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Leibniz Institute for Catalysis

LIKAT Rostock

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FOREWORD

Dr. Barbara Heller, Commercial Director, and
Prof. Dr. Matthias Beller, Scientific Director.

KEEPING AN EYE ON GLOBAL CHALLENGES

Catalysts get chemical reactants moving: they control and thus accelerate almost all chemical and biochemical processes. In the chemical industry, catalysts help save energy and raw materials. They increase yields and avoid by-products by enabling starting materials to react specifically and selectively at the molecular level. In short, catalysis can save resources and the environment to a great extent. And it is the key technology for the global economic transition to renewable raw materials and renewable energy.

The Leibniz Institute for Catalysis in Rostock, LIKAT, has been exploring the phenomena of catalysis from its fundamentals for almost 70 years and developing innovative solutions for the implementation of scientific findings together with industry. With their topics, researchers at LIKAT address major goals of the global community: climate-neutral society, food security, preservation of the natural environment, protection against pandemics. Our projects are part of international and national cooperations, such as the EU hydrogen strategy and the BMBF initiative 'Hydrogen Republic of Germany'. And they lay the foundations for a new, 'green' chemistry.

Research highlights in the reporting period include a process for bio-based polymers to produce PEF plastic, a sustainable alternative to PET. Highlights also include catalytic solutions for the ecologically sound production of platform chemicals and basic materials, e.g. from renewable raw materials and biowaste or using CO_2 from the air as well as sunlight and photocatalysis (Prophecy and Prodegy). New catalysts and building blocks in the promising field of fluorine chemistry should also be mentioned. And in the field of artificial metalloenzymes, a research hotspot, we are currently expanding our expertise (ComBioCat).

In the application-oriented field, LIKAT chemists explored, for example, processes for replacing expensive precious metal catalysts in the pharmaceutical industry and for the degradation of pollutants in wastewater. A new process developed by LIKAT as part of the Metha-Cycle joint project is the first to successfully couple wind power, electrolysis and CO_2-based methanol synthesis, enabling hydrogen to be stored for on-demand power generation, especially in rural regions.

Our research led to a good three dozen patents in the reporting period. The transfer of our catalysts or processes to an industrial pilot scale will also be facilitated in the future by a 'zero carbon' pilot plant, the inauguration of which is planned for early 2022. We generate about one third of our budget with successful acquisition of competitive third-party funding, for example through industrial cooperations and from public funding programs.

LIKAT's success has many sources. Just two may be mentioned: Our expertise of seven decades of catalysis research at the Rostock site and our almost 300 institute members - whether in research, workshop or administration, whether as specialists, professors or doctoral students and regardless of their main color and nation. Especially in the difficult time of the corona pandemic they are doing a great job. LIKAT's success is also based on our willingness to keep ourselves 'on our toes' and to overcome boundaries – between disciplines, between theory and application, between heterogeneous and homogeneous catalysis. And finally, between the individual research departments of the previous institute structure, which we have supplemented with a matrix structure now comprising seven future-oriented topics.

Barbara Heller

Barbara Heller *Matthias Beller*

A LOOK INSIDE

TOPICS
& PROJECTS

RESEARCH GROUPS

February

Thieme Chemistry Journal Award 2019 for Jola Pospech

Dr. Jola Pospech has been awarded the 'Thieme Chemistry Journal Award 2019'. Every year, the Georg Thieme Verlag honors 'promising junior professors at the beginning of their careers'. In 2019, seven young researchers from Germany were among the award winners selected from around the world.

Jola Pospech is the first to bring this Thieme Verlag prize to the Leibniz Institute for Catalysis in Rostock.

April

Spiers Memorial Award for Matthias Beller

Prof. Matthias Beller was honored with the 2019 Spiers Memorial Award for the development of applied homogeneous and heterogeneous catalysts for sustainable chemical conversions at the Artificial Photosynthesis Faraday Discussion, March 25-27, 2019, in Cambridge. The Spiers Memorial Award is given to individuals who have made outstanding contributions to the field of Faraday Discussion. These are unique international discussion events that address current and rapidly evolving areas of chemistry and their interfaces with other scientific disciplines.

May

3D Printing for the ISS: Rostock Pupils at the World's Largest Youth Science Competition in Arizona

The national winners of the 'Jugend forscht' competition 2018 came from Rostock and participate with their project in the world's largest pre-academic science competition, the 70th Intel ISEF, in Arizona (USA) from May 12 to 17.

Lara Neubert and Adrian Schorowsky prepared for this at the Leibniz Institute for Catalysis. There, they investigated the production of a raw material from packaging waste for 3D printing on board the International Space Station ISS in the laboratory. A great deal of packaging waste is generated on board the ISS during supply operations. Until now, this plastic has been left to burn up in the Earth's atmosphere, although it can be used according to their findings.

May

Rui Sang Receives "Chinese Government Award for Outstanding Self-financed Students Abroad"

Rui Sang, PhD student in the research group 'Applied Carbonylations' (headed by Dr. Ralf Jackstell) in the area of Applied Homogeneous Catalysis (Prof. Matthias Beller) was awarded the '2018 Chinese Government Award for Outstanding Self-financed Students Abroad'.

The award is given annually to Chinese PhD students for their outstanding achievements. The award is one of the highest honors given by the Chinese government to doctoral students who study outside China and are not supported by a scholarship from the Chinese government.

Leibniz Association

March

LIKAT in Central German Network '4chiral'

The LIKAT was able to expand its network by an important cooperation partner and is now a member of the Central German network '4chiral'.

'The primary goal of the network partners is to work together on the rapidly expanding field of organic fine synthesis and to be present here.' One research focus at LIKAT is the development of catalyzed processes for the synthesis of fine chemicals.

April

1,1 Million EUR for New Science Campus in Rostock and Greifswald

At the beginning of April 2019, the Leibniz Association decided to fund six new Leibniz Science Campi across Germany. The Leibniz Institute for Catalysis (LIKAT), together with the Leibniz Institute for Plasma Research and Technology e.V. (INP) in Greifswald and the Universities of Greifswald and Rostock, succeeded in bringing the *ComBioCat* science campus to Mecklenburg-Vorpommern.

The researchers involved will be looking for solutions to one of the major challenges facing society: the transition from fossil resources to renewable raw materials for the production of chemicals and energy sources. The key technology here is catalysis.

May

Esteban Mejia Received Scholarship to Attend the 'Bürgenstock Konferenz'

Dr. Esteban Mejia, a junior researcher at LIKAT, is one of 15 young scientists who have been awarded the coveted scholarship. The scholarships are awarded by leading researchers for scientific excellence and diversity.

The 'SCS Conference on Stereochemistry' or 'Bürgenstock Conference' is held annually in Brunnen (Switzerland) and brings together young and established scientists for interdisciplinary exchange.

June

Third Alumni Meeting at LIKAT

On June 27 and 28, the third alumni meeting took place, welcoming a good dozen LIKAT graduates. After short reports about their current position and tasks, they briefly reported about their career after leaving LIKAT.

The interest was not only great on the part of the graduates. Also, the PhD students and postdocs took the opportunity to exchange ideas with the alumni and to benefit from their experiences. In addition, some alumni support potential LIKAT graduates in the context of a mentoring program at the start of their professional lives.

June

Rostocks Eleven

Jacob Schneidewind, PhD student in the research group ‘Catalysis for Energy Technologies’ (headed by Dr. Henrik Junge), represented LIKAT at the annual competition ‘Rostock’s 11’. Under the aspect of science communication, it offers eleven young scientists from Rostock’s eleven scientific institutions the chance to present their research projects to a non-scientific audience of eleven journalists.

October

Start of Construction of the ‘Zero Carbon’ Transfer Technology Center

In October, construction of the Transfer Technology Center ‘ZeroCarbon-Catalysis’ at LIKAT begins. The institute’s own Technology Center is intended to simplify the transfer of innovative laboratory results from catalysis research for SMEs and non-chemical user industries that do not have the corresponding facilities themselves.

November

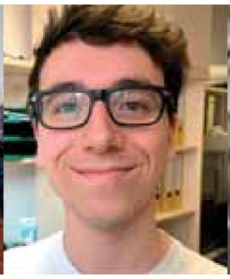
‘Wippengespräch’ with Matthias Beller

Smart heads discuss climate change: Under the motto ‘Solving global problems globally’, the University of Rostock invited to the ‘Wippengespräch’ in the Konrad-Zuse-Haus. Different experts from science, economy and politics lead a ‘balanced’ discussion on the controversial but current topic ‘How and at what price can we stop the anthropogenic influences on the climate?’. Among the representatives of science, Prof. Matthias Beller took part in this event.

November

Highly Cited Researchers

With Dr. Kathrin Junge and Prof. Dr. Matthias Beller, two LIKAT researchers are on the 2019 Highly Cited Researcher list, which has been published annually since 2002 by the Web of Science Group, a Clarivate Analytics company. The list recognizes scientists who have produced multiple scientific papers and whose publications are in the top 1% of published citations in their field, demonstrating significant research impact. In 2019, a total of 327 German researchers are listed, 16 of them in the field of chemistry. Among them, Dr. Kathrin Junge is the only woman.



August

S1-Lab Begins Operation

As part of the LeibnizCampus *ComBioCat*, an S1 safety laboratory was set up at LIKAT. The scientists in the field of ‘Bioinspired Homogeneous Catalysis’ of Prof. Paul Kamer were now able to start their research work, which requires the establishment of cell cultures for the production of proteins as well as their harvesting, genetic modification and purification, sterile work according to the legal requirements of the Genetic Engineering Protection Ordinance.

October

Starting Signal for the New LeibnizCampus *‘ComBioCat’*

As one of the four partner institutions of ComBioCat, the participants at LIKAT officially start their research work. Through the collaboration of all catalysis disciplines, catalysis as a key technology has the potential to provide solutions to the challenges of the 21st century: The shift from fossil resources to renewable raw materials for the production of chemicals and energy sources. Previously inaccessible biomass is to be made usable and catalyst systems for sustainable chemical and energy production are to be developed.

November

Awards for Lars Longwitz und Fabian Reiß

P-Campus Publication Award for Lars Longwitz

Lars Longwitz, PhD student from the Werner group, received one of the P-Campus publication awards during the P-Campus Symposium on November 12/13, 2019 at the IOW in Warnemünde. The prerequisite for the award, which is endowed with 300 €, is the interdisciplinarity of the project within the P-Campus. The publication must therefore be written by at least two authors from different P-Campus institutions.

Poster Award for Fabian Reiß

Dr. Fabian Reiß, group leader ‘Catalysis of Early Transition Metals’ was awarded the ‘Best Poster Award’ at the meeting ‘Chemistry of Organoelement Compounds and Polymers 2019’ (INEOS, 18. – 22. Novermber) in Moscow.

January

Honorary Membership of the 'Chinese Chemical Society' for Prof. Matthias Beller

The 'Chinese Chemical Society"' (CCS) appoints Prof. Matthias Beller as an honorary member. This highest honor of the CCS is awarded exclusively to the 100 most distinguished chemists in the world. The prerequisite for honorary membership is 'significant contributions to the promotion of chemistry and the development of Chinese chemistry and society', according to the CCS letter.

Angelika Brückner Elected to the GDCh Board of Directors

Prof. Angelika Brückner was elected to the Board of the 'Gesellschaft Deutscher Chemiker' (GDCh) for the term of office 2020 – 2023.

April

Klaus Tschira Boost Fund for Christian Hering-Junghans

For the first time, the Klaus Tschira Foundation and the German Scholars Organization e.V. selected young researchers to be supported by the Klaus Tschira Boost Fund. In addition to Dr. Christian Hering-Junghans, ten other young scientists will receive funding for their projects over the next two years. The program is aimed at excellent scientists in the natural sciences, mathematics and computer science.

