of Biomass-Derived Methyl Levulinate to Methyl Vinyl Ketone.

[68] A. Fedorov, D. Linke, J.  $CO_2$  Utilization **2022**, 61, 102034, Data analysis of  $CO_2$  hydrogenation catalysts for hydrocarbon production.

[69] M. Feldt, Q. M. Phung, *Eur. J. Inorg. Chem.* **2022**, n/a, e202200014, Ab Initio Methods in First-Row Transition Metal Chemistry.

[70] M. T. Flynn, X. Liu, A. Dell'Acqua, J. Rabeah, A. Brueckner, E. Baráth, S. Tin, J. G. de Vries, *ChemSusChem* **2022**, n/a, e202201264, Glycolaldehyde as a Bio-Based C1 Building Block for Selective N-Formylation of Secondary Amines.

[71] M. Frahm, A. Voss, M. Brasholz, *Chem. Commun.* **2022**, *58*, 5467-5469, A short total synthesis of (±)-mersicarpine via visible light-induced cascade photooxygenation.

[72] R. Francke, in Nature (London, U. K.), Vol. 603, Nature Portfolio, **2022**, pp. 229-230.

[73] R. Francke, *Curr. Opinion Electro-chem.* **2022**, *36*, 101111, Concepts for sustainable organic electrosynthesis.

[74] R. Francke, M. Májek, in Sustainable and Functional Redox Chemistry (Ed.: S. Inagi), The Royal Society of Chemistry, **2022**, pp. 119-153.

[75] F. Gai, X. Guo, G. Ding, K. Zhang, Y. Zhang, Y. Zuo, *New J. Chem.* **2022**, 46, 10213-10218, Turn-on silicon-based fluorescent probe for visualizing endogenous CO during hypoxia.

[76] J. Gao, L. Feng, R. Ma, B.-J. Su, A. M. Alenad, Y. Liu, M. Beller, R. V. Jagadeesh, *Chem. Catal.* **2022**, *2*, 178-194, Cobalt single-atom catalysts for domino reductive amination and amidation of levulinic acid and related molecules to N-heterocycles.

[77] L. Gausas, R. Jackstell, T. Skrydstrup, M. Beller, *ACS Sustainable Chem. Eng.* **2022**, *10*, 16046-16054, Toward a Practical Catalyst for Convenient Deaminative Hydrogenation of Amides under Mild Conditions.

[78] H.-Q. Geng, R. Franke, X.-F. Wu, Org. Lett. **2022**, 24, 7993-7996, Copper-Catalyzed Synthesis of Multideuterium-Labeled Alcohols from Styrenes with CO and  $D_2$  as the Source of the Hydroxymethyl Group.

[79] H.-Q. Geng, W. Li, Y. Zhao, X.-F. Wu, *Org. Chem. Front.* **2022**, *9*, 4943-4948, Copper-catalyzed synthesis of cyclopropyl bis(boronates) from aryl olefins and carbon monoxide.

[80] H.-Q. Geng, X.-F. Wu, *Chem. Commun.* **2022**, *58*, 6534-6537, Copper-catalyzed hydroaminocarbonylation of benzylidenecyclopropanes: synthesis of  $\gamma$ , $\delta$ -unsaturated amides.

[81] S. Ghimire, K. Oldenburg, S. Bartling, R. Lesyuk, C. Klinke, ACS Energy Lett. 2022, 7, 975-983, Structural Reconstruction in Lead-Free Two-Dimensional Tin Iodide Perovskites Leading to High Quantum Yield Emission.

[82] Y. R. Girish, Udayabhanu, G. Alnaggar, A. Hezam, M. B. Nayan, G. Nagaraju, K. Byrappa, J. Sci.: Adv. Mater. Devices **2022**, 7, 100419, Facile and rapid synthesis of solar-driven  $TiO_2/g-C_3N_4$  heterostructure photocatalysts for enhanced photocatalytic activity.

[83] B. Golub, D. Ondo, R. Ludwig, D. Paschek, *J. Phys. Chem. Lett.* **2022**, *13*, 3556-3561, Why Do Liquids Mix? The Mixing of Protic Ionic Liquids Sharing the Same Cation Is Apparently Driven by Enthalpy, Not Entropy.

[84] B. Golub, D. Ondo, V. Overbeck, R. Ludwig, D. Paschek, *Phys. Chem. Chem. Phys.* **2022**, *24*, 14740-14750, Hydrogen bond redistribution effects in mixtures of protic ionic liquids sharing the same cation: non-ideal mixing with large negative mixing enthalpies.

[85] B. Guo, J. G. de Vries, E. Otten, Adv. Synth. Catal. 2022, 364, 179-186, Selective  $\alpha$ -Deuteration of Cinnamonitriles using D<sub>2</sub>O as Deuterium Source.

[86] X. Guo, F. Unglaube, U. Kragl, E. Mejía, *Chem. Commun.* **2022**, *58*, 6144-6147,  $B(C_6F_5)_3$ -Catalyzed transfer hydrogenation of esters and organic carbonates towards alcohols with ammonia borane.

[87] P. Gupta, T. Taeufer, J.-E. Siewert, F. Reiß, H.-J. Drexler, J. Pospech, T. Beweries, C. Hering-Junghans, *Inorg. Chem.* **2022**, *61*, 11639-11650, Synthesis, Coordination Chemistry, and Mechanistic Studies of P,N-Type Phosphaalkene-Based Rh(I) Complexes.

[88] Q. L. M. Ha, H. Atia, C. Kreyenschulte, H. Lund, S. Bartling, G. Lisak, S. Wohlrab, U. Armbruster, *Fuel* **2022**, *312*, 122823, Effects of modifier (Gd, Sc, La) addition on the stability of low Ni content catalyst for dry reforming of model biogas.

[89] A. Hamza, D. Moock, C. Schlepphorst, J. Schneidewind, W. Baumann, F. Glorius, *Chem. Sci.* **2022**, *13*, 985-995, Unveiling a key catalytic pocket for the ruthenium NHC-catalysed asymmetric heteroarene hydrogenation.

[90] F. He, E. Klein, S. Bartling, S. Saeidpour, B. Corzilius, R. Lesyuk, C. Klinke, *J. Phys. Chem. C* **2022**, *126*, 20498-20504, Template-Mediated Formation of Colloidal Two-Dimensional Tin Telluride Nanosheets and the Role of the Ligands.

[91] Y. He, Y. Yin, C. Liu, X.-F. Wu, Z. Yin, *New J. Chem.* **2022**, *46*, 663-667, Electrochemical oxidative cyclization of N-allylcarboxamides: efficient synthesis of halogenated oxazolines.

[92] M. Heilmann, C. Prinz, R. Bienert, R. Wendt, B. Kunkel, J. Radnik, A. Hoell, S. Wohlrab, A. Guilherme Buzanich, F. Emmerling, *Adv. Eng. Mater.* **2022**, *24*, 2101308, Size-Tunable Ni–Cu Core–Shell Nanoparticles— Structure, Composition, and Catalytic Activity for the Reverse Water–Gas Shift Reaction.

[93] A. Hezam, Q. A. Drmosh, D. Ponnamma, M. A. Bajiri, M. Qamar, K. Namratha, M. Zare, M. B. Nayan, S. A. Onaizi, K. Byrappa, *Chem. Record* **2022**, *22*, e202100299, Strategies to Enhance ZnO Photocatalyst's Performance for Water Treatment: A Comprehensive Review.

[94] D. T. Hieu, H. Kosslick, M. Riaz, A. Schulz, A. Springer, M. Frank, C. Jaeger, N. T. M. Thu, L. T. Son, *Catalysts* **2022**, 12, *253*, Acidity and Stability of Brønsted Acid Sites in Green Clinoptilolite Catalysts and Catalytic Performance in the Etherification of Glycerol.

[95] Y. Hu, R. Sang, R. Vroemans, G. Mollaert, R. Razzaq, H. Neumann, H. Junge, R. Franke, R. Jackstell, B. U. W. Maes, M. Beller, *Angew. Chem. Int. Ed.* **2022**, n/a, e202214706, Efficient Synthesis of Novel Plasticizers by Direct Palladium-Catalyzed Di- or Multi-carbonylations.

[96] W. Huang, X. Tian, H. Jiao, R. Jackstell, M. Beller, *Chem. Eur. J.* **2022**, *28*, e202104012, Iridium-Catalyzed Domino Hydroformylation/Hydrogenation of Olefins to Alcohols: Synergy of Two Ligands.

[97] M. Huettenschmidt, H. Lange, M. A. A. Cordero, A. Villinger, S. Lochbrunner, W. W. Seidel, *Dalton Trans.* **2022**, *51*, 852-856, Development and application of redox-active cyclometallating ligands based on W(ii) alkyne complexes.

[98] L. Hunger, L. Al-Sheakh, D. H. Zaitsau, S. P. Verevkin, A. Appelhagen, A. Villinger, R. Ludwig, *Chem. Eur. J.* **2022**, *28*, e202200949, Dissecting Noncovalent Interactions in Carboxyl-Functionalized Ionic Liquids Exhibiting Double and Single Hydrogens Bonds Between Ions of Like Charge.

[99] Y.-W. Huo, X. Qi, X.-F. Wu, Org. Lett. **2022**, 24, 4009-4013, Nickel-Catalyzed Carbonylative Synthesis of  $\alpha$ , $\beta$ -Unsaturated Thioesters from Vinyl Triflates and Arylsulfonyl Chlorides.