NFDI4Cat

June

External Funding Successes and Digitalization: NFDI4Cat – Research Data Treasures Become Available, Digitization of Science

In the first of three rounds of call for proposals, the LIKAT in Rostock and the Universities of Rostock and Greifswald, as a significant part of the catalysis-related sciences, are benefiting from the BMBF's 90 million euro project for the digitization of science.

The new project promotes digitization in key scientific areas with the aim of networking important research data from the participating partners and making it more widely available. In addition to LIKAT, the universities in Rostock and Greifswald will be supported as part of NFDI4Cat with approximately 2 million euros for the next 5 years.

July

Virtual Poster Event via Twitter: Award for Master Student at LIKAT

Alternatives in demand:
Due to COVID-19, all events in which people meet directly with each other were cancelled. In order to maintain the important exchange among researchers in science as well, the Canadian Institute of Chemistry (CIC) organized a 48-hour poster event on Twitter, in which a total of 166 scientists from over 20 nations participated.

Jan-Erik Siewert, a master's student in the junior research group 'Activation of Small Molecules' led by Dr. Christian Hering-Junghans, also participated in the GIDW (Global Inorganic Discussion Weekdays) poster event with his work from his methods and research internship.

2020
GREEN TALENTS

March/April

'Research Is Going on' – Signal from the Chemistry Lab

The Leibniz Institute for Catalysis in Rostock maintained its research operations despite the lockdowns. Even though the Covid-19 disease caused by the new coronavirus posed a logistical challenge to the management board and staff, experiments continued in the laboratories.

Strict hygiene regulations and the greatest possible flexibility with regard to working hours and mobile working made it possible to maintain the research work. In addition, young parents were individually supported in order to be able to look after their children at home.

May

Transfer in Politics and Society – Leibniz im Bundestag

Within the framework of this Leibniz format, Prof. Dr. Jennifer Strunk (Head of Department 'Heterogeneous Photocatalysis') and Norbert Altenkamp (CDU, direct mandate Main-Taunus district) found each other – this year virtually. They talked about the topic 'Recycling instead of emitting: Returning carbon dioxide to chemical production with the help of renewable energies.' The Leibniz format is a good example of successful science communication at the interface between politics and research. In addition to new impulses for both sides, the dialog also increases understanding for each other.

June

P-Campus Starts into Second Funding Phase

The P-research in the network of the Leibniz research campus 'P-Campus' is secured until 2023. The second funding phase was secured in a cooperation agreement between the Leibniz Association, the state of Mecklenburg-Vorpommern and the University of Rostock.

LEIBNIZ SCIENCE CAMPUS
PHOSPHORUS RESEARCH
ROSTOCK

September

Angelika Brückner Appointed to Advisory Board of Karl Ziegler Foundation

Prof. Angelika Brückner, member of the board at LIKAT and head of the department 'Catalytic *in-situ*-studies', was appointed to the advisory board of the Karl Ziegler Foundation by the GDCh board. Her term of office will begin on January 1, 2021. The Foundation's Advisory Board will select the next awardee in spring 2021.

September

Green Talents at LIKAT

Young scientific visionaries, the 25 winners of the BMBF's *Green Talents* competition, made a virtual stop at LIKAT.
They were awarded for their outstanding research on the topic of sustainability. Their research range from climate change to new energy systems, which also determine the research program at LIKAT.
Even if only online in 2020: the stations of the Science Forum offer the young researchers a good opportunity to establish contacts for collaborations and for a future research stay in Germany. These stays of the Green Talents are funded by the BMBF for three months.

October

Evgenii Kondratenko Receives extraordinary professorship

PD Dr. Evgenii Kondratenko, group leader of the research group 'Reaction Mechanisms', receives a professorship 'Prof. apl.' from the University of Rostock. His research has been dedicated to the detailed analysis of chemical processes for many years.

November

Honoring - Highly Cited Researchers 2020

In 2020, Dr. Kathrin Junge and Prof. Dr. Matthias Beller again made it onto the 2020 Highly Cited Researcher list, which recognizes scientists whose publications are among the top 1% of published citations in their field. In total, only 14 German chemists were honored this year, including Dr. Junge as the only woman in the field of chemistry.

December

Best Master's Graduate in Chemistry: MNF Faculty Award Goes to Jan-Erik Siewert

M.Sc. Jan-Erik was awarded the Faculty Prize of the Faculty of Mathematics and Natural Sciences of the University of Rostock (MNF) as the best Master's graduate of the Institute of Chemistry 2020. He wrote his master thesis on 'DFT studies on the mechanism of reactions of phospha-Wittig reagents with N-heterocyclic carbenes and N-heterocyclic olefins' under the supervision of junior group leader Dr. Christian Hering-Junhans and Prof. Johannes de Vries.

October

Kick-Off-Symposium for LeibnizCampus *ComBioCat*

On October 13, the first 'ComBioCat Symposium' took place in Rostock. Despite strict corona regulations, all PhD students had the chance to network and to present and discuss first research results.

Eqality – LIKAT Receives TEQ Award for the 4th Time in a Row

LIKAT has been awarded the 'Total E-Quality' predicate for the fourth time in a row. The jury's statement emphasized that the equal opportunities policy at the Leibniz Institute for Catalysis has been firmly integrated and institutionalized for many years.

November

Matthias Beller Again Vice President and Member of the Board of the Leibniz Association

Prof. Dr. Matthias Beller was re-elected to the Executive Board and as Vice President of the Leibniz Association at the Leibniz Annual Meeting on 26.11.2020.

Prof. Paul C. J. Kamer

The LIKAT mourns the death of Paul Kamer, an excellent researcher and university teacher, a pioneer in his field. His death deeply shocked us, his colleagues. Paul Kamer's extraordinarily productive research was reflected in some 250 widely cited publications and a number of patents. He was co-editor of CATALYSIS SCIENCE AND TECHNOLOGY and a visiting professor at universities in Milan, Eindhoven, Tarragona, Amsterdam and Caltech.

November

Successful Audit at LIKAT

As an advisory body, the Scientific Advisory Board evaluates the scientific performance of Leibniz institutions. Of great importance are the audits, in the context of which scientific quality as well as questions of further structural development and orientation play a role.
The Audit for LIKAT, scheduled for summer 2020, was postponed to November 30 due to corona and conducted virtually. The scientific advisory board rates the audit as outstanding in all respects.

December

Successful Habilitation of Esteban Mejia

On 16.12. Esteban Mejia, junior research group leader 'Polymer Chemistry & Catalysis' successfully defended his habilitation. In the working group of Prof. Udo Kragl he asserted himself as a successful and creative junior researcher and group leader.

Research Structure

TOPICS

Topic 01
Structure-Reactivity Relationships
Angelika Brückner, Wolfgang Baumann (deputy)

Topic 02
Kinetics, Theory & Mechanisms
Evgenii Kondratenko, Haijun Jiao (deputy)

Topic 03
Reaction Engineering & Implementation
David Linke, Udo Armbruster (deputy)

Topic 04
Renewable Resources
Johannes de Vries, Thomas Werner (deputy)

Topic 05
Energy & Environment
Jennifer Strunk, Henrik Junge (deputy)

Topic 06
More Efficient Processes
Sebastian Wohlrab, Bernd Müller (deputy)

Topic 07
New Products & Processes
Torsten Beweries, Christian Hering-Junghans (deputy)

Towards a Matrix Structure

Until now, LIKAT was organized in three program focuses consisting of several research departments. However, the operational research work at the Leibniz Institute for Catalysis has already been organized for many years in the form of a project matrix structure in which projects have been assigned to several research departments.

The focus of our research approach is not the separation into the classical areas of catalysis – homogeneous and heterogeneous – but the answering of important research questions. In order to better reflect these operational research activities, the former program department structure is replaced by the so-called matrix structure and the research activities are assigned to so-called *Topics* across departments.

One important goal is to achieve greater synergy effects. If all groups and their expertise are visible to everyone, opportunities for collaboration will be found more quickly. Basically, a holistic view of the phenomenon of catalysis is aimed at. This will put the institute in a better position to use its research results to make significant contributions to solving the global 'Grand Challenges' of the 21st century, such as health, sustainability, energy supply or climate change.

A total of seven topics have been identified as future-oriented research areas, which are being worked on by the existing research departments with their individual *research groups*. Three of them (*Topic 01 - 03*) are methodologically oriented and four (*Topic 04 - 07*) are materially oriented. All topics are coordinated by a speaker and his or her deputy speaker.

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

This does not affect the granting of research freedom for all scientific staff. Researchers are encouraged to independently develop solutions for existing projects or to propose new project topics. Explorative topics, which have been set up specifically for this purpose, offer the opportunity to explore research ideas and to react flexibly to current problems and challenges.

TOPIC 01

Prof. Angelika Brückner
PD Dr. Wolfgang Baumann

STRUCTURE-REACTIVITY RELATIONSHIPS

In Topic 01, modern experimental methods are established and combined as an essential basis for knowledge-based catalyst design. This includes the development, optimization and application of innovative methods, processes and setups for carrying out catalytic reactions and catalyst syntheses. The aim is to accelerate the development of new catalytic processes and to make existing processes more efficient.

One focus is on the development of new spectroscopic reaction cells in which different *in situ* and *operando* methods can be coupled simultaneously. Of particular note is the 5-in-1 coupling of FTIR-ATR/UV-Vis/EPR/EXAFS/XANES at a measurement site of the Synchrotron Soleil near Paris, which allows, for example, the elucidation of complex reaction mechanisms. In addition, a low temperature FTIR cell was developed to analyze exposed metal centers on the surface of solid catalysts by adsorption of probe molecules (NO, CO).

New experimental solutions were developed for *operando* spectroscopy at elevated pressure up to 20 bar. Worth mentioning here are the FTIR spectroscopic investigation of the Fischer-Tropsch synthesis with CO_2 and the combination of EPR spectroscopy and EXAFS/XANES for mechanistic studies of the homogeneous chromium-catalyzed tetramerization of ethylene.