[100] N. Jannsen, C. Fischer, C. Selle, C. Pribbenow, H.-J. Drexler, F. Reiß, T. Beweries, D. Heller, *Dalton Trans*. **2022**, *51*, 18068-18076, How solvents affect the stability of cationic Rh(i) diphosphine complexes: a case study of MeCN coordination.

[101] J. Jašík, S. Valtera, M. Vaidulych, M. Bunian, Y. Lei, A. Halder, H. Tarábková, M. Jindra, L. Kavan, O. Frank, S. Bartling, Š. Vajda, *Faraday Disc.* **2022**, Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer Cu4-nPdn ( $0 \le n \le 4$ ) tetramer clusters: the effect of cluster composition and support on performance.

[102] Y. Jin, H. Yang, X. Yu, P. Ren, Y. Yang, H. Xiang, Y.-W. Li, H. Jiao, X. Wen, J. Phys. Chem. C 2022, 126, 6241-6248, Unraveling the Synergetic Effect of the FeO<sub>x</sub>–Cu Model System in Catalyzing the Water–Gas Shift Reaction.

[103] M. N. Jorabchi, M. Abbaspour, E. K. Goharshadi, S. Wohlrab, *J. Mol. Liq.* **2022**, *360*, 119447, Ag, Au, Pt, and Au-Pt nanoclusters in  $[N_{1114}]$  $[C_1SO_3]$  ionic liquid: A molecular dynamics study.

[104] S. K. Kaiser, E. Fako, I. Surin, F. Krumeich, V. A. Kondratenko, E. V. Kondratenko, A. H. Clark, N. López, J. Pérez-Ramírez, *Nat. Nanotechnol.* **2022**, *17*, 606-612, Performance descriptors of nanostructured metal catalysts for acetylene hydrochlorination.

[105] S. Keller, U. Bentrup, J. Rabeah, A. Brueckner, J. Catal. 2022, 408, 453-464, Impact of dopants on catalysts containing Ce<sub>1-x</sub> $M_xO_{2-\delta}$  (M = Fe, Sb or Bi) in NH<sub>3</sub>-SCR of NO<sub>x</sub> – A multiple spectroscopic approach.

[106] A. E. Khudozhitkov, M. Donoshita, A. G. Stepanov, F. Philippi, D. Rauber, R. Hempelmann, H. Kitagawa, D. I. Kolokolov, R. Ludwig, *Chem. Eur. J.* **2022**, *28*, e202200257, High-Temperature Quantum Tunneling and Hydrogen Bonding Rearrangements Characterize the Solid-Solid Phase Transitions in a Phosphonium-Based Protic Ionic Liguid.

[107] A. E. Khudozhitkov, P. Stange, D. Paschek, A. G. Stepanov, D. I. Kolokolov, R. Ludwig, *ChemPhysChem* **2022**, *23*, e202200557, The Influence of Deuterium Isotope Effects on Structural Rearrangements, Ensemble Equilibria, and Hydrogen Bonding in Protic Ionic Liquids.

[108] A. E. Khudozhitkov, P. Stange, A. G. Stepanov, D. I. Kolokolov, R. Ludwig, *Phys. Chem. Chem. Phys.* **2022**, *24*, 6064-6071, Structure, hydrogen bond dynamics and phase transition in a model ionic liquid electrolyte.

[109] S. Kopf, F. Bourriquen, W. Li, H. Neumann, K. Junge, M. Beller, *Chem. Rev.* **2022**, *122*, 6634-6718, Recent Developments for the Deuterium and Tritium Labeling of Organic Molecu-

#### les.

[110] S. Kopf, J. Liu, R. Franke, H. Jiao, H. Neumann, M. Beller, *Eur. J. Org. Chem.* **2022**, *2022*, e202200204, Base-Mediated Remote Deuteration of N-Heteroarenes – Broad Scope and Mechanism.

[111] L. Korel, A. S. Behr, N. Kockmann, M. Holeňa, **2022**, Using Artificial Neural Networks to Determine Ontologies Most Relevant to Scientific Texts.

[112] B. Kortewille, O. Pfingsten, G. Bacher, J. Strunk, *ChemPhotoChem* **2022**, *6*, e202100120, Supported Vanadium Oxide as a Photocatalyst in the Liquid Phase: Dissolution Studies and Selective Laser Excitation.

[113] E. F. Krake, H. Jiao, W. Baumann, J. Mol. Struct. 2022, 1247, 131309, NMR and DFT analysis of the major diastereomeric degradation product of clopidogrel under oxidative stress conditions.

[114] C.-S. Kuai, L.-C. Wang, J.-X. Xu, X.-F. Wu, *Org. Lett.* **2022**, *24*, 451-456, Palladium-Catalyzed Direct Dicarbonylation of Amines with Ethylene to Imides.

[115] C.-S. Kuai, J.-X. Xu, B. Chen, X.-F. Wu, *Org. Lett.* **2022**, *24*, 4464-4469, Palladium-Catalyzed Regio- and Stereoselective Hydroaminocarbonylation of Unsymmetrical Internal Alkynes toward  $\alpha$ , $\beta$ -Unsaturated Amides.

[116] P. Kucmierczyk, S. Behrens, C. Kubis, W. Baumann, Z. Wei, H. Jiao, K. Dong, A. Spannenberg, H. Neumann, R. Jackstell, A. Boerner, R. Franke, M. Beller, *Catal. Sci. Technol.* **2022**, *12*, 3175-3189, (*In situ*) spectroscopic studies on state-of-the-art Pd(II) catalysts in solution for the alkoxycarbonylation of alkenes.

[117] P. Kucmierczyk, R. Duehren, R. Sang, R. Jackstell, M. Beller, R. Franke, *ACS Sustainable Chem. Eng.* **2022**, *10*, 4822-4830, Palladium-Catalyzed Methoxycarbonylation Investigated by Design of Experiments.

[118] A. Kutuzova, T. Dontsova, W. Kwapinski, J. J. Leahy, J. Strunk, *Mol. Crystals Liq. Crystals* **2022**, 1-13, Photocatalytic activity to ciprofloxacin and physico-chemical properties of  $TiO_2$  synthesized by different methods.

[119] T. Lange, S. Reichenberger, S. Ristig, M. Rohe, J. Strunk, S. Barcikow-

ski, R. Schloegl, Progress in Mater. Sci. 2022, 124, 100865, Zinc sulfide for photocatalysis: White angel or black sheep?

[120] P. Langer, *Synlett* **2022**, *33*, 207-223, Domino Reactions of Chromones with Heterocyclic Enamines.

[121] P. Langer, *Synlett* **2022**, *33*, 440-457, Synthesis of Purines and Related Molecules by Cyclization Reactions of Heterocyclic Enamines.

[122] P. Langer, *Synlett* **2022**, *33*, 728-736, Adventures in 1,3-Selenazole Chemistry.

[123] P. Langer, *Synlett* **2022**, *33*, 1029-1051, Cross-Coupling Reactions of Polyhalogenated Heterocycles.

[124] P. Langer, *Synlett* **2022**, *33*, 1215-1226, Palladium-Catalyzed Synthesis of Heterocyclic Ring Systems by Combination of Regioselective C–C with Twofold C–N Couplings.

[125] P. Langer, *Synlett* **2022**, *33*, 1707-1715, Synthesis of Nitrogen Heterocycles by a C–C Cross-Coupling/ Cycloisomerization Strategy.

[126] P. Langer, *Synlett* **2022**, *33*, 1596-1606, Synthesis of Nitrogen Heterocycles by Domino C–N Coupling/ Hydroamination Reactions.

[127] D. K. Leonard, P. Ryabchuk, M. Anwar, S. Dastgir, K. Junge, M. Beller, *ChemSusChem* **2022**, *15*, e202102315, A Convenient and Stable Heterogeneous Nickel Catalyst for Hydrodehalogenation of Aryl Halides Using Molecular Hydrogen.

[128] C.-L. Li, X.-F. Wu, in The Chemical Transformations of C1 Compounds, **2022**, pp. 1647-1665.

[129] W. Li, J. Rabeah, F. Bourriquen, D. Yang, C. Kreyenschulte, N. Rockstroh, H. Lund, S. Bartling, A.-E. Surkus, K. Junge, A. Brueckner, A. Lei, M. Beller, *Nat. Chem.* **2022**, Scalable and selective deuteration of (hetero) arenes.

[130] W. Li, X.-F. Wu, in The Chemical Transformations of C1 Compounds, **2022**, pp. 157-247.

[131] Y. Li, X. Yu, Q. Zhang, V. A. Kondratenko, Y. Wang, G. Cui, M. Zhou, C. Xu, E. V. Kondratenko, G. Jiang, *J. Catal.* **2022**, *413*, 658-667, The nature of  $VO_x$  structures in HMS supported vanadium catalysts for non-oxidative propane dehydrogenation.

[132] H.-Q. Liang, T. Beweries, R. Francke, M. Beller, *Angew. Chem. Int. Ed.* **2022**, *61*, e202200723, Molecular Catalysts for the Reductive Homocoupling of  $CO_2$  towards  $C_{2+}$  Compounds.

[133] K. Lindenau, A. Spannenberg, F. Reiß, T. Beweries, *RSC Adv.* **2022**, *12*, 26277-26283, Mono- and dinuclear zirconocene(IV) amide complexes for the catalytic dehydropolymerisation of phenylsilane.