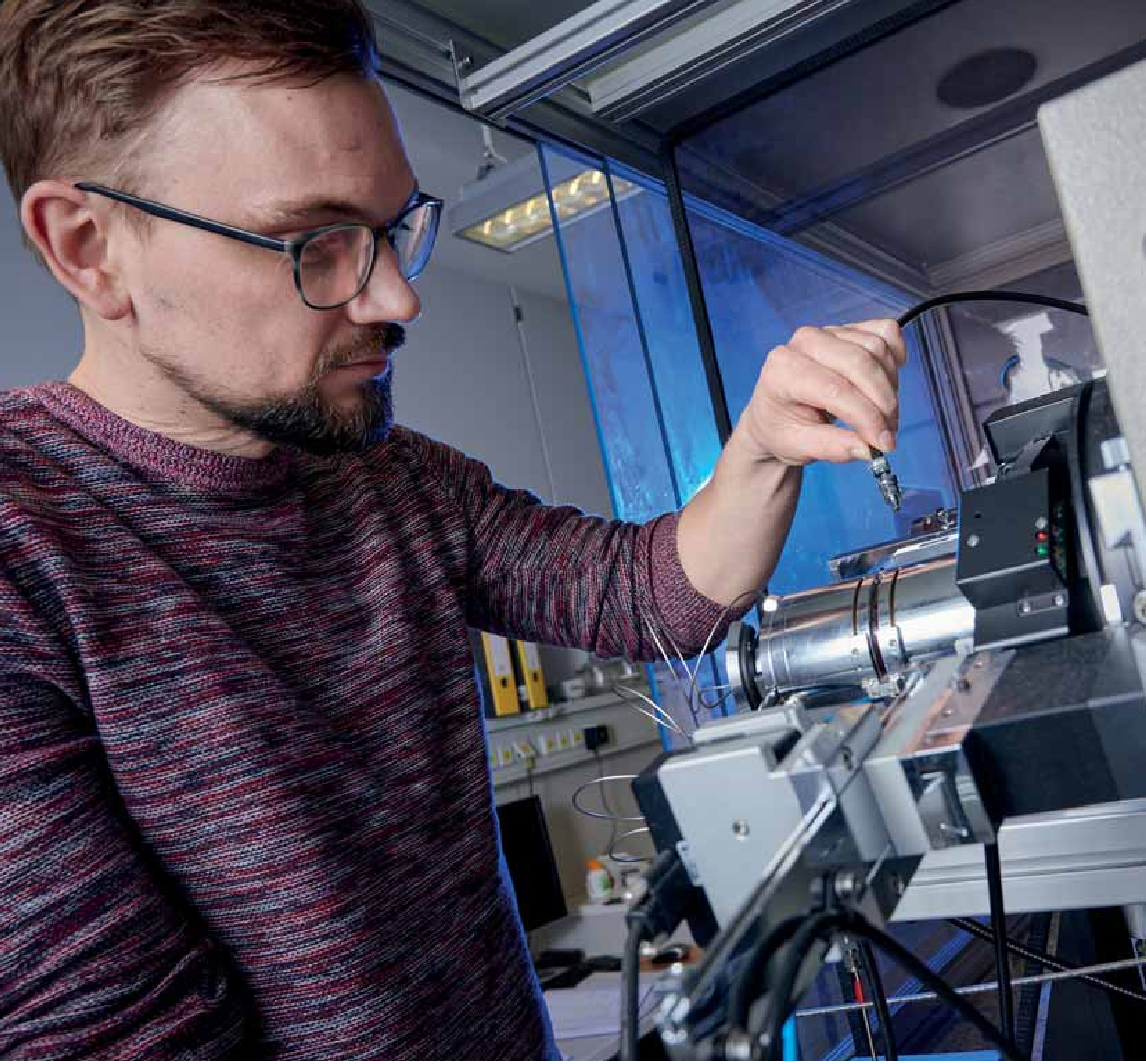
Further milestones on the way to relevant reaction conditions for *in situ* investigations of catalysts are (i) the installation of a new NAP-XPS spectrometer (Near Ambient Pressure) at LIKAT and (ii) an innovative TEM setup with special sample holders for in situ investigations at elevated temperatures and pressures at the interdisciplinary faculty ‘Life, Light & Matter’ of the University of Rostock (funds for this were jointly obtained). The measurements under near-real conditions allow conclusions to be drawn, for example, about reaction conditions or catalyst properties that need to be adjusted.

The comprehensive set of *operando* techniques has been used for monitoring selective oxidations, hydrogenations, photocatalytic as well as environmentally relevant reactions such as selective catalytic reduction of NO_x (NH_3-SCR) and photocatalytic ozonation of organic contaminants in wastewater.

A very illustrative example of the collaboration between different groups in Topic 01 is the development of a special ‘spin-trapping’ method in the research group ‘Magnetic Resonance & X-ray Methods’, which can selectively distinguish between different radicals. With the help of this method, predominantly preparative groups can detect whether reactions are driven by radical mechanisms.

Investigation of structural and electronic properties of heterogeneous and homogeneous photocatalyst and electrocatalyst systems in CO_2 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 a 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, the combination of *operando* FTIR spectroscopy and kinetics as well as chemometrics will be a new experimental advance in the subject area.



RESEARCH GROUPS

Sustainable Redox Reactions
Dr. Kathrin Junge

Optical Spectroscopy & Thermoanalytical Methods
Dr. Christoph Kubis

Magnetic Resonance & X-ray Methods
Dr. Jabor Rabeah

Catalysis with Renewable Resources & Platform Chemicals
Dr. Sergey Tin

Structure-Function Correlations
Prof. Jennifer Strunk

Reaction Mechanisms
Prof. Evgenii Kondratenko

Catalysis of Late Transition Metals
PD Dr. Torsten Beweries

Catalysis of Early Transition Metals
Dr. Fabian Reiß

Bioinspired Catalysis
Prof. Paul Kamer

Inorganic Functional Materials
Dr. Sebastian Wohlrab

Catalytic Functionalizations
Dr. Jola Pospech

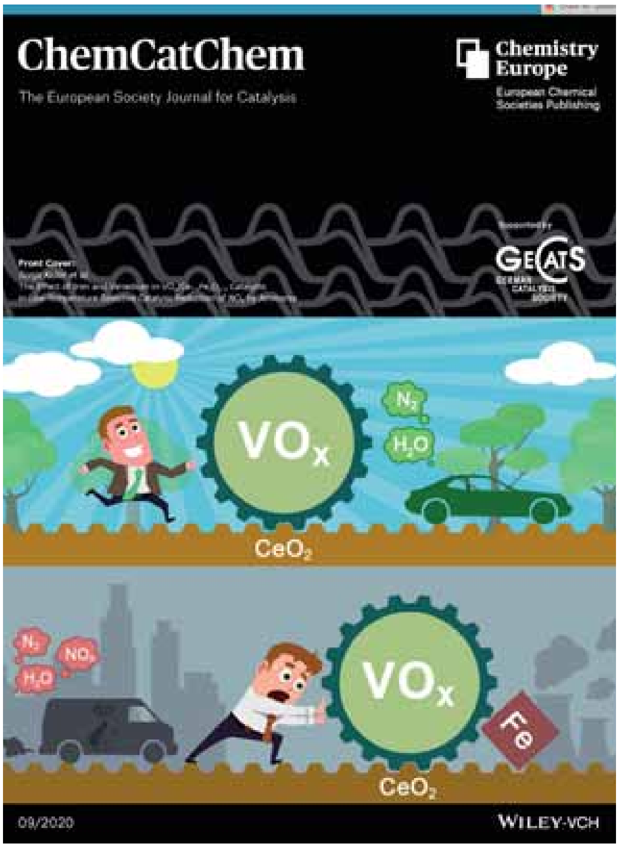
Small Molecule Activation
Dr. Christian Hering-Junghans

Catalytic Cycloadditions
Prof. Dr. Marko Hapke - J. Kepler Univ. of Linz

IMPACT OF V AND M ON MECHANISM AND PERFORMANCE OF $VO_y/Ce_{1-x}M_xO_{2-\delta}$ CATALYSTS IN LOW-TEMPERATURE NH_3-SCR OF NO_x

ABSTRACT: The selective catalytic reduction (SCR) of NO_x by NH_3 is highly important for cleaning of exhaust gases, yet common catalysts such as V_2O_5-WO_3/TiO_2 and Fe- or Cu-containing zeolites work properly only between 300 and 500 °C, which is too high for application in diesel and lean-burn engines. Promising candidates are CeO_2-based catalysts, which show high activity already well below 200 °C, due to their high oxygen mobility and interesting redox properties. Therefor we tried to improve supported $VO_y/Ce_{1-x}MxO_{2-\delta}$ catalysts by doping with metal ions of different valence and redox potential. This work has been performed in close cooperation between the research groups of U. Armbruster and J. Rabeah.

OBJECTIVE: The aim was to explore the effect of replacing Ce^{4+} lattice ions by isovalent M^{4+} (Zr, Ti, Mn) or lower-valent M^{3+} (Fe, Sb, Bi) with different redox potential. While M^{4+} should modify oxygen mobility due to lattice distortion caused by the difference of Ce^{4+} and M^{4+} radii, incorporation of M^{3+} was expected to create oxygen vacancies. Various techniques such as DRIFTS, EPR, UV-vis and XANES/EXAFS spectroscopy were applied in *operando* or *in situ* mode together with catalytic tests for elucidating structure-reactivity relationships and mechanisms.



RESULTS: Almost complete NO_x conversion and N_2 selectivity were obtained at T < 200°C and high flow rates with $VO_y/Ce_{1-x}MxO_{2-\delta}$ (M^{4+} = Zr, Ti, Mn)[1, 2]. The high activity has been related to the unique oxygen transport ability of such $Ce_{1-x}M_xO_{2-\delta}$ solid solutions which was shown to govern the redox activity of the supported VO_y species.
In $Ce_{1-x}M_xO_{2-\delta}$ solid solutions with M^{3+} = Fe, Bi, Sb, catalytic activity of V-free supports follows the order CeSb>CeFe>CeO_2>CeBi and correlates with the formation of Ce-O surface species which promote initial NO oxidation. $VO_y/Ce_{1-x}M_xO_{2-\delta}$ catalysts are more active than corresponding V-free supports, yet the order of NO_x conversion (VSbCe>VCe>VFeCe>VBiCe) is governed by the efficiency of the V^{5+}/V^{4+} redox shuttle which is faster in $VO_y/Ce_{1-x}Sb_xO_{2-\delta}$ than in VO_y/CeO_2 but lower when M=Fe and Bi. Activity of V-free supports is raised by increasing Brønsted acidity after treatment with H_2O/SO_2 containing feed while no positive effect was observed for $VO_y/Ce_{1-x}MxO_{2-\delta}$, since the redox properties of VO_y dominate over the impact of surface acidity.

OUTLOOK: We are now going to use the acquired knowledge on the redox properties of $Ce_{1-x}M_xO_{2-\delta}$ solid solutions to optimize those materials for simultaneous absorption of CO_2 from air and its selective conversion to methanol within a new collaboration project sponsored by the Leibniz-Gemeinschaft within the 'Pakt für Forschung'.

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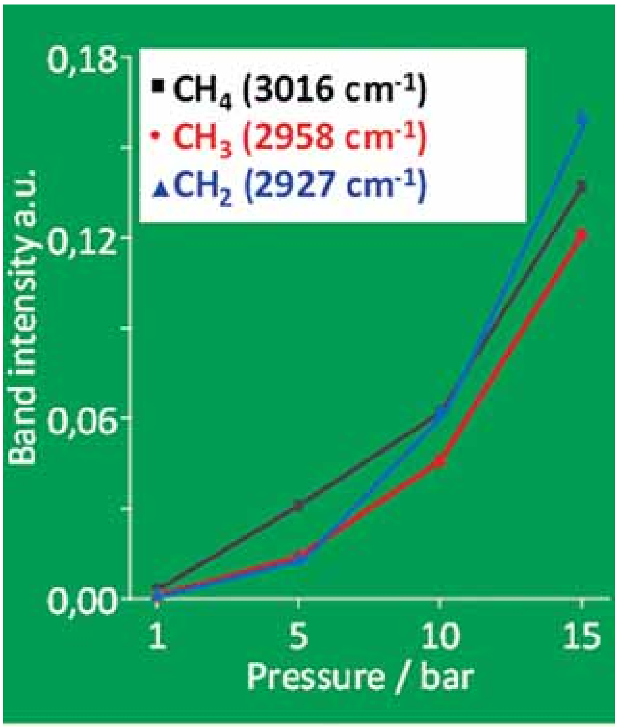
IRON-BASED CATALYSTS FOR CO_2 CONVERSION INTO HIGHER HYDROCARBONS UNDER DYNAMIC CONDITIONS

ABSTRACT: CO_2 hydrogenation to higher hydrocarbons offers a sustainable path to valuable chemicals if H_2 is produced using renewable energy. As such energy is provided in a non-continuous manner, applied catalysts should be robust to changes in reaction temperature or feed composition without losing their desired performance. To address these challenges, we develop catalysts for dynamic operation.

OBJECTIVE: The main objective of this project in the frame of the DFG SPP 2080 is to understand basics for the purposeful development of Fe-based catalysts for CO_2 hydrogenation to higher hydrocarbons (CO_2-FT) with low selectivity to CH_4 under dynamic conditions. We focus especially on mechanistic and kinetics aspects related to reaction-induced changes of catalyst structure/composition and to the hydrogenation reaction itself.

RESULTS: In this project, the research groups Bentrup, Kondratenko from LIKAT and Kraehnert from TU Berlin are working together in a complementary manner. They possess broad expertise in *operando* studies, transient and steady-state kinetic/mechanistic analysis, and controlled material synthesis.



Effect of total pressure on the formation of various adsorbates.

As a first step towards targeted catalyst design, literature data about CO_2-FT were analyzed by various statistical methods.[1] The Pauling electronegativity of metal dopant for Fe_2O_3 was identified to be an appropriate descriptor affecting catalyst activity and selectivity. In addition, the selectivity to higher hydrocarbons and the olefin/paraffin ratio are improved when combining promoters based on oxides of alkali and transition metals. On this basis, we developed a K-Mn/Fe_2O_3 catalyst with the selectivity to higher hydrocarbons of 83.1 % at CO_2 conversion of 42 %.

We also proved that catalyst composition changes along the bed length under CO_2-FT. A correlation between product selectivity and the steady-state composition was established. In addition, reduction treatment prior CO_2-FT was shown to affect the dynamics of reaction-induced catalyst restructuring and accordingly product distribution.

A cell for operando catalyst characterization by means of IR spectroscopy was developed and successfully validated for CO_2-FT at pressures up to 15 bar (Figure). It is possible to monitor both surface adsorbates and gas-phase under real reaction conditions. Such analysis is instrumental for deriving molecular insights into product formation in CO_2-FT under dynamic and steady-state operation.

OUTLOOK: Our activities are further focused on (i) establishing the rules regulating catalyst structure/composition under dynamic and steady-state CO_2-FT conditions and (ii) identifying the relationships between operando catalyst composition and

In-house developed cell for *operando* IR-studies of catalytic material.

activity/selectivity. The derived insights should enable a rational design of improved catalysts and be used as general guidelines for efficient catalyst operation.

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TOPIC 02

Prof. Evgenii Kondratenko
Prof. Haijun Jiao

KINETICS, THEORY & MECHANISMS

The focus of Topic 02 is on mechanistic and kinetic aspects of heterogeneous, homogeneous, electro- and photocatalysis.

The subject of ongoing investigations are various large-scale, future-oriented and sustainable catalytic processes. The main goal is to derive correlations between macroscopic observations in reactors with the microscopic structure of catalytic active sites/phases and reaction microkinetics at as elementary a level as possible.

Several research groups from complementary fields are collaborating to achieve this goal.

Transient (time-resolved) experiments with isotope-labeled molecules, steady-state kinetic and mechanistic measurements, and spectroscopic catalyst characterization are used to identify individual reaction steps and determine their kinetic parameters. With mathematical modeling and numerical analysis of time-resolved experiments and density functional theory (DFT) calculations, it is possible to obtain nearly elementary kinetic and mechanistic information. The combination provides a very detailed view of the mode of action of a wide variety of catalysts.

One focus is on catalyst development supported by mechanistic and kinetic investigations as well as optimization of reactor operation in order to carry out catalyzed reactions as efficiently as possible. For this purpose, various techniques and methods are applied and combined.

Chemometric methods allow the extraction of pure component spectra and concentration profiles of substrates and products as well as catalyst complexes and intermediates from time-resolved FTIR spectra. These are used for the qualitative description of the reaction network.

An integral part of the Topic's research is the combination of kinetic measurements (*in situ/operando* NMR, UV-Vis spectroscopy, catalytic studies) coordination chemistry studies (NMR, UV-Vis, X-ray), time-resolved product analysis, steady-state isotopic transient kinetic analysis and DFT calculations to elucidate reaction mechanisms and to obtain reaction kinetics.

The establishment of vibrational spectroscopy (such as high pressure in situ spectroscopy) supported by DFT calculations offers the potential to identify catalytically active species and develop kinetics for complex and cluster formation. Simultaneous combination with electrochemistry (for spectrochemistry) provides information on structural changes and charge transfer of reactants.

Collaboration in Topic 02 promotes rationalization of experimental results, based on which suggestions can be made for optimizing reaction conditions, improving reaction sequences, and planning new experiments.

RESEARCH GROUPS

Theory of Catalysis
Prof. Haijun Jiao

Optical Spectroscopy &
Thermoanalytical Methods
Dr. Christoph Kubis

Magnetic Resonance & X-ray Methods
Dr. Jabor Rabeah

Reaction Mechanisms
Prof. Evgenii Kondratenko

Mechanisms in Homogeneous Catalysis
Prof. Detlef Heller

Small Molecule Activation
Dr. Christian Hering-Junghans

Vibrational Spectroscopy
Prof. Ralf Ludwig - Univ. of Rostock

Numerical Analysis
Prof. Klaus Neymeyr - Univ. of Rostock

DEVELOPMENT OF ALTERNATIVE-TYPE CATALYSTS FOR NON-OXIDATIVE DEHYDROGENATION OF PROPANE TO PROPENE

ABSTRACT: Owing to the developments of shale gas technology and demand for propene, non-oxidative propane dehydrogenation (PDH) has attracted growing attention. However, commercial catalysts suffer from costs of Pt or toxicity of Cr(VI). To overcome these faults, we developed and validated a concept for preparation of alternative-type catalysts based on ZrO_2. They became novel ‘state-of-the-art catalysts’.

OBJECTIVE: In contrast to the most of literature studies using supported catalysts, we develop bulk catalysts. Our idea behind is that surface defects of non-reducible metal oxides can catalyze alkane transformations. This concept was proven in our previous studies using ZrO_2-based catalysts for PDH. The main aims of our recent studies in the frame of a DFG project (E. Kondratenko and H. Jiao, 2017 – 2020) were to identify structure of active sites, to understand basics relevant for catalyst synthesis and to check applicability of catalysts developed.

RESULTS: The performed work includes synthesis of well-defined catalysts, their detailed characterization, mechanistic tests and density functional theory (DFT) calculations in cooperation with the research groups Rabeah, Bentrup/Kubis, Rodemerck, and ‘Analytics’ of LIKAT, Prof. Grunwaldt (Karlsruhe), and Prof. Jiang (Beijing). DFT calculations predict that two coordinatively unsaturated Zr cations (Zr_{cus}) of tetragonal or monoclinic ZrO_2 form the active site for PDH.[1] Their concentration depends on the ability of ZrO_2 to release lattice oxygen. This property can be tuned through the usage of a metal (Cr, La, Sm or Y) oxide promoter for ZrO_2 or/and supported metal (Ru, Rh, Ir or Pt)[2] or ZnO_x.[3] The highest positive promoter effect was established when ZrO_2 was doped with Cr_2O_3[4]. Ru, Rh, Ir or Pt particles deposited on ZrO_2 increase intrinsic activity of Zrcus located at them[5] and influence side reactions[2], with Ir and Pt effectively hindering coke formation.

The derived knowledge was successfully applied for the development of novel catalysts based on Gd_2O_3 or Eu_2O_3.[6] Thus, our approach is of general character and may be used for synthesis of other alternative-type catalysts.

Finally, our best materials outperform an analogue of commercial K-CrO_x/Al_2O_3 tested under same conditions (Fig. 1) and have already aroused interest of several companies.

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OUTLOOK: The application potential of our catalysts for PDH will be further analyzed. Besides, the concept developed for ZrO_2-based catalysts will be extended to other metal oxides to identify general descriptors affecting formation and catalytic properties of defective metal cations in dehydrogenation of C_2-C_4 alkanes.

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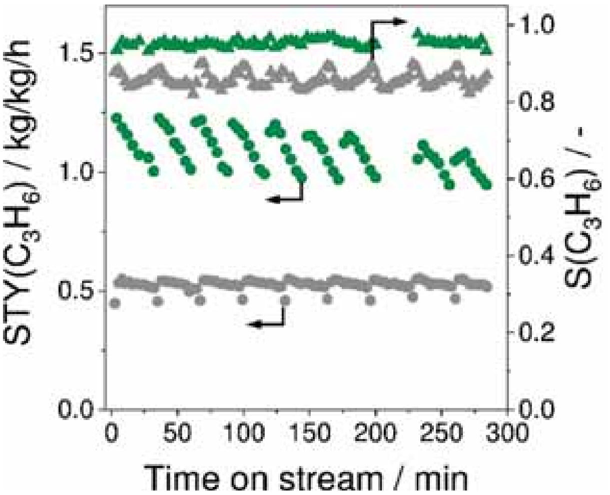

Fig. 1. Space time yield of propene formation ($STY(C_3H_6)$) and the selectivity to propene ($S(C_3H_6)$) over $ZnO_x/TiZrO_x$ (green) and $K\text{-}CrO_x/Al_2O_3$ (grey) in 10 PDH/regeneration cycles.

Synergy Effect between ZrO_2 and CrO_x in Supported $CrZrO_x$ for Propene Formation in Non-oxidative Propane Dehydrogenation.

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THEORY OF CATALYSIS

ABSTRACT: Different collaborations in Topic 02 dedicated to the understanding the mechanisms of catalytic hydrogenation[1,2], dehydrogenation[3,4], transfer hydrogenation[5] and dehydrocoupling[6,7,8] reactions using non-noble Mn-, Fe-, Co- and Ni-based catalysts.

OBJECTIVE: The main goal is the synergistic cooperation between experiment and theory to understand the experimental findings and in turn to make rational suggestions for optimizing reaction conditions, improving reaction procedures and planning new experiments.

RESULTS: In the reaction of manganese catalyzed isomerization of allylic alcohols to ketones (Fig. 1), the following mechanistic aspect was found: (a) Allylic alcohol (**1**) dehydrogenation has the highest barrier and is the rate-determining step. This explains the need of high temperature. (b) The catalyst interconversion has lower barrier than allylic alcohol dehydrogenation what explains the need of high pressure to maintain the stability of catalysts. (c) The subsequent 1,4-hydrogenation of α,β-unsaturated ketone (**4**) is more favored kinetically than 1,2-addition. This could be verified by the isolation of the α,β-unsaturated ketone as intermediate and deuterium labeling experiment. (d) The ketone (**2**) from the isomerization of allylic alcohol is the main product as found experimentally. (e) Direct hydrogenation of allylic alcohol (1) to saturated alcohol (**3**) is not competitive due to the much high barrier. (f) The saturated alcohol can be formed from ketone hydrogenation due to the close barrier to allylic alcohol dehydrogenation. A short reaction time is needed for high yield of desired product. (g) It also provided a rationale for the observed selectivity and the higher efficiency of phenyl over isopropyl substitution at the phosphorous.

In the chemoselective semihydrogenation of alkynes catalyzed by manganese(I)-PNP pincer complexes (Fig. 2), it is found that (a) the catalyst has high stability toward CO dissociation and is also stable for the semihydrogenation; (b) an outer-sphere mechanism is operative. (c) The high selectivity of the *Z*-product (**2a**) was due to the low barrier. (d) Low H_2 pressure (5 bar), low temperature (30 °C) and short reaction time (4 h) lead to high yield (99 %) and *Z*-selectivity (99 %). (e) A too high temperature lowers H_2 concentration in solution and suppresses the reaction.

OUTLOOK: On the basis of our very cooperative and productive work, we will continue our cooperation not only in the reactions involving H_2 but also reactions relating with practical applications. We wish to design new generation catalysts with

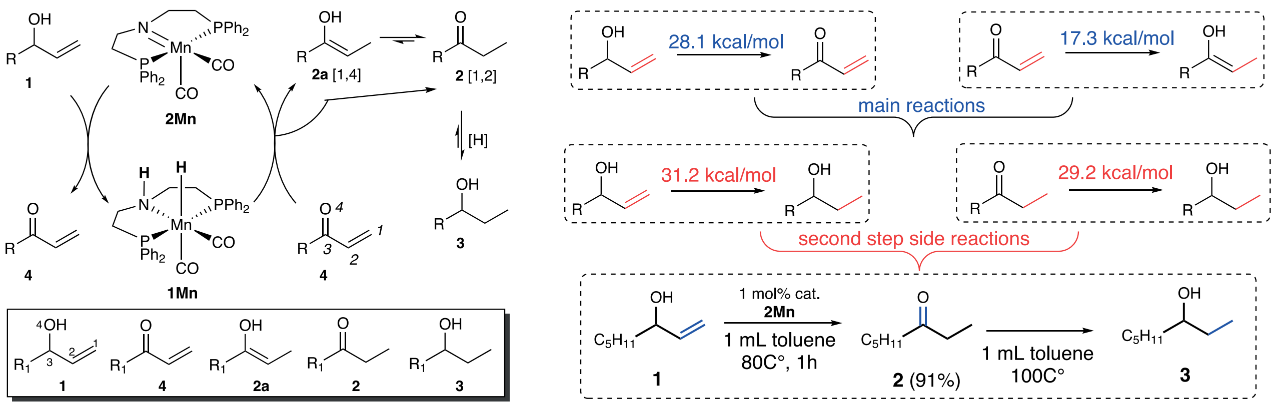

Fig. 1. Proposed reaction mechanisms of allyl alcohol dehydrogenation and isomerization to ketone (left) and computed Gibbs free energy profile for the isomerization of **1** to **2** (right).[5]

the respect of economy, ecology and green and sustainable chemistry.