[134] A. Linke, D. Decker, H.-J. Drexler, T. Beweries, *Dalton Trans*. **2022**, *51*, 10266-10271, Iridium(III) bis(thiophosphinite) pincer complexes: synthesis, ligand activation and applications in catalysis.

[135] J.-L. Liu, W. Wang, X. Qi, X.-F. Wu, *Org. Lett.* **2022**, *24*, 2248-2252, Palladium-Catalyzed Reductive Aminocarbonylation of o-lodophenol-Derived Allyl Ethers with o-Nitrobenzaldehydes to 3-Alkenylquinolin-2(1H)-ones.

[136] X. Liu, Y. Zuo, F. Kallmeier, E. Mejía, S. Tin, J. G. de Vries, E. Baráth, *Chem. Commun.* **2022**, *58*, 5415-5418, Hydrogenative depolymerization of silicon-modified polyureas.

[137] Y. Liu, Z.-P. Bao, X. Qi, X. F. Wu, *Org. Chem. Front.* **2022**, *9*, 2079-2083, Palladium-catalyzed reductive desulfonative aminocarbonylation of benzylsulfonyl chlorides with nitroarenes towards arylacetamides.

[138] F. Lorenz, N. G. Moustakas, T. Peppel, J. Strunk, *Chem. Ing. Tech.* **2022**, *94*, 1776-1783, Comparative Studies of Oxygen-Free Semiconductors in Photocatalytic  $CO_2$  Reduction and Alcohol Degradation.

[139] S.-N. Lu, Y. Sun, J. Zhang, Z. Chen, X.-F. Wu, Mol. Catal. 2022, 524, 112336, Metal-free Synthesis of 5-Trifluoromethyl-1,2,4-triazoles via elemental sulfur promoted oxidative cyclization of trifluoroacetimidohydrazides with benzylic and aliphatic amines.

[140] S.-N. Lu, J. Zhang, J. Li, Z. Chen, X. F. Wu, Green Synth. Catal. 2022, 3, 385-388, Metal-free synthesis of 3-trifluoromethyl-1,2,4-triazoles via oxidative cyclization of trifluoroacetimidohydrazides with N,N-dimethylformamide as carbon synthons.

[141] Z. Ma, V. G. Chandrashekhar, B. Zhou, A. M. Alenad, N. Rockstroh, S. Bartling, M. Beller, R. V. Jagadeesh, *Chem. Sci.* **2022**, *13*, 10914-10922, Stable and reusable Ni-based nanoparticles for general and selective hydrogenation of nitriles to amines.

[142] Z. Ma, B. Zhou, X. Li, R. G. Kadam, M. B. Gawande, M. Petr, R. Zbořil, M. Beller, R. V. Jagadeesh, *Chem. Sci.* **2022**, *13*, 111-117, Reusable Co-nanoparticles for general and selective N-alkylation of amines and ammonia with alcohols.

[143] M. S. Macedo, E. Kraleva, H. Ehrich, M. A. Soria, L. M. Madeira, *Int. J. Hydrogen Energy* **2022**, *47*, 33239-33258, Hydrogen production from glycerol steam reforming over Co-based catalysts supported on  $La_2O_3$ , AlZnO<sub>x</sub> and AlLaO<sub>x</sub>.

[144] S. A. Mahyoub, F. A. Qaraah, S. Yan, A. Hezam, C. Chen, J. Zhong, Z. Cheng, J.  $CO_2$  Utilization 2022, 61, 102033, 3D Cu/In nanocones by morphological and interface engineering design in achieving a high current density for electroreduction of  $CO_2$  to syngas under elevated pressure.

[145] S. A. Mahyoub, F. A. Qaraah, S. Yan, A. Hezam, J. Zhong, Z. Cheng, *Mater. Today Energy* **2022**, *24*, 100923, Rational design of low loading Pd-alloyed Ag nanocorals for high current density  $CO_2$ -to-CO electroreduction at elevated pressure.

[146] S. Mao, S. Budweg, A. Spannenberg, X. Wen, Y. Yang, Y.-W. Li, K. Junge, M. Beller, *ChemCatChem* **2022**, *14*, e202101668, Iron-Catalyzed Epoxidation of Linear α-Olefins with Hydrogen Peroxide.

[147] S. Mao, P. Ryabchuk, S. Dastgir, M. Anwar, K. Junge, M. Beller, *ACS Appl. Nano Mater.* **2022**, *5*, 5625-5630, Silicon-Enriched Nickel Nanoparticles for Hydrogenation of N-Heterocycles in Aqueous Media.

[148] I. C. B. Martins, D. Al-Sabbagh, U. Bentrup, J. Marquardt, T. Schmid, E. Scoppola, W. Kraus, T. M. Stawski, A. Guilherme Buzanich, K. V. Yusenko, S. Weidner, F. Emmerling, *Chem. Eur. J.* **2022**, *28*, e202200079, Formation Mechanism of a Nano-Ring of Bismuth Cations and Mono-Lacunary Keggin-Type Phosphomolybdate.

[149] M. Marx, H. Frauendorf, A. Spannenberg, H. Neumann, M. Beller, JACS Au 2022, 2, 731-744, Revisiting Reduction of  $CO_2$  to Oxalate with First-Row Transition Metals: Irrepro-

ducibility, Ambiguous Analysis, and Conflicting Reactivity.

[150] P. McNeice, M.-A. Mueller, J. Medlock, W. Bonrath, N. Rockstroh, S. Bartling, H. Lund, K. Junge, M. Beller, *ACS Sustainable Chem. Eng.* **2022**, *10*, 9787-9797, Designing a Green Replacement for the Lindlar Catalyst for Alkyne Semi-hydrogenation Using Silica-Supported Nickel Nanoparticles Modified by N-Doped Carbon.

[151] P. McNeice, M.-A. Mueller, J. Medlock, W. Bonrath, N. Rockstroh, S. Bartling, H. Lund, K. Junge, M. Beller, *Green Chem.* **2022**, *24*, 6912-6922, The development of a lead-free replacement for the Lindlar catalyst for alkyne semi-hydrogenation using silica supported, N-doped carbon modified cobalt nanoparticles.

[152] D. Meinhardt, H. Schröder, J. Hellwig, E. Steimers, A. Friebel, T. Beweries, M. Sawall, E. von Harbou, K. Neymeyr, *J. Magn. Res.* **2022**, *339*, 107212, Model-based signal tracking in the quantitative analysis of time series of NMR spectra.

[153] K. Melin, J. O. Strueven, P. Eidam, J. Appelt, C. Hummel, U. Armbruster, Y. Chapellière, C. Mirodatos, Y. Schuurman, A. Oasmaa, *Energy & Fuels* **2022**, *36*, 12004-12009, Hybrid Gasoline Production from Black Liquor through Coprocessing.

[154] M. J. Menke, A. S. Behr, K. Rosenthal, D. Linke, N. Kockmann, U. T. Bornscheuer, M. Doerr, *Chem. Ing. Tech.* **2022**, *94*, 1827-1835, Development of an Ontology for Biocatalysis.

[155] D. Michalik, H. Jiao, P. Langer, *Mag. Reason. Chem.* **2022**, *60*, 845-856, NMR spectroscopic and theoretical study on the isomerism of dimethyl benzodiazepine(diylidene) diacetates.

[156] J. Michalke, K. Faust, T. Boegl, S. Bartling, N. Rockstroh, C. Topf, *Int. J. Mol. Sci.* **2022**, *23*, 8742, Mild and Efficient Heterogeneous Hydrogenation of Nitroarenes Facilitated by a Pyrolytically Activated Dinuclear Ni(II)-Ce(III) Diimine Complex.

[157] J. Michalke, M. Haas, D. Krisch, T. Boegl, S. Bartling, N. Rockstroh, W. Schoefberger, C. Topf, *Catalysts* **2022**, *12*, 11, Generation of Cobalt-Containing Nanoparticles on Carbon via Pyrolysis of a Cobalt Corrole and Its Application in the Hydrogenation of Nitroarenes. [158] L. Milaković, Y. Liu, E. Baráth, J. A. Lercher, *Catal. Sci. Technol.* **2022**, *12*, 6084-6091, Dehydration of fatty alcohols on zirconia supported tungstate catalysts.

[159] A. Moazezbarabadi, D. Wei, H. Junge, M. Beller, *ChemSusChem* **2022**, *15*, e202201502, Improved CO<sub>2</sub> Capture and Catalytic Hydrogenation Using Amino Acid Based Ionic Liquids.

[160] N. Mohebbati, I. Sokolovs, P. Woite, M. Lõkov, E. Parman, M. Ugandi, I. Leito, M. Roemelt, E. Suna, R. Francke, *Chem. Eur. J.* **2022**, n/a, e202200974, Electrochemistry and Reactivity of Chelation-stabilized Hypervalent Bromine(III) Compounds.

[161] P. Naliwajko, T. Peppel, J. Strunk, *Reac. Kinetics, Mechan. Catal.* **2022**, *135*, 2291-2305, Thermal and light induced infrared blackening of ZnO revisited: rediscovery of fundamental scientific knowledge.

[162] E. G. Narváez-Ordoñez, K. A. Pabón-Carcelén, D. A. Zurita-Saltos, P. M. Bonilla-Valladares, T. G. Yánez-Darquea, L. A. Ramos-Guerrero, S. E. Ulic, J. L. Jios, G. A. Echeverría, O. E. Piro, P. Langer, C. D. Alcívar-León, J. Heredia-Moya, *Molecules* **2022**, *27*, 2636, Synthesis, Experimental and Theoretical Study of Azidochromones.

[163] K. Natte, R. V. Jagadeesh, in Surface Modified Nanomaterials for Applications in Catalysis (Eds.: M. B. Gawande, C. Mustansar Hussain, Y. Yamauchi), *Elsevier*, **2022**, pp. 251-266.

[164] H. Neumann, R. Jackstell, in Encyclopedia of Reagents for Organic Synthesis, **2022**, pp. 1-4.

[165] T. A. Nguyen Tien, M. Miliutina, J. Radolko, R. Thom, T. T. Dang, P. Ehlers, P. Langer, *Tetrahedron* **2022**, *104*, 132608, Synthesis of chromeno[2,3-c] pyrrol-9(2H)-ones by domino Michael-Claisen-SNAr reactions of amino acid esters with 2-chlorophenylpropynones.

[166] S. Nieß, U. Armbruster, S. Dietrich, M. Klemm, *Catalysts* **2022**, *12*, 374, Recent Advances in Catalysis for Methanation of CO<sub>2</sub> from Biogas.

[167] A. C. Olivieri, K. Neymeyr, M. Sawall, R. Tauler, *Chemom. Intell. Lab. Syst.* **2022**, *220*, 104472, How noise affects the band boundaries in multivariate curve resolution.

[168] A. C. Olivieri, M. Sawall, K. Neymeyr, R. Tauler, *Chemom. Intell. Lab. Syst.* **2022**, *228*, 104636, Noise effects on band boundaries in multivariate curve resolution of three-component systems.

[169] N. Ortner, H. Lund, U. Armbruster, S. Wohlrab, E. V. Kondratenko, *Catal. Today* **2022**, *387*, 47-53, Factors affecting primary and secondary pathways in CO<sub>2</sub> hydrogenation to methanol over CuZnIn/MZrO<sub>x</sub> (La, Ti or Y).

[170] A. G. Oshchepkov, P. A. Simonov, A. N. Kuznetsov, S. A. Shermukhamedov, R. R. Nazmutdinov, R. I. Kvon, V. I. Zaikovskii, T. Y. Kardash, E. A. Fedorova, O. V. Cherstiouk, A. Bonnefont, E. R. Savinova, *ACS Catal.* **2022**, *12*, 15341-15351, Bimetallic NiM/C (M = Cu and Mo) Catalysts for the Hydrogen Oxidation Reaction: Deciphering the Role of Unintentional Surface Oxides in the Activity Enhancement.

[171] J. Oswald, M. T. Scharnhölz, P. Coburger, H. Beer, J. Bresien, A. Schulz, H. Gruetzmacher, *Zeitschr. f. anorg. und allgem. Chem.* **2022**, *648*, e202200093, Insertion of Ruthenium into an inorganic, cyclic biradicaloid.

[172] T. Otroshchenko, Q. Zhang, E. V. Kondratenko, *Catal. Lett.* **2022**, *152*, 2366-2374, Room-Temperature Metathesis of Ethylene with 2-Butene to Propene Over MoO<sub>x</sub>-Based Catalysts: Mixed Oxides as Perspective Support Materials.

[173] S. Pantoom, L. Hules, C. Schoell, A. Petrosyan, M. Monticelli, J. Pospech, M. V. Cubellis, A. Hermann, J. Lukas, *Int. J. Mol. Sci.* **2022**, *23*, 3536, Mechanistic Insight into the Mode of Action of Acid  $\beta$ -Glucosidase Enhancer Ambroxol.

[174] J.-B. Peng, X.-L. Liu, L. Li, X.-F. Wu, *Sci. China Chem.* **2022**, Palladium-catalyzed enantioselective carbonylation reactions.

[175] M. Peng, L. Wang, L. Guo, J. Guo, L. Zheng, F. Yang, Z. Ma, X. Zhao, *Coatings* **2022**, *12*, 1397, A Durable Nano-SiO<sub>2</sub>-TiO<sub>2</sub>/Dodecyltrimethoxy-silane Superhydrophobic Coating for Stone Protection.

[176] A. Petrosyan, L. Zach, T. Taeufer, T. S. Mayer, J. Rabeah, J. Pospech, *Chem. Eur. J.* **2022**, *28*, e202201761, Pyrimidopteridine-catalyzed Photo-mediated Hydroacetoxylation. [177] F. Poovan, V. G. Chandrashekhar, K. Natte, R. V. Jagadeesh, *Catal. Sci. Technol.* **2022**, *12*, 6623-6649, Synergy between homogeneous and heterogeneous catalysis.

[178] J. Pospech, in *Nachr. Chem.*, Vol. 70, **2022**, pp. 76-80.

[179] J. Pospech, T. S. Mayer, in *Nachr. Chem.*, Vol. 70, **2022**, pp. 81-85.

[180] R. Puchta, S. Đorđević, S. Radenković, H. Jiao, N. Van Eikema Hommes, *J. Serbian Chem. Soc.* **2022**, *87*, 1439-1446, 25 years of NICS – much more than nothing! Letter to the Editor.

[181] F. A. Qaraah, S. A. Mahyoub, A. Hezam, A. Qaraah, Q. A. Drmosh, G. Xiu, *Chinese J. Catal.* **2022**, *43*, 2637-2651, Construction of 3D flowers-like O-doped  $g-C_3N_4$ -[N-doped Nb<sub>2</sub>O<sub>5</sub>/C] heterostructure with direct S-scheme charge transport and highly improved visible-light-driven photocatalytic efficiency.

[182] F. A. Qaraah, S. A. Mahyoub, A. Hezam, A. Qaraah, F. Xin, G. Xiu, *Appl. Catal. B* **2022**, *315*, 121585, Syner-gistic effect of hierarchical structure and S-scheme heterojunction over O-doped  $g-C_3N_4/N$ -doped  $Nb_2O_5$  for highly efficient photocatalytic  $CO_2$  reduction.

[183] F. Reiß, A. Villinger, H. Brand, W. Baumann, D. Hollmann, A. Schulz, *Chem. Eur. J.* **2022**, *28*, e202200854, Low-Temperature Isolation of a Labile Silylated Hydrazinium-yl Radical Cation, [(Me<sub>3</sub>Si)<sub>2</sub>N–N(H)SiMe<sub>3</sub>]<sup>+</sup>.

[184] C. Ren, A. Spannenberg, T. Werner, *Asian J. Org. Chem.* **2022**, *11*, e202200156, Synthesis of Bifunctional Phosphonium Salts Bearing Perfluorinated Side Chains and Their Application in the Synthesis of Cyclic Carbonates from Epoxides and CO<sub>2</sub>.

[185] C. Rieg, D. Dittmann, Z. Li, A. Kurtz, E. Kaya, S. Peters, B. Kunkel, M. Parlinska-Wojtan, S. Wohlrab, A. M. Abdel-Mageed, M. Dyballa, *J. Phys. Chem. C* 2022, *126*, 13213-13223, Introducing a Novel Method for Probing Accessibility, Local Environment, and Spatial Distribution of Oxidative Sites on Solid Catalysts Using Trimethylphosphine.

[186] M. A. Rodriguez-Olguin, H. Atia, M. Bosco, A. Aguirre, R. Eckelt, E. D. Asuquo, M. Vandichel, J. G. E. Gardeniers, A. Susarrey-Arce, *J. Catal.* **2022**, *405*, 520-533, Al<sub>2</sub>O, nanofibers prepared from aluminum Di(sec-butoxide)acetoacetic ester chelate exhibits high surface area and acidity.

[187] M. A. Rodriguez-Olguin, R. N. Cruz-Herbert, H. Atia, M. Bosco, E. L. Fornero, R. Eckelt, D. A. De Haro Del Río, A. Aguirre, J. G. E. Gardeniers, A. Susarrey-Arce, *Catal. Sci. Technol.* **2022**, *12*, 4243-4254, Tuning the catalytic acidity in  $Al_2O_3$  nanofibers with mordenite nanocrystals for dehydration reactions.

[188] J. Rosenboom, L. Chojetzki, T. Suhrbier, J. Rabeah, A. Villinger, R. Wustrack, J. Bresien, A. Schulz, *Chem. Eur. J.* **2022**, *28*, e202200624, Radical Reactivity of the Biradical [ $P(\mu$ -NTer)<sub>2</sub>P ·] and Isolation of a Persistent Phosphorus-Cantered Monoradical [ $P(\mu$ -NTer)<sub>2</sub>P-Et].

[189] J. Rosenboom, A. Villinger, A. Schulz, J. Bresien, *Dalton Trans.* **2022**, *51*, 13479-13487, Concerted addition of aldehydes to the singlet biradical  $[P(\mu-NTer)]_{n}$ .

[190] U. Rosenthal, *Organometallics* **2022**, *41*, 3478-3492, How Serendipity and Chance Can Be Transformed into Knowledge: Examples from 50 Years of Research in Organometallic Chemistry and Homogeneous Catalysis.

[191] U. Rosenthal, A. Schulz, *Eur. J. Inorg. Chem.* **2022**, *2022*, e202100749, Contributions of Erhard Kurras to Organochromium Chemistry – From a Historical Perspective.

[192] J. Rothe, J. Bresien, F. Reiß, A. Villinger, T. Beweries, A. Schulz, *Zeitschr. anorg. allgem. Chem.* **2022**, n/a, e202200174, A 2-Aza-3,4-Diphospha-1-Bora-Butadiene.