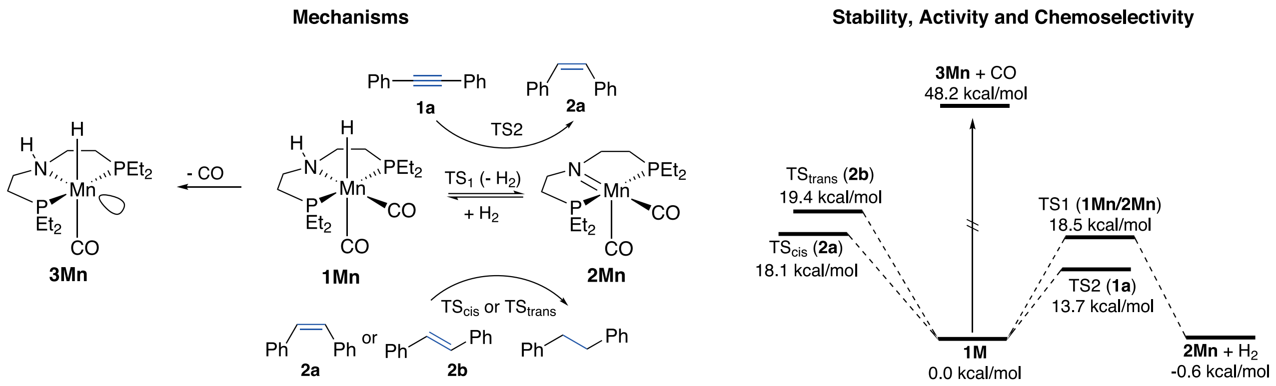

Figure 2. Proposed bifunctional outer-sphere mechanism for the Mn-catalysed hydrogenation of alkyne **1a** and alkenes **2** (left) and the computed Gibbs free energy surfaces (right).[2]

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TOPIC 03

Dr. David Linke
Dr. Udo Armbruster

REACTION ENGINEERING & IMPLEMENTATION

Along with Topics 01 and 02, Topic 03 is one of the methodologically and technologically oriented topics at LIKAT.

With regard to reaction technology, the core task of Topic 03 is the development of the best possible design and the determination of an optimal mode of operation for reactors to carry out homogeneously and heterogeneously catalyzed chemical reactions. Different reactor concepts can be evaluated, but also reactor and process concepts can be developed together. Core elements are reaction kinetics, fluid dynamics, and mass and heat transport, which form the basis for modeling and optimizing reactor performance. In addition to the catalytic reaction, process engineering aspects of catalyst synthesis are also addressed.

Core implementation tasks include (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.

Construction of the LIKAT *Transfer Technology Center* began in the fall of 2019. Since SMEs and non-chemistry-specific user industries usually do not have facilities for transferring innovative laboratory results to pilot scale, it makes sense to keep the know-how for piloting available at LIKAT to support these users in transferring.

To realize this vision, research groups from different research departments work together. For industry, Topic 03 is a competent partner for the transfer of new developments in catalysis from basic research to application. In both heterogeneous and homogeneous catalysis, several projects with industry target reaction engineering or upscaling aspects. To support these activities, Topic 03 operates and (partly) develops experimental facilities of different scale (from microreactor to miniplant scale) that provide high quality data.

To guarantee controlled synthesis of catalysts, it is important to monitor all parts of the synthesis, such as dosing of solutions or precipitants, mixing, control of pH, etc. This involves the combination of different reactor techniques and analytical methods. A more detailed knowledge of the role of the different parameters on the synthesis also minimizes the risk of failure when upscaling a catalyst synthesis

Currently, various modern and sustainable catalytic processes for fine and bulk chemistry are being developed in Topic 03. This includes, among other things, studies on catalyst activation and deactivation as well as start-up and shut-down behavior. Scale-up of catalyst synthesis is also becoming increasingly important.

In the future, ‘Data Science’ within NFDI4Cat will add another focus on research data management.

RESEARCH GROUPS

Applied Carbonylations
Dr. Ralf Jackstell

Homogeneous Catalysis for Life Sciences
Dr. Helfried Neumann

Synergy betrween Homogeneous & Heterogeneous Catalysis
Dr. Jagadeesh Rajenahally

Micro Reaction Engineering
Dr. Norbert Steinfeldt

Reaction Engineering
Dr. David Linke

High-Throughput Technologies
Dr. Uwe Rodemerck

Mechanisms in Homogeneous Catalysis
Prof. Detlef Heller

New Hydroformylation Catalysts
Dr. Detlef Selent

Technology-Oriented Processes
Dr. Udo Armbruster

Liquid Phase Oxidations
Dr. Angela Köckritz

Inorganic Functional Materials
Dr. Sebastian Wohlrab

Polymer Chemistry & Catalysis
Prof. Udo Kragl - Univ. of Rostock
Dr. habil. Esteban Mejia

STUDY OF REACTION NETWORK OF THE ETHYLENE-TO-PROPENE REACTION BY MEANS OF ISOTOPICALLY LABELLED REACTANTS

ABSTRACT: The reaction network of direct conversion of ethylene to propene (EtP) is still under debate. Particularly it is controversially discussed, if metathesis is part of the reaction network. By using 13C- and 12C-labelled feed components we could show that metathesis does not play a major role in the reaction. Instead a complicated set of reactions of forming longer olefins by C-C coupling and cracking them to lower olefins happens.[1]

OBJECTIVE: Ethylene can be directly converted to propene over different Ni containing catalysts; the highest propene yields have been obtained over Ni/Al-MCM-41 prepared by complicated template-ion exchange method[2] and over Ni/silica-alumina prepared by incipient wetness impregnation method.[3] A reaction network comprising three steps has been suggested in the past: (1) ethylene dimerization to 1-butene on Ni sites, (2) 1-butene isomerization to 2-butene on acidic sites of the support and (3) metathesis of 2-butene with ethylene to propene on Ni sites.[2, 4] The third step is under debate since Ni was never shown before to be active for metathesis. Alternatively, a conjunct polymerization producing a complex mixture of saturated and unsaturated hydrocarbons has been suggested.[5]

The aim of the present study was to investigate the reaction mechanism of the third step in the reaction sequence of the EtP reaction, the reaction of ethylene with trans-2-butene. Particularly, it should be checked if propene is formed via metathesis of these two molecules or through another reaction pathway(s). To this end we used ethylene labelled with the isotope ^{13}C and let it react with trans-2-butene containing only ^{12}C atoms. In case of metathesis the formed propene should contain one ^{13}C and two ^{12}C atoms. We also analyzed the fraction of ^{12}C and ^{13}C atoms in all other reaction products.

RESULTS: We studied the reaction of ^{13}C labelled ethylene with ^{12}C containing trans-2-butene over two catalysts, Ni/Al-MCM-41 and Ni/silica-alumina. The reaction products were separated by gas chromatography and their isotopic composition was analyzed by mass spectrometer. Pure metathesis reaction should result in propene containing one ^{13}C and two ^{12}C atoms. However, different isotopologues of propene were formed; the majority contains only ^{12}C atoms showing that it must be formed from the butene feed molecule (Fig. 1). Propene containing one ^{13}C and two ^{12}C atoms was observed only in traces excluding metathesis as a major pathway of its formation.

Besides propene, other olefins with up to six C atoms were obtained, and their isotopic composition was analyzed, too. As an example, the isotopologues of 1-butene are shown in Fig. 1. 1-Butene with four ^{12}C atoms can be easily formed at acidic sites of the catalyst by isomerization of the ^{12}C-trans-2-butene and thus represents the majority among 1-butene isotopologues (not shown in Fig. 1). However, besides ^{12}C-1-butene other

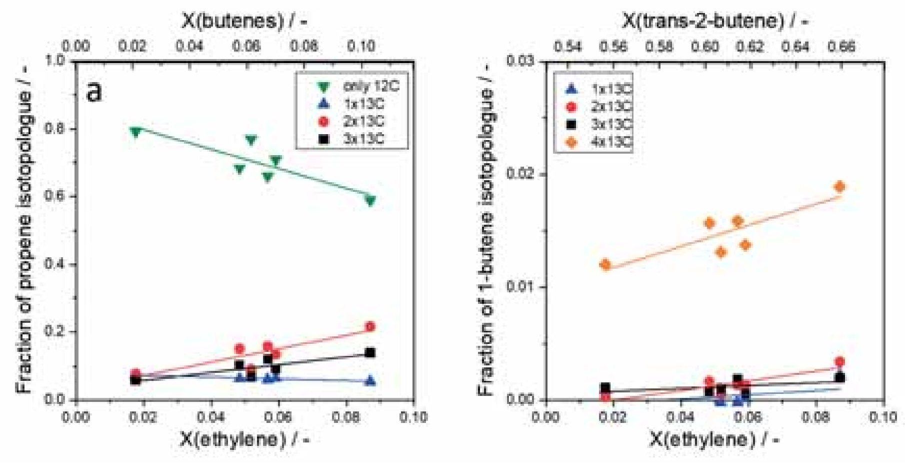

Fig. 1. Reaction between ^{13}C-ethylene and ^{12}C-trans-2-butene over Ni/silica-alumina. Fractions of ^{12}C und ^{13}C atoms in the reaction products propene und 1-butene in dependence of conversion. 1-Butene with four ^{12}C atoms is not shown. Adapted from [1].