[193] I. Salahshoori, M. Namayandeh Jorabchi, K. Valizadeh, A. Yazdanbakhsh, A. Bateni, S. Wohlrab, *J. Mol. Liq.* **2022**, *363*, 119793, A deep insight of solubility behavior, mechanical quantum, thermodynamic, and mechanical properties of Pebax-1657 polymer blends with various types of vinyl polymers: A mechanical quantum and molecular dynamics simulation study.

[194] E. Salaya-Gerónimo, D. S. García-Zaleta, G. Jácome-Acatitla, E. Huerta-García, R. López-González, A. Reyes-Montero, A. M. Abdel-Mageed, J. Chem. Technol. Biotechnol. 2022, 97, 2970-2983, Structural, optical and photocatalytic properties of Sr-doped and Ca-doped BiFeO<sub>3</sub> compounds prepared by Pechini method.

[195] R. Sang, Y. Hu, R. Razzaq, G. Mollaert, H. Atia, U. Bentrup, M. Sharif, H. Neumann, H. Junge, R. Jackstell, B. U. W. Maes, M. Beller, *Nat. Commun.* **2022**, *13*, 4432, A practical concept for catalytic carbonylations using carbon dioxide.

[196] S. Sarfaraz, M. Yar, M. Ans, M. A. Gilani, R. Ludwig, M. A. Hashmi, M. Hussain, S. Muhammad, K. Ayub, *RSC Adv.* **2022**, *12*, 3909-3923, Computational investigation of a covalent triazine framework (CTF-0) as an efficient electrochemical sensor.

[197] N. Sarki, V. Goyal, A. Narani, R. V. Jagadeesh, K. Natte, in Biomass, Biofuels, Biochemicals (Eds.: H. Li, S. Saravanamurugan, A. Pandey, S. Elumalai), Elsevier, **2022**, pp. 593-612.

[198] M. Sawall, T. Andersons, H. Abdollahi, S. K. Karimvand, B. Hemmateenejad, K. Neymeyr, *Chemom. Intell. Lab. Sys.* **2022**, *226*, 104577, Calculation of lower and upper band boundaries for the feasible solutions of rank-deficient multivariate curve resolution problems.

[199] M. Sawall, C. Ruckebusch, M. Beese, R. Francke, A. Prudlik, K. Neymeyr, *Anal. Chim. Acta* **2022**, *1233*, 340448, An active constraint approach to identify essential spectral information in noisy data.

[200] D. Schallenberg, N. Pardemann, A. Villinger, W. W. Seidel, *Dalton Trans.* **2022**, *51*, 13681-13691, Synthesis and coordination behaviour of 1H-1,2,3-triazole-4,5-dithiolates.

[201] S. Schimmler, T. Bönisch, M. Horsch, T. Petrenko, B. Schembera, V. Kushnarenko, B. Wentzel, F. Kirstein, H. Viemann, M. Holeňa, D. Linke, **2022**, NFDI4Cat: Local and overarching data infrastructures.

[202] J. Schneidewind, *Adv. Energy Mater.* **2022**, *12*, 2200342, How Much Technological Progress is Needed to Make Solar Hydrogen Cost-Competitive?

[203] M. Schroeder, D. Rauber, C. Matt, C. W. M. Kay, *Appl. Mag. Reson.* **2022**, *53*, 1043-1052, Pentacene in 1,3,5-Tri(1-naphtyl)benzene: A Novel Standard for Transient EPR Spectroscopy at Room Temperature.

[204] R. Schwarz, E. R. D. Seiler, S. Sender, A. Pews-Davtyan, H. Murua

Escobar, D. Zechner, M. Beller, C. Junghanß, B. Hinz, *Molecules* **2022**, *27*, 974, A Simple LC-MS/MS Method for the Quantification of PDA-66 in Human Plasma.

[205] M. Schwarze, T. A. Thiel, A. G. Rana, J. Yang, A. Acharjya, A. D. Nguyen, S. Tameu Djoko, E. M. Kutorglo, M. Tasbihi, M. Minceva, S. Huseyinova, P. Menezes, C. Walter, M. Driess, R. Schomäcker, A. Thomas, *Chem. Ing. Tech.* **2022**, *94*, 1739-1746, Screening of Heterogeneous Photocatalysts for Water Splitting.

[206] T. Senthamarai, V. G. Chandrashekhar, N. Rockstroh, J. Rabeah, S. Bartling, R. V. Jagadeesh, M. Beller, *Chem* **2022**, *8*, 508-531, A "universal" catalyst for aerobic oxidations to synthesize (hetero)aromatic aldehydes, ketones, esters, acids, nitriles, and amides.

[207] T. Senthamarai, F. Poovan, A. M. Alenad, N. Rockstroh, J. Rabeah, S. Bartling, E. Baráth, K. Natte, R. V. Jagadeesh, *Adv. Sustainable Sys.* **2022**, n/a, 2200263, Cu-Oxide Nanoparticles Catalyzed Synthesis of Nitriles and Amides from Alcohols and Ammonia in Presence of Air.

[208] I. Y. Shchapin, A. I. Nekhaev, D. N. Ramazanov, M. Al-Yusufi, V. O. Samoilov, A. L. Maximov, *Catalysts* **2022**, *12*, 409, Hydrocarbon Oxidation Depth:  $H_2O_2/Cu_2Cl_4 \cdot 2DMG/CH_3CN$ System.

[209] H. Shen, M. Yang, L. Hao, J. Wang, J. Strunk, Z. Sun, *Nano Research* **2022**, *15*, 2773-2809, Photocatalytic nitrogen reduction to ammonia: Insights into the role of defect engineering in photocatalysts.

[210] G. Sieg, M. Fischer, F. Dankert, J.-E. Siewert, C. Hering-Junghans, C. G. Werncke, *Chem. Commun.* **2022**, *58*, 9786-9789, A diarsene radical anion.

[211] A. S. Skrypnik, S. A. Petrov, V. A. Kondratenko, Q. Yang, H. Lund, A. A. Matvienko, E. V. Kondratenko, *ACS Catal.* **2022**, *12*, 11355-11368, Descriptors Affecting Methane Selectivity in CO<sub>2</sub> Hydrogenation over Unpromoted Bulk Iron(III)-Based Catalysts.

[212] M. Sobhani, R. M. Figueira de Abreu, A. Villinger, P. Ehlers, P. Langer, Org. Biomol. Chem. 2022, 20, 9207-9216, Synthesis of imidazo[1,2-a]benzoazepines by alkyne-carbonyl-metathesis. [213] M. Sobhani, A. Villinger, P. Ehlers, P. Langer, J. Org. Chem. 2022, 87, 4560-4568, Regioselective Synthesis of Naphthothiophenes by Pd Catalyzed Cross-Coupling Reactions and Alkyne-Carbonyl Metathesis.

[214] Y. Song, Y. Zhang, Z. Chen, X.-F. Wu, *Asian J. Org. Chem.* **2022**, *11*, e202200237, Recent Advances in Copper-Catalyzed Carboxylation Reactions with CO<sub>2</sub>.

[215] A. A. Sosa, V. Palermo, P. Langer, R. Luque, G. P. Romanelli, L. R. Pizzio, *Mol. Catal.* **2022**, *517*, 112046, Tungstophosphoric acid/mesoporous silicas as suitable catalysts in quinoxaline synthesis.

[216] B. Spiegelberg, H. Jiao, R. Grauke, C. Kubis, A. Spannenberg, A. Brandt, A. Taden, H. Beck, S. Tin, J. G. de Vries, *Adv. Synth. Catal.* **2022**, *364*, 1251-1263, Use of Iridium-Catalyzed Transfer Vinylation for the Synthesis of Bio-Based (bis)-Vinyl Ethers.

[217] J. Strunk, *Nachr. Chem.* **2022**, 70, 8-10, Kommunikation: Fremdsprache für die Führungsposition.

[218] P. Sudarsanam, A. Brueckner, *Catal. Commun.* **2022**, *170*, 106489, Preface to the special issue on "Analysis of solid-liquid interfaces in heterogeneous catalysis".

[219] T. Suhrbier, J. Bresien, A. Villinger, A. Schulz, *Cell Reports Phys. Sci.* **2022**, *3*, 100777, A four-membered heterocyclic prevented biradical that can be described as a zwitterion or masked N-heterocyclic phosphinidene.

[220] K. Sun, H. Shan, R. Ma, P. Wang, H. Neumann, G.-P. Lu, M. Beller, *Chem. Sci.* **2022**, *13*, 6865-6872, Catalytic oxidative dehydrogenation of N-heterocycles with nitrogen/ phosphorus co-doped porous carbon materials.

[221] K. Sun, H. Shan, H. Neumann, G.-P. Lu, M. Beller, *Nat. Commun.* **2022**, *13*, 1848, Efficient iron single-atom catalysts for selective ammoxidation of alcohols to nitriles.

[222] Y. Sun, J. Harloff, H. Kosslick, A. Schulz, C. Fischer, S. Bartling, M. Frank, A. Springer, *Mol. Catal.* **2022**, *517*, 112005, Influence of the framework on the catalytic performance of Rh-supported Zr-MOFs in the hydroformylation of n-alkenes.

[223] Y. Sun, Z. Yang, S.-N. Lu, Z.

Chen, X.-F. Wu, *Org. Lett.* **2022**, *24*, 6822-6827, Formal [4+1] Annulation of Azoalkenes with  $CF_3$ -Imidoyl Sulfoxonium Ylides and Dual Double Bond Isomerization Cascade: Synthesis of Trifluoromethyl-Containing Pyrazole Derivatives.

[224] J. Surkau, K. Blaesing, J. Bresien, D. Michalik, A. Villinger, A. Schulz, *Chem. Eur. J.* **2022**, n/a, e202201905, A Lewis Acid Stabilized Ketenimine in an Unusual Variant of the Electrophilic Aromatic Substitution.

[225] L. S. Szych, Y. Pilopp, J. Bresien, A. Villinger, J. Rabeah, A. Schulz, *Angew. Chem. Int. Ed.* **2022**, *61*, e202114792, A Persistent Phosphanyl-Substituted Thioketyl Radical Anion.

[226] L. Tadiello, H.-J. Drexler, T. Beweries, *Organometallics* **2022**, *41*, 2833-2843, Low-Field Flow <sup>31</sup>P NMR Spectroscopy for Organometallic Chemistry: On-Line Analysis of Highly Air-Sensitive Rhodium Diphosphine Complexes.

[227] L. Tadiello, T. Gandini, B. M. Stadler, S. Tin, H. Jiao, J. G. de Vries, L. Pignataro, C. Gennari, *ACS Catal.* **2022**, *12*, 235-246, Regiodivergent Reductive Opening of Epoxides by Catalytic Hydrogenation Promoted by a (Cyclopentadienone)iron Complex.

[228] T. Taeufer, M. Quasdorf, P. Ehlers, P. Langer, *Tetrahedron* **2022**, *103*, 132537, Synthesis and properties of Tetraaryl-1,8-naphthyridines.

[229] J. Tang, Z. Yang, Y. Song, Z. Chen, X.-F. Wu, *Mol. Catal.* **2022**, *524*, 112320, Palladium-catalyzed norbornene-mediated dehydrogenative annulation of 3-iodochromones with trifluoroacetimidoyl chlorides for the construction of trifluoromethyl-substituted chromeno[2,3-c]quinolin-12-ones.

[230] Z. Tang, I. Surin, A. Rasmussen, F. Krumeich, E. V. Kondratenko, V. A. Kondratenko, J. Pérez-Ramírez, *Angew. Chem. Int. Ed.* **2022**, *61*, e202200772, Ceria-Supported Gold Nanoparticles as a Superior Catalyst for Nitrous Oxide Production via Ammonia Oxidation.

[231] C. Terazzi, K. Laatz, J. von Langermann, T. Werner, *ACS Sustainable Chem. Eng.* **2022**, *10*, 13335-13342, Synthesis of Cyclic Carbonates Catalyzed by Cal<sub>2</sub>–Et<sub>3</sub>N and Studies on Their Biocatalytic Kinetic Resolution. [232] T. A. Thiel, X. Zhang, B. Radhakrishnan, R. van de Krol, F. F. Abdi, M. Schroeter, R. Schomäcker, M. Schwarze, *RSC Adv.* **2022**, *12*, 30860-30870, Kinetic investigation of para-nitrophenol reduction with photodeposited platinum nanoparticles onto tunicate cellulose.

[233] P. Thiem, S. Ludwig, A. Villinger, W. W. Seidel, *Eur. J. Inorg. Chem.* **2022**, *2022*, e202200552, Boosting the Donor Effect of Side-On W(II) Alkyne Complex Based Diphosphines.

[234] C. Timmermann, P. Thiem, D. Wanitschke, M. Hüttenschmidt, J. Romischke, A. Villinger, W. W. Seidel, *Chem. Sci.* **2022**, *13*, 123-132, Migratory insertion of isocyanide into a ketenyl–tungsten bond as key step in cyclization reactions.

[235] M. Traxler, S. Gisbertz, P. Pachfule, J. Schmidt, J. Roeser, S. Reischauer, J. Rabeah, B. Pieber, A. Thomas, *Angew. Chem. Int. Ed.* **2022**, *61*, e202117738, Acridine-Functionalized Covalent Organic Frameworks (COFs) as Photocatalysts for Metallaphotocatalytic C–N Cross-Coupling.

[236] M. Traxler, S. Reischauer, S. Vogl, J. Roeser, J. Rabeah, C. Penschke, P. Saalfrank, B. Pieber, A. Thomas, *Chem. Eur. J.* **2022**, n/a, e202202967, Programmable Photocatalytic Activity of Multicomponent Covalent Organic Frameworks Used as Metallaphotocatalysts.

[237] D. D. Truong, P. T. M. Pham, E. V. Kondratenko, M. T. Le, *ACS Sustainable Chem. Eng.* **2022**, *10*, 16548-16554, Au/SiO<sub>2</sub>-Based Catalysts for Propanol/Propanal Synthesis from  $CO_{2^{\prime}}C_{2}H_{4^{\prime}}$  and  $H_{2}$  in a Dual-reactor System.

[238] F. Unglaube, J. Schlapp, A. Quade, J. Schaefer, E. Mejía, *Catal. Sci. Technol.* **2022**, *12*, 3123-3136, Highly active heterogeneous hydrogenation catalysts prepared from cobalt complexes and rice husk waste.

[239] A. Vardanyan, S. Boldt, A. Villinger, P. Ehlers, P. Langer, *J. Org. Chem.* **2022**, *87*, 11296-11308, Synthesis and Properties of 1-Azapyrenes.

[240] S. P. Verevkin, D. H. Zaitsau, R. Ludwig, *Molecules* **2022**, *27*, 2321, Aprotic Ionic Liquids: A Framework for Predicting Vaporization Thermo-dynamics.

[241] D. Verspeek, S. Ahrens, A. Spannenberg, X. Wen, Y. Yang, Y.-W. Li, K. Junge, M. Beller, *Catal. Sci. Technol.* **2022**, *12*, 7341-7348, Manganese N,N,N-pincer complex-catalyzed epoxidation of unactivated aliphatic olefins.

[242] P. N. X. Vo, N. H. A. Thu, M. Stoehr, M. N. Jorabchi, S. Wohlrab, *Chem. Ing. Tech.* **2022**, *94*, 157-165, Condensation-Assisted Separation of Alkanes by Silica Membranes with Wide Pore Size Distribution

[243] B. Wang, Y. Sun, A. Cheng, Y. Zhu, J. Wang, Z. Chen, X.-F. Wu, *Front. in Chem.* **2022**, *10*, Metal-free synthesis of 3-trifluoromethyl-1,2,4-triazoles via multi-component reaction of trifluoroacetimidoyl chlorides, hydrazine hydrate and benzene-1,3,5-triyl triformate.

[244] C. Wang, L. M. Azofra, P. Dam, M. Sebek, N. Steinfeldt, J. Rabeah, O. El-Sepelgy, *ACS Catal.* **2022**, *12*, 8868-8876, Catalytic Desaturation of Aliphatic Amides and Imides Enabled by Excited-State Base-Metal Catalysis.

[245] E. Wang, A. Mahmood, S.-G. Chen, W. Sun, T. Muhmood, X. Yang, Z. Chen, ACS Catal. 2022, 12, 11206-11215, Solar-Driven Photocatalytic Reforming of Lignocellulose into  $H_2$ and Value-Added Biochemicals.

[246] H. Wang, R. Schmack, S. Sokolov, E. V. Kondratenko, A. Mazheika, R. Kraehnert, *ACS Catal.* **2022**, *12*, 9325-9338, Oxide-Supported Carbonates Reveal a Unique Descriptor for Catalytic Performance in the Oxidative Coupling of Methane (OCM).

[247] H. Wang, H. Yang, Y. Jiao, X. Wen, H. Jiao, *Appl. Surface Sci.* **2022**, *593*, 153396, Surface hydroxyl dependent adsorption of ruthenium on  $SiO_2(001)$  – Understanding metal– support interaction.

[248] J.-S. Wang, C. Li, J. Ying, T. Xu, W. Lu, C.-Y. Li, X.-F. Wu, *J. Catal.* **2022**, *408*, 81-87, Supported palladium-catalyzed carbonylative cyclization of 2-bromonitrobenzenes and alkynes to access quinolin-4(1H)-ones.

[249] J.-S. Wang, C. Li, J. Ying, T. Xu, W. Lu, C.-Y. Li, X.-F. Wu, J. Catal. 2022, 413, 713-719, Activated carbon fibers supported palladium as efficient and easy-separable catalyst for carbonylative cyclization of o-alkynylphenols with nitroarenes: Facile construction of benzofuran-3-carboxamides.

[250] J.-S. Wang, J. Zhang, S. Wang, J. Ying, C.-Y. Li, X.-F. Wu, *J. Catal.* **2022**, *414*, 313-318, Palladium-catalyzed domino carbonylative cyclization to access functionalized heterocycles.

[251] L.-C. Wang, B. Chen, X.-F. Wu, Angew. Chem. Int. Ed. **2022**, 61, e202203797, Cobalt-Catalyzed Direct Aminocarbonylation of Ethers: Efficient Access to  $\alpha$ -Amide Substituted Ether Derivatives.

[252] L.-C. Wang, B. Chen, Y. Zhang, X.-F. Wu, *Angew. Chem. Int. Ed.* **2022**, *61*, e202207970, Nickel-Catalyzed Four-Component Carbonylation of Ethers and Olefins: Direct Access to *y*-Oxy Esters and Amides.

[253] L.-C. Wang, J.-X. Xu, X.-F. Wu, J. Catal. 2022, 414, 84-89, Cobalt-catalyzed alkoxycarbonylation of ethers: Direct synthesis of  $\alpha$ -oxy esters from phenols and alcohols.