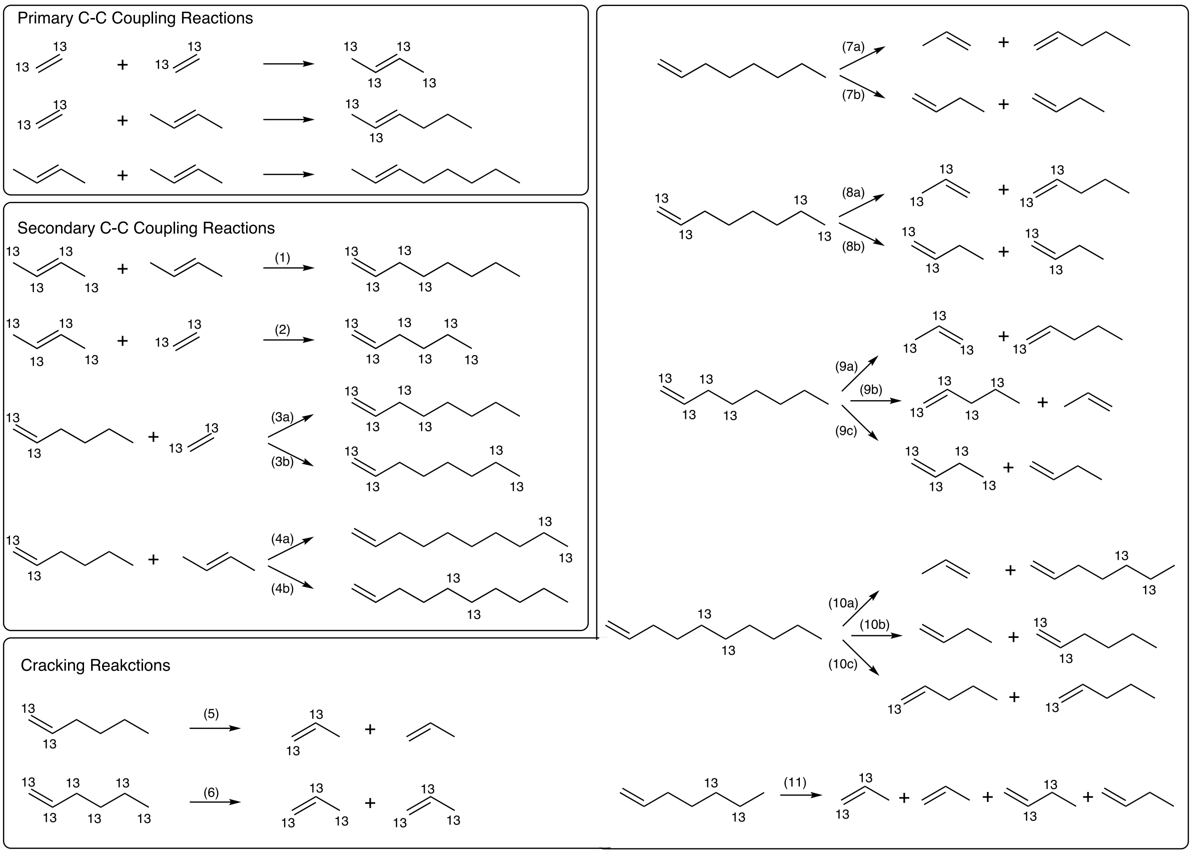

Fig. 2. Reaction between ^{13}C-ethylene and ^{12}C-trans-2-butene. Formation of intermediates and reaction products containing different numbers of ^{12}C und ^{13}C isotopes. Adapted from [1].

isotopologues containing one to four ^{13}C atoms, were obtained, too. Among them, the molecule with four ^{13}C atoms presents the majority. It is most likely, that it was formed by dimerization of ^{13}C-ethylene. Also, the formed ethylene, pentenes and hexenes contain different numbers of ^{12}C and ^{13}C atoms. From the occurrence and fractions of the C isotopes in the different products a complex reaction scheme was deduced that contains various C-C coupling and cracking reactions (Fig. 2). The former can be catalyzed by both Ni and acidic sites whereas for cracking reactions acidic sites are mandatory.

The two studied catalysts, Ni/Al-MCM-41 and Ni/silica-alumina differ in strength and number of surface acidic sites with the latter being more acidic. Consequently, over the two catalysts, a different distribution of ^{12}C and ^{13}C atoms in the produced olefins was obtained.

OUTLOOK: Our study excluded metathesis as a major reaction in the reaction scheme of EtP reaction. Instead, complex scheme of C-C coupling and cracking reactions can explain all reaction products and the fractions of ^{12}C and ^{13}C atoms contained therein. Besides Ni sites, acidic sites of the catalyst play a vital role. Consequently, tuning the surface acidity of supported Ni catalysts offers the way to improve catalyst selectivity.

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HYDROGENOLYSIS OF TETRAHYDROFURFURYL ALCOHOL TO 1,5-PENTANDIOL IN A CONTINUOUS-FLOW MICROREACTOR

ABSTRACT: Ni on various lanthanide oxides is a very selective, active and also long-term stable catalyst for the hydrogenolysis of bio-based tetrahydrofurfuryl alcohol (THFA) to 1,5-pentanediol (1,5-PeD) in the liquid phase. In isopropanol, yields of 1,5-PeD of 87 % were obtained in a batch reactor and of 72 % in a continuously operated microreactor.

OBJECTIVE: Terminal diols derived from renewables are desired building blocks for bio-based polyesters and polyurethanes. C5 monomers such as 1,5-PeD are attracting particular interest because they are not available in large quantities from petrochemical feedstocks. In polymers, 1,5-PeD contributes to a good balance between hardness and flexibility, and the materials possess a low viscosity and low glass transition temperature.[1] Furan-derived compounds accessible from cellulose should be investigated as starting material. Since continuous processes are favorable for technical applications, and very good selectivities to the desired products can often be achieved by setting an optimum residence time, continuous processing should be investigated. Since the best conversions and selectivities to 1,5-PeD were achieved in the literature mainly by means of expensive supported noble metal catalysts (e.g. Rh/ReOx/SiO_2),[2] we looked for cheaper alternatives for active and selective catalysts.

RESULTS: After an extensive catalyst screening in the batch reactor, nickel catalysts on lanthanide oxides, such as La_2O_3, Pr_2O_3, Sm_2O_3, and Nd_2O_3, were identified as particularly active, but more importantly, selective to 1,5-PeD. The best yield (87 %) of 1,5-PeD at 88 % selectivity was obtained with Ni/Pr_2O_3. The four types of catalysts were then used in a commercial modular microreactor system (Fig. 1, Ehrfeld Mikrotechnik BTS) under continuous liquid phase flow conditions. The preparation methods of catalysts and reaction conditions, such as temperature, H_2 pressure, concentration, and solvent, were optimized.

The reaction was found to proceed mainly as a transfer hydrogenation, and the most suitable solvent, and hydrogen donor at the same time, was isopropanol. However, the presence of molecular hydrogen significantly increased partly the catalyst activity and selectivity. With Ni/La_2O_3, up to 82 % conversion of THFA at 88 % selectivity to 1,5-PeD, and with Ni/Sm_2O_3, up to 70 % conversion of THFA at 72 % selectivity to 1,5-PeD could be achieved. In a long-term experiment (Fig. 2), where the reac-

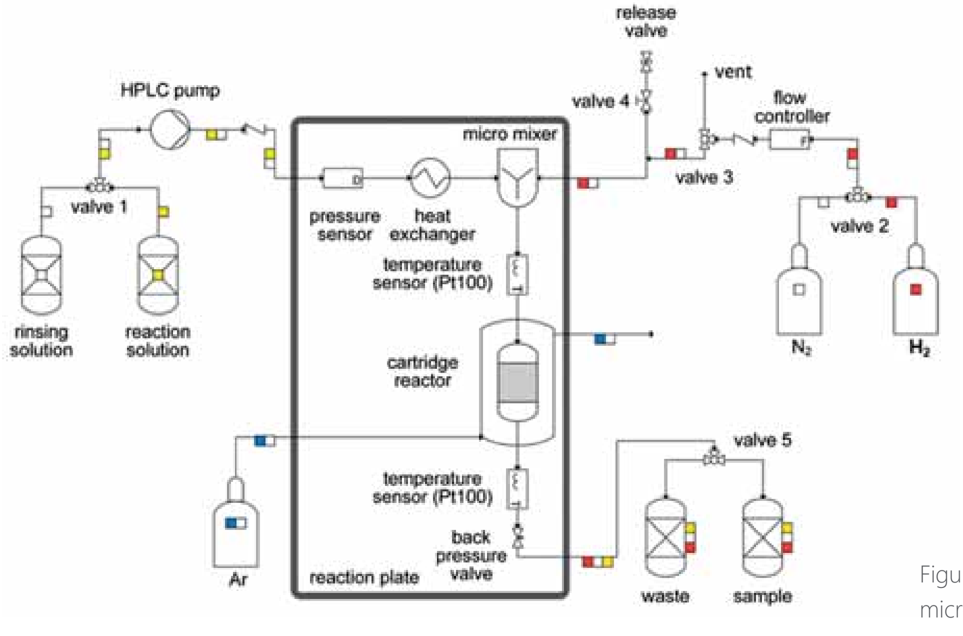

Figure 1. Scheme of the microreactor set-up.[3]

tion temperature was simultaneously varied between 135 and 150 °C, a Ni/La$_2$O$_3$ catalyst was still as active after 384 h as at the beginning of the experiment. The best selectivity obtained to 1,5-PeD was 94 % at 72 % conversion.

Very active, selective, and long-term stable catalysts have been provided for the continuous production of 1,5-PeD from bio-based feedstock.[4]

OUTLOOK: Other suitable substrates, bio-based if possible, will be included into the studies to generate diols of different chain length. In addition, investigations of the reaction mechanism are to be continued.

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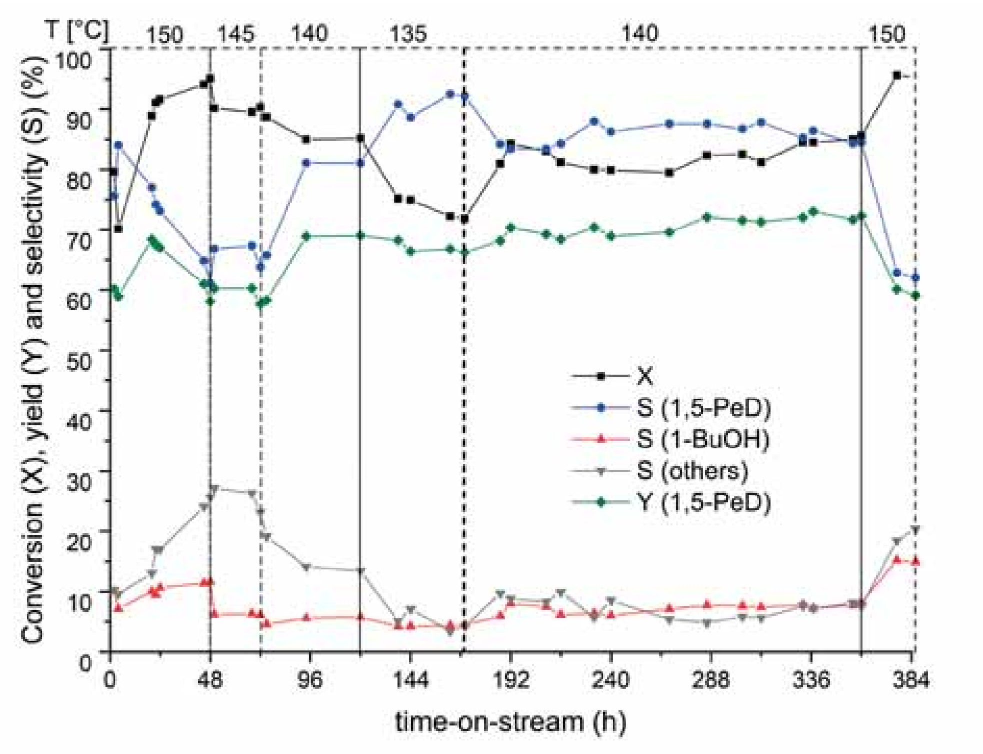


Figure 2. Influence of reaction temperature on conversion, yield of 1,5-PeD and product selectivities in the hydrogenolysis of THFA in a continuous microreactor with Ni/La$_2$O$_3$ (m_{cat} = 3.0 g, $\dot{n}_{THFA}$ = 0.024 mmol/min, Q_{liquid}= 0.25 mL/min, p = 30 bar).