[254] P. Wang, Z. Cao, Y. X. Wang, H. Neumann, M. Beller, *Eur. J. Org. Chem.* **2022**, *2022*, e202200663, Palladium-Catalyzed Carbonylation of Allylic Chlorides to  $\beta$ , $\gamma$ -Unsaturated Esters/Amides under Mild Conditions.

[255] P. Wang, Y. Wang, H. Neumann, M. Beller, *Chem. Sci.* **2022**, *13*, 13459-13465, Rh-catalyzed alkoxycarbonylation of unactivated alkyl chlorides.

[256] P. Wang, Y. Wang, H. Neumann, M. Beller, *Chem. Eur. J.* **2022**, n/a, e202203342, Rhodium-Catalyzed Formylation of Unactivated Alkyl Chlorides to Aldehydes.

[257] P. Wang, J. Yang, K. Sun, H. Neumann, M. Beller, *Org. Chem. Front.* **2022**, *9*, 2491-2497, A general synthesis of aromatic amides via palladium-catalyzed direct aminocarbonylation of aryl chlorides.

[258] Q. Wang, L. Yao, J.-S. Wang, J. Ying, X.-F. Wu, *Mol. Catal.* **2022**, *524*, 112302, Palladium-catalyzed aminocarbonylative cyclization of benzyl chlorides with 2-nitroaryl alkynes to construct indole derivatives.

[259] Q. Wang, L. Yao, J.-S. Wang, J. Ying, X.-F. Wu, *J. Org. Chem.* **2022**, *87*, 3874-3882, Additive-Controlled Divergent Synthesis of Indole and 4H-Benzo[d][1,3]oxazine Derivatives: Palladium-Catalyzed Carbonylative Cyclization of 2-Alkynylanilines and Benzyl Chlorides.

[260] S. Wang, L. Yao, J.-S. Wang, J. Ying, X.-F. Wu, *Mol. Catal.* **2022**, *524*, 112303, Cobalt-catalyzed C-H annulation of N-aroylpicolinamides with alkynes for (NH)-isoquinolones synthesis.

[261] S. Wang, J. Zhang, J.-S. Wang, J. Ying, X.-F. Wu, *Org. Lett.* **2022**, *24*, 8843-8847, Palladium-Catalyzed Cascade Carbonylative Synthesis of Perfluoroalkyl and Carbonyl-Containing 3,4-Dihydroquinolin-2(1H)-one Derivatives.

[262] Y. Wang, Q. He, Z. Cao, P. Wang, G. Chen, M. Beller, *Org. Chem. Front.* **2022**, *9*, 5592-5598, Hypervalent-iodine promoted selective cleavage of C(sp<sup>3</sup>)–C(sp<sup>3</sup>) bonds in ethers.

[263] Z. Wang, X.-F. Wu, in The Chemical Transformations of C1 Compounds, **2022**, pp. 1439-1474.

[264] S. Weber, R. T. Zimmermann, J. Bremer, K. L. Abel, D. Poppitz, N. Prinz, J. Ilsemann, S. Wendholt, Q. Yang, R. Pashminehazar, F. Monaco, P. Cloetens, X. Huang, C. Kübel, E. Kondratenko, M. Bauer, M. Bäumer, M. Zobel, R. Gläser, K. Sundmacher, T. L. Sheppard, *ChemCatChem* **2022**, *14*, e202101878, Digitization in Catalysis Research: Towards a Holistic Description of a Ni/Al<sub>2</sub>O<sub>3</sub> Reference Catalyst for CO<sub>2</sub> Methanation.

[265] D. Wei, R. Sang, A. Moazezbarabadi, H. Junge, M. Beller, *JACS Au* **2022**, *2*, 1020-1031, Homogeneous Carbon Capture and Catalytic Hydrogenation: Toward a Chemical Hydrogen Battery System.

[266] D. Wei, R. Sang, P. Sponholz, H. Junge, M. Beller, *Nat. Energy* **2022**, *7*, 438-447, Reversible hydrogenation of carbon dioxide to formic acid using a Mn-pincer complex in the presence of lysine.

[267] D. Wei, X. Shi, R. Qu, K. Junge, H. Junge, M. Beller, *ACS Energy Lett.* **2022**, *7*, 3734-3752, Toward a Hydrogen Economy: Development of Heterogeneous Catalysts for Chemical Hydrogen Storage and Release Reactions.

[268] D. Wei, X. Shi, P. Sponholz, H. Junge, M. Beller, *ACS Centr. Sci.* **2022**, *8*, 1457-1463, Manganese Promoted (Bi)carbonate Hydrogenation and Formate Dehydrogenation: Toward a Circular Carbon and Hydrogen Economy.

[269] L. Wei, H. Yang, P. Ren, Y. Yang, Y.-W. Li, R. Li, X.-D. Wen, H. Jiao, *Microporous Mesoporous Mater.* **2022**, *344*, 112184, Distribution of multiple Al substitution in HY zeolite and Brønsted acid strength - A periodic DFT study.

[270] P. Wei, Y. Zhu, J. Zhang, J. Ying, X.-F. Wu, *J. Catal.* **2022**, *414*, 349-355, Cobalt-catalyzed direct functionalization of indoles with isocyanides.

[271] J. Weiß, Q. Yang, U. Bentrup, E. V. Kondratenko, A. Brueckner, C. Kubis, *ChemCatChem* **2022**, *14*, e202200577, Operando DRIFT and In situ Raman Spectroscopic Studies on Aspects of CO<sub>2</sub> Fischer-Tropsch Synthesis Catalyzed by Bulk Iron Oxide-Based Catalysts.

[272] D. Wen, Z. Shen, X. Qi, X.-F. Wu, *Eur. J. Org. Chem.* **2022**, *2022*, e202200971, Palladium-Catalyzed Cascade Carbonylative Synthesis of Functionalized Isoquinoline-1,3-diones and Oxindoles Using Dimethyl Carbonate as both Solvent and Reactant.

[273] F.-P. Wu, H.-Q. Geng, X.-F. Wu, *Angew. Chem. Int. Ed.* **2022**, *61*, e202211455, Copper-Catalyzed Boroaminomethylation of Olefins to γ-Boryl Amines with CO as C1 Source.

[274] F.-P. Wu, X.-F. Wu, *Chem. Sci.* **2022**, *13*, 4321-4326, Catalyst-controlled selective borocarbonylation of benzylidenecyclopropanes: regiodivergent synthesis of  $\gamma$ -vinylboryl ketones and  $\beta$ -cyclopropylboryl ketones.

[275] F.-P. Wu, Y. Yang, D. P. Fuentes, X.-F. Wu, *Chem* **2022**, *8*, 1982-1992, Copper-catalyzed carbonylative catenation of olefins: Direct synthesis of  $\gamma$ -boryl esters.

[276] S.-M. Wu, M. Beller, X.-Y. Yang, *Matter* **2022**, *5*, 3104-3107, A clear view of zeolite-catalyzed processes.

[277] J.-X. Xu, Z.-P. Bao, X.-F. Wu, Org. Lett. **2022**, 24, 1848-1852, Palladium-Catalyzed Carbonylation of Disulfides and Ethylene: Synthesis of  $\beta$ -Thiopropionate Thioesters.

[278] J.-X. Xu, C.-S. Kuai, B. Chen, X.-F. Wu, *Chem Catal.* **2022**, *2*, 477-498, Transition-metal-catalyzed carbonylative cross-coupling with alkyl carbon nucleophiles.

[279] J.-X. Xu, C.-S. Kuai, X.-F. Wu, J. Org. Chem. 2022, 87, 6371-6377, Cobalt-Catalyzed Four-Component Carbonylation of Methylarenes with Ethylene and Alcohols.

[280] J.-X. Xu, L.-C. Wang, X.-F. Wu, Org. Lett. 2022, 24, 4820-4824, Palladium-Catalyzed Desulfonative Carbonylation of Thiosulfonates: Elimination of  $SO_2$  and Insertion of CO.

[281] J.-X. Xu, L.-C. Wang, X.-F. Wu, *Chem. Asian J.* **2022**, *17*, e202200928, Non-Noble Metal-Catalyzed Carbonylative Multi-Component Reactions.

[282] R.-R. Xu, X. Bao, Y.-W. Huo, R.-G. Miao, D. Wen, W. Dai, X. Qi, X.-F. Wu, *Org. Lett.* **2022**, *24*, 6477-6482, Palladium-Catalyzed Domino Carbopalladation/Carbonylative Cyclization: Synthesis of Heterocycles bearing Oxindoles and 3-Acylbenzofuran/3-Acylindole Moieties.

[283] R.-R. Xu, W. Wang, X. Qi, X.-F. Wu, *Org. Chem. Front.* **2022**, *9*, 1417-1421, Palladium-catalyzed cascade Heck-type thiocarbonylation for the synthesis of functionalized thioesters.

[284]R.-R. Xu, D. Wen, X. Qi, X.-F. Wu, *Org. Biomol. Chem.* **2022**, *20*, 2605-2608, Palladium-catalyzed cascade Heck-type cyclization and reductive aminocarbonylation for the synthesis of functionalized amides.

[285] H. Yang, X. Geng, Y. Yang, Y.-W. Li, X.-D. Wen, H. Jiao, *Appl. Surf. Sci.* **2022**, 600, 154151, Mechanisms of  $CO_2$  hydrogenative conversion on supported Ni/ZrO, catalyst.