TOPIC 04

Prof. Johannes G. de Vries
PD Dr. Thomas Werner

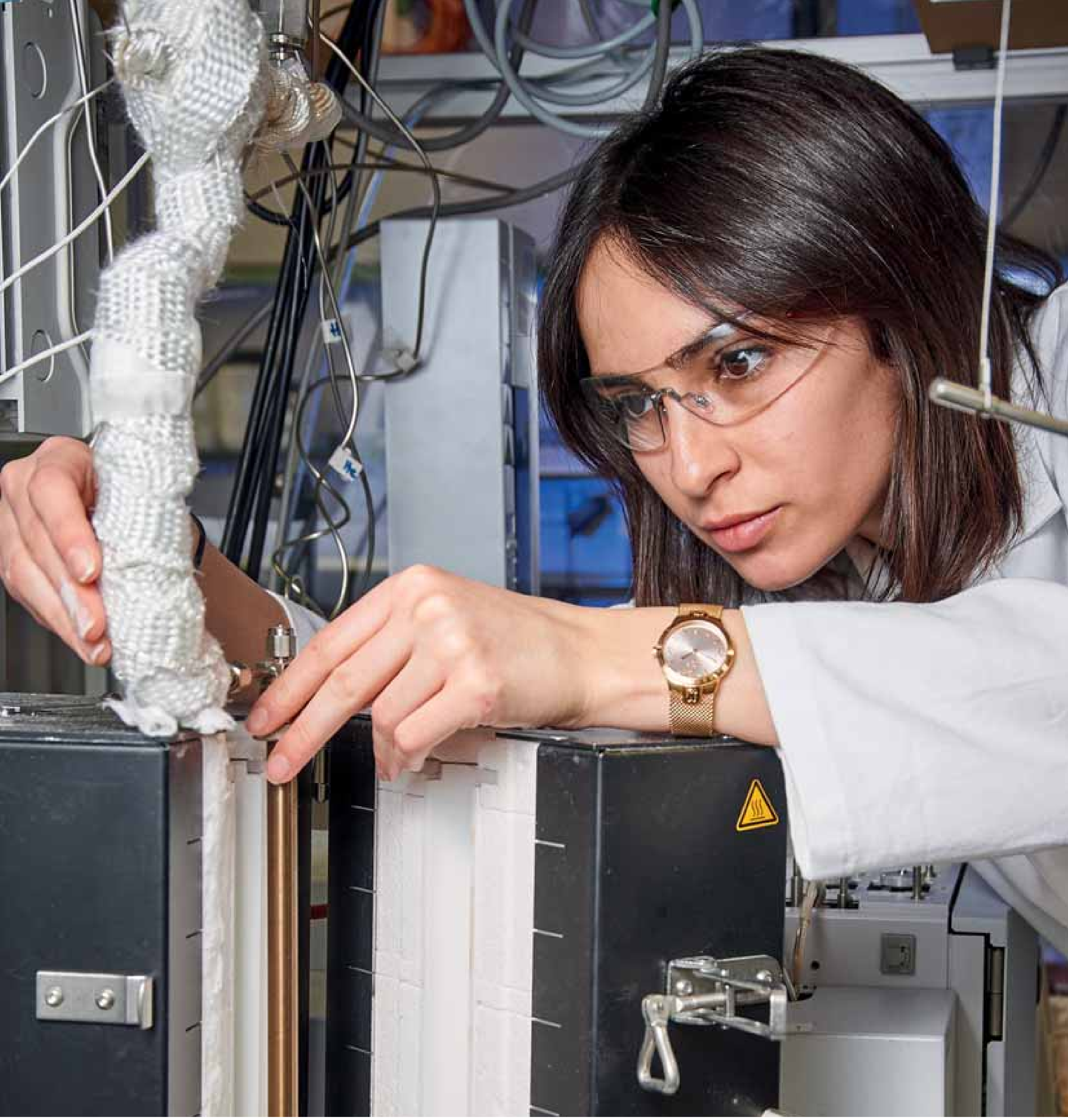
RENEWABLE RESOURCES

Topic 04 bundles expertise in the field of renewable raw materials. The focus is on research into the catalytic conversion of renewable raw materials into basic chemicals for products used in our daily lives. For example, lignocellulose obtained from wood waste and its components or fatty acids and terpenes can be used to produce various polymers, agrochemicals, solvents or flavorings.

The first step is to convert the biomass into so-called platform chemicals. These can usually be produced in large quantities in simple and high-yield reactions and are suitable as synthesis building blocks for numerous other compounds. Subsequently, these platform chemicals, such as glycerol, levulinic or lactic acid, HMF or furfural, are converted in further catalyzed steps into the desired existing or new chemicals with the desired properties. Carbon dioxide is also used as a raw material. The challenge lies in activating the thermodynamically extremely stable compound.

Until now, mainly homogeneous and heterogeneous catalysts have been used. Through our collaboration in new Leibniz Science Campus *ComBioCat*, biocatalysis (in cooperation with the University of Greifswald) and low-temperature plasma technologies (with INP Greifswald) can now also be used.

Topic 04 facilitates excellent cooperation with industry in many projects: Renewable monomers for use in adhesives are being developed together with the Henkel company. Long-standing cooperations with Symrise AG are dedicated to the production of fragrances and flavors based on biomass. Chitin, waste from shellfish, or residues from rice husks are also used as catalyst bases or carriers for heterogeneous catalysts.



RESEARCH GROUPS

Sustainable Redox Reactions
Dr. Kathrin Junge

Catalysis with Renewables & Platform Chemicals
Dr. Sergey Tin

Organocatalysis
PD Dr. Thomas Werner

Bioinspired Catalysis
Prof. Paul Kamer

Liquid Phase Oxidations
Dr. Angela Köckritz

Inorganic Functional Materials
Dr. Sebastian Wohlrab

Polymer Chemistry & Catalysis
Prof. Udo Kragl - Univ. of Rostock
Dr. habil. Esteban Mejia

GLUE FROM WOOD

ABSTRACT: Levulinic acid is a chemical that can be made from wood in excellent yield. In a large European project with several industrial and academic partners, this process was scaled up and processes were developed for further conversion to solvents and resins that will be used as components in glues.

OBJECTIVE: One of the major goals of the research group Tin is to prepare chemicals from renewables via catalytic routes. The group 'Renewable Ressources' is partner in a large European project called 'GreenSolRes' (https://greensolres.eu), funded by the Bio-Based Industry Joint Undertaking (BBI-JU), together with industrial partners (GFBiochemicals, BASF, Lenzing, Henkel) as well as other academic partners and research organisations. The goal of the project was the production of levulinic acid from wood on demonstration scale, hydrogenation of levulinic acid to three different molecules (GVL, 2-MeTHF and 1,4-pentanediol) and finding applications of the three hydrogenation products.

RESULTS: Our role in the project was to develop components for adhesives from these levulinic acid-derived compounds. In the end, successful oligomers for adhesives were prepared from 2-MeTHF and 1,4-pentanediol;[1,2] investigation of the applicability of the rather unreactive GVL is still on-going. These polymers are used as components for adhesives by the company Henkel, one of the partners in the project. A number of patents have been filed. As a bonus, one of the polymers based on 1,4-pentanediol showed a very interesting memory effect. A glue based on this material would have great potential, for example, for use on labels for bottles containing pharmaceuticals, which need to be kept at low temperatures. If the bottle is exposed at some point to higher temperatures, it would immediately become obvious from the label, which would come off.

OUTLOOK: Another goal pursued during the project was the recycling of polyesters. Our modern society uses large amounts of plastic objects that at the end of their large are either landfilled or float around in the environment. To deal with this problem we need to develop economic recycling methods. We have developed a method to upcycle (= convert to a higher value product) much used polyesters like PET to polyethers, that can be used as components in glues.[3]

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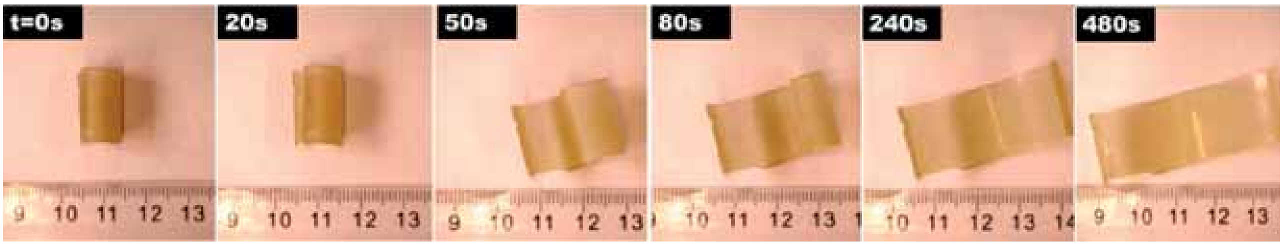
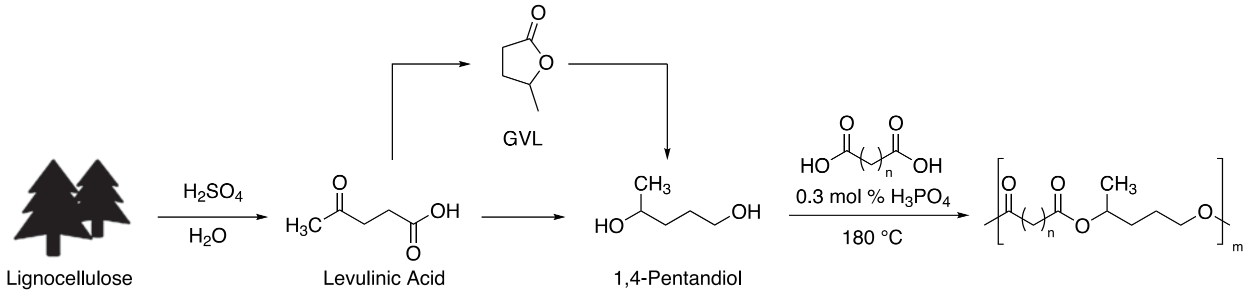



GVL
H2SO4
H2O
Lignocellulose
Levulinic Acid
1,4-Pentandiol
0.3 mol % H3PO4
180 °C
m
n

SUSTAINABLE SOLUTIONS TOWARDS GREEN POLYMERS: THE CASE OF PEF

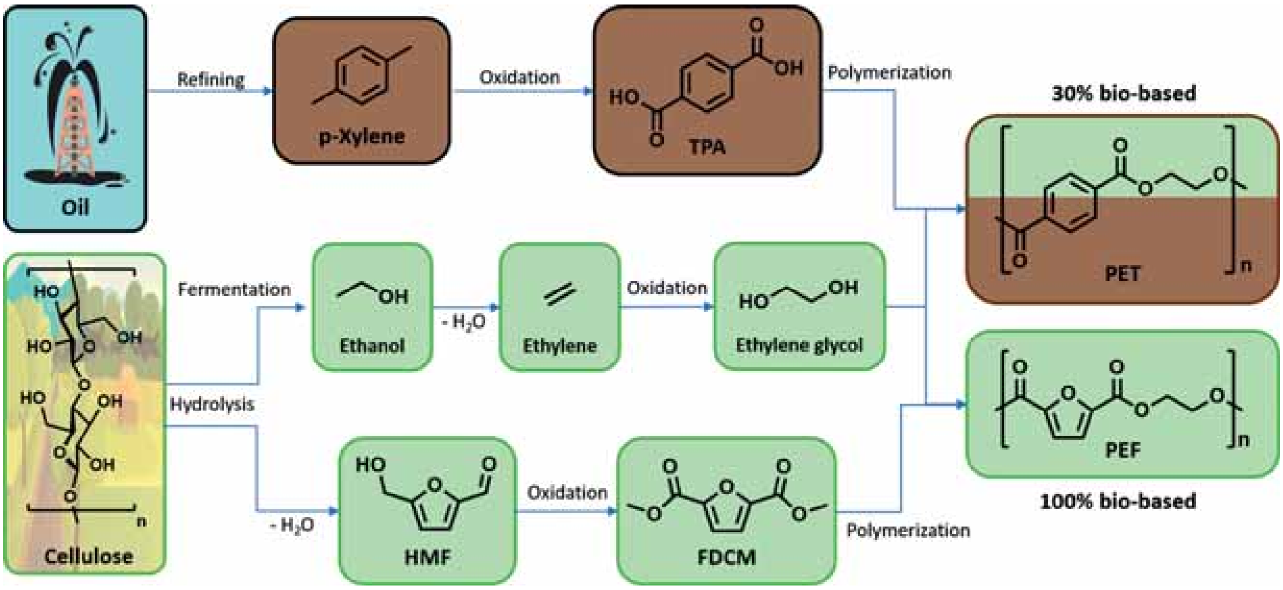
ABSTRACT: The large-scale production of 100% bio-derived PEF, the 'green brother' of PET, has been hampered by the poor processability of its building blocks. Here we describe an alternative process for the sustainable aerobic synthesis of PEF monomers under batch -and flow conditions.