[286] H. Yang, L.-C. Wang, Y. Zhang, D. Zheng, Z. Chen, X.-F. Wu, *Chem. Sci.* **2022**, *13*, 3526-3532, Controllable access to trifluoromethyl-containing indoles and indolines: palladium-catalyzed regioselective functionalization of unactivated alkenes with trifluoroacetimidoyl chlorides.

[287] H. Yang, J. Zhang, Z. Chen, X.-F. Wu, *Chem. Record* **2022**, *22*, e202100220, TFBen (Benzene-1,3,5-triyl triformate): A Powerful and Versatile CO Surrogate.

[288] J. Yang, F. G. Delolo, A. Spannenberg, R. Jackstell, M. Beller, *Angew. Chem. Int. Ed.* **2022**, *61*, e202112597, A Selective and General Cobalt-Catalyzed Hydroaminomethylation of Olefins to Amines.

[289] J. Yang, S. Ghosh, J. Roeser, A. Acharjya, C. Penschke, Y. Tsutsui, J. Rabeah, T. Wang, S. Y. Djoko Tameu, M.-Y. Ye, J. Grüneberg, S. Li, C. Li, R. Schomäcker, R. Van De Krol, S. Seki, P. Saalfrank, A. Thomas, *Nat. Commun.* **2022**, *13*, 6317, Constitutional isomerism of the linkages in donor-acceptor covalent organic frameworks and its impact on photocatalysis. [290] Q. Yang, V. A. Kondratenko, S. A. Petrov, D. E. Doronkin, E. Saraçi, H. Lund, A. Arinchtein, R. Kraehnert, A. S. Skrypnik, A. A. Matvienko, E. V. Kondratenko, *Angew. Chem. Int. Ed.* **2022**, *61*, e202116517, Identifying Performance Descriptors in CO<sub>2</sub> Hydrogenation over Iron-Based Catalysts Promoted with Alkali Metals.

[291] Z. Yang, J. Tang, Z. Chen, X.-F. Wu, Org. Lett. **2022**, 24, 7288-7293, Ruthenium-Catalyzed Hydroxyl-Directed peri-Selective C–H Activation and Annulation of 1-Naphthols with  $CF_3$ -Imidoyl Sulfoxonium Ylides for the Synthesis of 2-(Trifluoromethyl)-2,3-dihydrobenzo[de]chromen-2-amines.

[292] L. Yao, P. Wei, J. Ying, X.-F. Wu, *Org. Chem. Front.* **2022**, *9*, 2685-2689, Nickel-catalyzed carbonylative domino cyclization of arylboronic acid pinacol esters with 2-alkynyl nitroarenes toward N-aroyl indoles.

[293] Z. Yin, X.-F. Wu, in The Chemical Transformations of C1 Compounds, **2022**, pp. 249-288.

[294] U. Yorsh, A. S. Behr, N. Kockmann, M. Holena, in ITAT'22 / IW-CIDM CEUR Workshop, **2022**, pp. 28-34.

[295] Y. Yuan, J.-X. Xu, X.-F. Wu, *Chem. Commun.* **2022**, *58*, 12110-12113, Cooperative Cu/Pd-catalyzed borocarbonylation of ethylene.

[296] A. Zanina, V. A. Kondratenko, H. Lund, J. Li, J. Chen, Y. Li, G. Jiang, E. V. Kondratenko, *ACS Catal.* **2022**, *12*, 15361-15372, The Role of Adsorbed and Lattice Oxygen Species in Product Formation in the Oxidative Coupling of Methane over  $M_2WO_4/SiO_2$  (M = Na, K, Rb, Cs).

[297] B. Zhang, C. Kubis, R. Franke, *Science* **2022**, *377*, 1223-1227, Hydroformylation catalyzed by unmodified cobalt carbonyl under mild conditions.

[298] J. Zhang, S. Wang, J.-S. Wang, J. Ying, X.-F. Wu, *Org. Chem. Front.* **2022**, *9*, 5219-5224, Palladium-catalyzed carbonylative synthesis of indole-3-carboxamides from 2-ethynylanilines and nitroarenes.

[299] Q. Zhang, T. Otroshchenko, E. V. Kondratenko, *Catal. Sci. Technol.* **2022**, *12*, 5210-5216, Fundamentals and application potential of the synergy effect between ZnO and Mo/SiO<sub>2</sub> for propene production in the metathesis of ethylene and trans-2-butene.

[300] Y. Zhang, Z.-P. Bao, J.-X. Xu, X.-F. Wu, Org. Lett. **2022**, 24, 6845-6850, Palladium-Catalyzed Perfluoroalkylative Carbonylation of 2-Allylaryl Trifluoromethanesulfonates: Base-Controlled Selective Access to  $\beta$ -Perfluoroalkyl Amides.

[301] Y. Zhang, S. Ling, P. Li, Z. Chen, X.-F. Wu, *Org. Lett.* **2022**, *24*, 8864-8869, Rh(III)-Catalyzed Dual C–H Activation/Cascade Annulation of Benzimidates and CF3-Imidoyl Sulfoxonium Ylides for the Synthesis of Trifluoromethyl-Decorated Benzo[de] [1,8]naphthyridines.

[302] Y. Zhang, X.-F. Wu, *Chinese J. Org. Chem.* **2022**, *42*, 3007-3009, Switchable Radical Carbonylation by Philicity Regulation.

[303] Y. Zhang, Z. Yang, Z. Chen, L. Liu, X.-F. Wu, *Adv. Synth. Catal.* **2022**, *364*, 1044-1049, Copper-Catalyzed Decarbonylative Cyclization of Isatins and Trifluoroacetimidohydrazides for the Synthesis of 2-(5-Trifluoromethyl-1,2,4-triazol-3-yl)anilines.

[304] Y. Zhang, Y. Yuan, H.-Q. Geng, J.-X. Xu, X.-F. Wu, *J. Catal.* **2022**, *413*, 214-220, Visible light-induced perfluoroalkylative carbonylation of unactivated alkenes.

[305] D. Zhao, K. Guo, S. Han, D. E. Doronkin, H. Lund, J. Li, J.-D. Grunwaldt, Z. Zhao, C. Xu, G. Jiang, E. V. Kondratenko, *ACS Catal.* **2022**, *12*, 4608-4617, Controlling Reaction-Induced Loss of Active Sites in ZnO<sub>x</sub>/ Silicalite-1 for Durable Nonoxidative Propane Dehydrogenation.

[306] F. Zhao, H.-J. Ai, X.-F. Wu, Angew. Chem. Int. Ed. **2022**, 61, e202200062, Copper-Catalyzed Substrate-Controlled Carbonylative Synthesis of  $\alpha$ -Keto Amides and Amides from Alkyl Halides.

[307] F. Zhao, X.-W. Gu, R. Franke, X.-F. Wu, *Angew. Chem. Int. Ed.* **2022**, *61*, e202214812, Copper-Catalyzed 1,2-Dicarbonylative Cyclization of Alkenes with Alkyl Bromides via Radical Cascade Process.

[308] F. Zhao, P. Russo, R. Mancuso, B. Gabriele, X.-F. Wu, *J. Catal.* **2022**, *413*, 907-912, Copper-catalyzed carbonylative coupling of alkyl iodides with phenols for the synthesis of esters. [309] P. Zhao, Y. He, X. Wen, H. Jiao, Surf. Sci. 2022, 715, 121936, Dissociative adsorption of  $H_2O$  and  $CO_2$ on the clean and O-pre-covered high index Ru surfaces: Corrugated Ru(11–21) and stepped Ru(20–21) surfaces.

[310] S. Zhao, H.-Q. Liang, X.-M. Hu, S. Li, K. Daasbjerg, *Angew. Chem. Int. Ed.* **2022**, *61*, e202204008, Challenges and Prospects in the Catalytic Conversion of Carbon Dioxide to Formal-dehyde.

[311] S. Zheng, S. Chakrabortty, E. Baráth, S. Tin, J. G. de Vries, ACS Sustainable Chem. Eng. 2022, 10, 15642-15647, Synthesis of N-Substituted 3-Hydroxypyridinium Salts from Bioderived 5-Hydroxymethylfurfural in Water.

[312] S. Zheng, W. Smit, A. Spannenberg, S. Tin, J. G. de Vries, *Chem. Commun.* **2022**, *58*, 4639-4642, Synthesis of  $\alpha$ -keto aldehydes via selective Cu(I)-catalyzed oxidation of  $\alpha$ -hydroxy ketones.

[313] B. Zhou, Z. Ma, A. M. Alenad, C. Kreyenschulte, S. Bartling, M. Beller, R. V. Jagadeesh, *Green Chem.* **2022**, *24*, 4566-4572, Cobalt-catalysed CH-alkylation of indoles with alcohols by borrowing hydrogen methodology.

[314] F. Zhu, P. Yin, X.-F. Wu, *Chem. Sci.* **2022**, *13*, 12122-12126, Regioselective catalytic carbonylation and borylation of alkynes with aryldiazonium salts toward  $\alpha$ -unsubstituted  $\beta$ -boryl ketones.

[315] Y. Zhu, B. Guo, S. Gao, J. Ying, X.-F. Wu, *Org. Chem. Front.* **2022**, *9*, 5005-5009, Cobalt-catalyzed carbonylative synthesis of free (NH)-tetrahydro- $\beta$ -carbolinones from tryptamine derivatives.

[316] Y. Zhu, J. Ying, X.-F. Wu, *Mol. Catal.* **2022**, *524*, 112267, Cobalt-catalyzed carbonylative cyclization of N-(2-Vinylphenyl)nicotinamides to access (NH)-quinolin-2(1H)-ones.

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