OBJECTIVE: Polyethylene terephthalate (PET) is general-purpose thermoplastic which finds commercial application in many sectors including beverage bottles and food packaging, fabrics, films, parts for automotive, and electronics, among others. PET is a polyester made traditionally from petroleum-derived terephthalic acid (TPA) and ethylene glycol.

The 'green brother' of PET is polyethylenefuranoate (PEF), produced from plant-derived furandicarboxylic acid (FDCA) and ethylene glycol, making it a 100 % biobased polymer. PEF can replace PET in many applications, sometimes even surpassing its performance. The sustainable production of PEF can be entirely made from cellulose, for instance derived from agricultural bio-waste. The bottleneck of this otherwise 'dream-process' lies in the physical and chemical properties of FDCA which make its synthesis, purification and downstream processing challenging. Hence, we have embarked on the synthesis of a more stable, easier to handle FDCA surrogate, namely dimethyl-2,5-furandicarboxylate (FDCM). This diester is easier to purify and is more stable in the polymerization process to produce PEF, therefore, it is economically more suited as starting material than FDCA.

RESULTS: We developed a green batch process for the quantitative and selective oxidative esterification of Hydroxymethylfurfural (HMF) to FDCM.[1] The conversion was achieved using a bimetallic heterogeneous catalytic system containing ruthenium and cobalt oxide over nitrogen-doped carbon which work in synergy. Each catalyst has his own mechanism of action and the sum of both mechanisms leads to the improved synthesis of FDCM. The process works at mild temperatures (50 °C), uses oxygen from air as oxidant and does not require additional solvents.

With this technology in our hands, we transferred our batch process to micro-flow conditions,[2] for



which a new set of catalysts had to be developed to circumvent certain technical limitations like the catalyst's particle size. The products are continuously collected with a HMF conversion of 98 % and selectivity towards FDCM up to 57 %. The use and adaptation of flow chemistry to this challenging reaction led to a >15-fold increase in the production of FDCM from HMF compared to batch conditions.

OUTLOOK: With this work on the synthesis of FDCM, we set the starting point in the use of flow chemistry for the synthesis of this important molecule and hope the interest of the industry is renewed, as FDCM is the building block for biobased furan polymers, which widens the possibilities of establishing the use of a 100 % biobased polymer like PEF in our everyday life.

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TOPIC 05

Prof. Jennifer Strunk
Dr. Henrik Junge

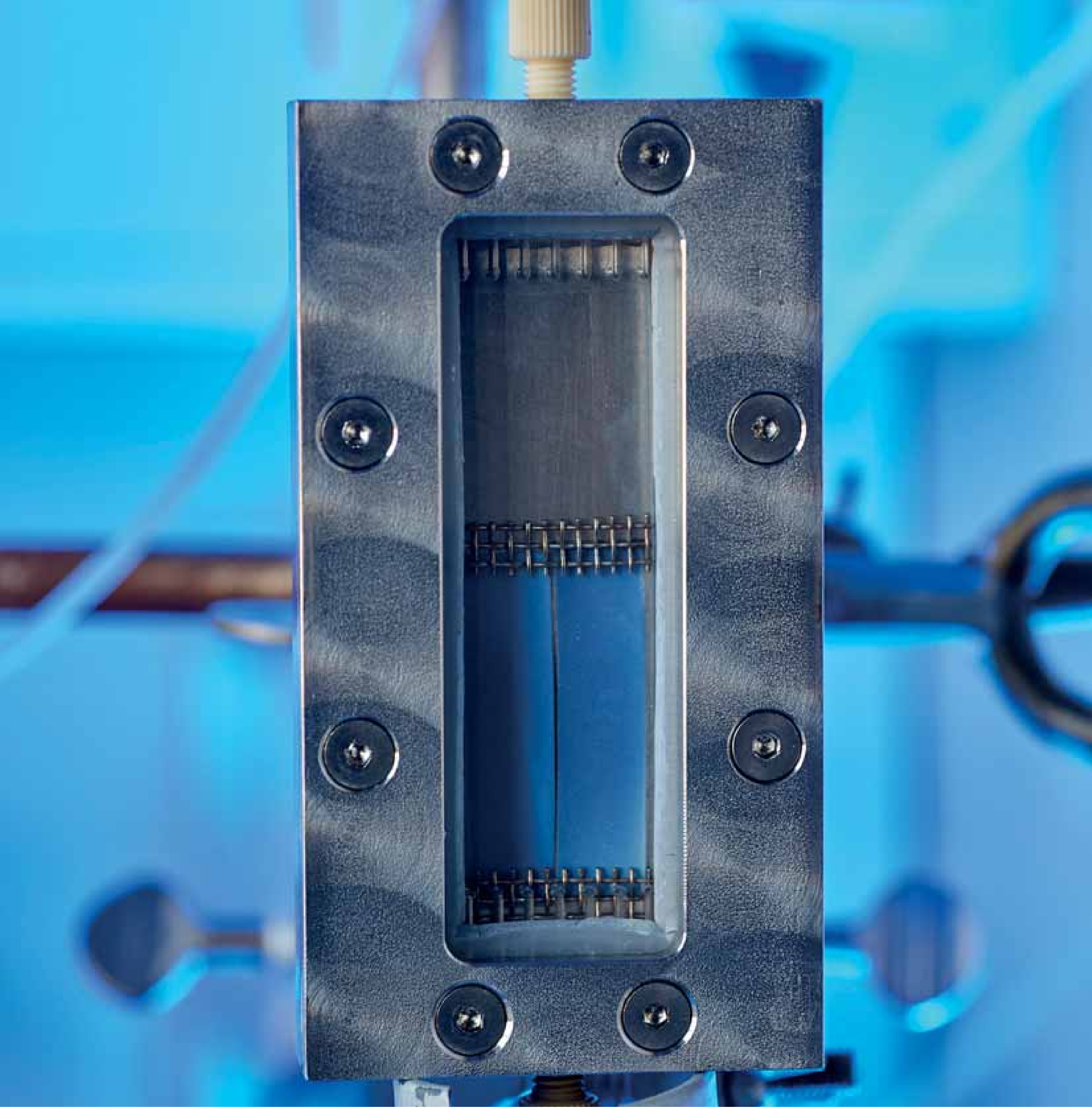
ENERGY & ENVIRONMENT

Topic 05 deals with basic and applied research aimed at enabling a circular economy and securing clean resources for future generations. To this end, the research work focuses on three main lines of research.

‘Utilization of renewable energy for chemical production’, e.g. in electrochemical or photocatalytic processes, bundles research efforts on hydrogen production, its storage and reconversion into electrical energy. This includes H_2 production from renewable resources and its storage in small energy-rich molecules such as methanol and formic acid under mild conditions, as well as the photo- and electrocatalytic splitting of water and reduction of CO_2.

Another focus is on the ‘reintroduction of greenhouse gases into chemical production’. Various research approaches of Topic 05 are dedicated to CO_2, which is considered a climate gas and is thermodynamically stable, as a potential raw material. Using suitable catalysts and reaction conditions, it can be converted to methanol, which in turn can be used as a CO_2-neutral fuel or energy storage medium. The reaction of CO_2 with the greenhouse gas methane CH_4 in dry reforming is also the subject of intensive research. The synthesis gas (H_2/CO) produced in this process is relevant for numerous industrial processes.

Another focus of Topic 05 is on the ‘purification of exhaust gas streams’, e.g. of NO_x, and ‘wastewater’, e.g. of organic substances that are difficult to degrade. The selective catalytic reduction of nitrogen oxides (NO_x) with ammonia at low temperatures (NH_3-SCR) is a promising method for removing the toxic gases from exhaust gases. At the same time, influences of other components, such as formaldehyde, on the catalyst‘s mode of action are also being investigated. The close collaboration of different research groups with expertise in catalytic testing, *in situ/operando* FTIR and EPR spectroscopy as well as transient studies with temporal resolution enables detailed findings in this context, which form the basis for knowledge-based catalyst design. Hardly degradable inorganic and organic compounds in wastewater, e.g. from pharmaceuticals, can be heterogeneously photocatalytically degraded using UV and visible light.



RESEARCH GROUPS

Catalysis for Energy Dr. Henrik Junge	High-Throughput Technologies Dr. Uwe Rodemerck
Optical Spectroscopy & Thermoanalytical Methods Dr. Christoph Kubis	Reaction Engineering Dr. David Linke
Magnetic Resonance & X-ray methods Dr. Jabor Rabeah	Technology-Oriented Processes Dr. Udo Armbruster
Photocatalytic Carbon Dioxide Reduction Prof. Jennifer Strunk	Numerical Analysis Prof. Klaus Neymeyr - Univ. of Rostock
Reaction Mechanisms Prof. Evgenii Kondratenko	

EMISSION OF HCN FROM FORMALDEHYDE DURING NH_3-SELECTIVE CATALYTIC REDUCTION OF NO_X OVER DIFFERENT V_2O_5-WO_3/TIO_2 CATALYSTS

ABSTRACT: Selective catalytic reduction of nitrogen oxides (NO_x) by ammonia (NH_3-SCR) is an important technology for the abatement of these harmful substances from the environment.[1-3] Recent investigations showed that catalytic reactions of formaldehyde, stemming from incomplete combustion of fuel, may form toxic hydrogen cyanide (HCN) with NH_3.[4] We investigated this widely neglected effect on commercial catalysts to understand and tackle this issue.

OBJECTIVE: The main goal of this work in the frame of ROHAN project between Hanoi University of Science and Technology (Vietnam) and LIKAT (J. Rabeah, U. Armbruster and E. Kondratenko) was to study the impact of formaldehyde on HCN production during NH_3-SCR of NO_x over commercial V_2O_5-WO_3/TiO_2 and home-made catalysts having different redox and acidic properties. This side reaction generates a novel serious emission problem during operation of combined heat and power plants. To this end, the interaction of HCHO with different feed components as well as with the total SCR feed has been investigated in detail.

RESULTS: The effect of HCHO on NH_3-SCR has been studied on commercial V_2O_5-WO_3/TiO_2 catalyst and analyzed in detail by tailored catalytic tests, in situ EPR and FTIR experiments, and transient studies using temporal analysis of products (TAP). To explore the effect of the different catalyst components on the reaction of HCHO, model catalysts WO_3/TiO_2 and V_2O_5/TiO_2 have also been investigated. Significant amounts of HCN were detected during the NH_3-SCR in the presence of formaldehyde over the most active catalyst V_2O_5-WO_3/TiO_2, while the effect of HCHO was negligible on the less active catalysts WO_3/TiO_2 and V_2O_5/TiO_2.

In a first step, HCHO is oxidized to adsorbed formate species, which compete with adsorbed nitrate species for NH_3. The first leads to formamide and the second to N_2. The acidic and redox properties of V_2O_5-WO_3/TiO_2 catalysts play essential roles in the subsequent reaction pathways to formamide as precursor for HCN. Above 450 °C, formamide was oxidized to CO_2 and nitrogen oxides on V_2O_5-WO_3/TiO_2 catalyst while in the range from 250 to 400 °C it was mainly dehydrated to form HCN together with minor amount of CO via decarbonylation. This overall reaction sequence consumes NH_3 and hence lowers the SCR activity and N_2 selectivity in addition to the emission of a highly toxic substance.

OUTLOOK: This work provides evidence for HCN emission due to the direct reaction between formaldehyde and NH_3 and should offer a basis for designing highly active and selective catalysts either to prevent HCN emissions or to convert it to non-toxic gases. Extra efforts are required to deeply understand the roles of water and SO_2, which are present in the exhaust gas, for HCN formation. Such kind of investigations is essential for practical application. Therefore, the groups of J. Rabeah, U Armbruster and E. Kondratenko are planning to continue their collaboration through ROHAN project to provide a solid scientific knowledge for catalyst improvement to minimize the formation of HCN.

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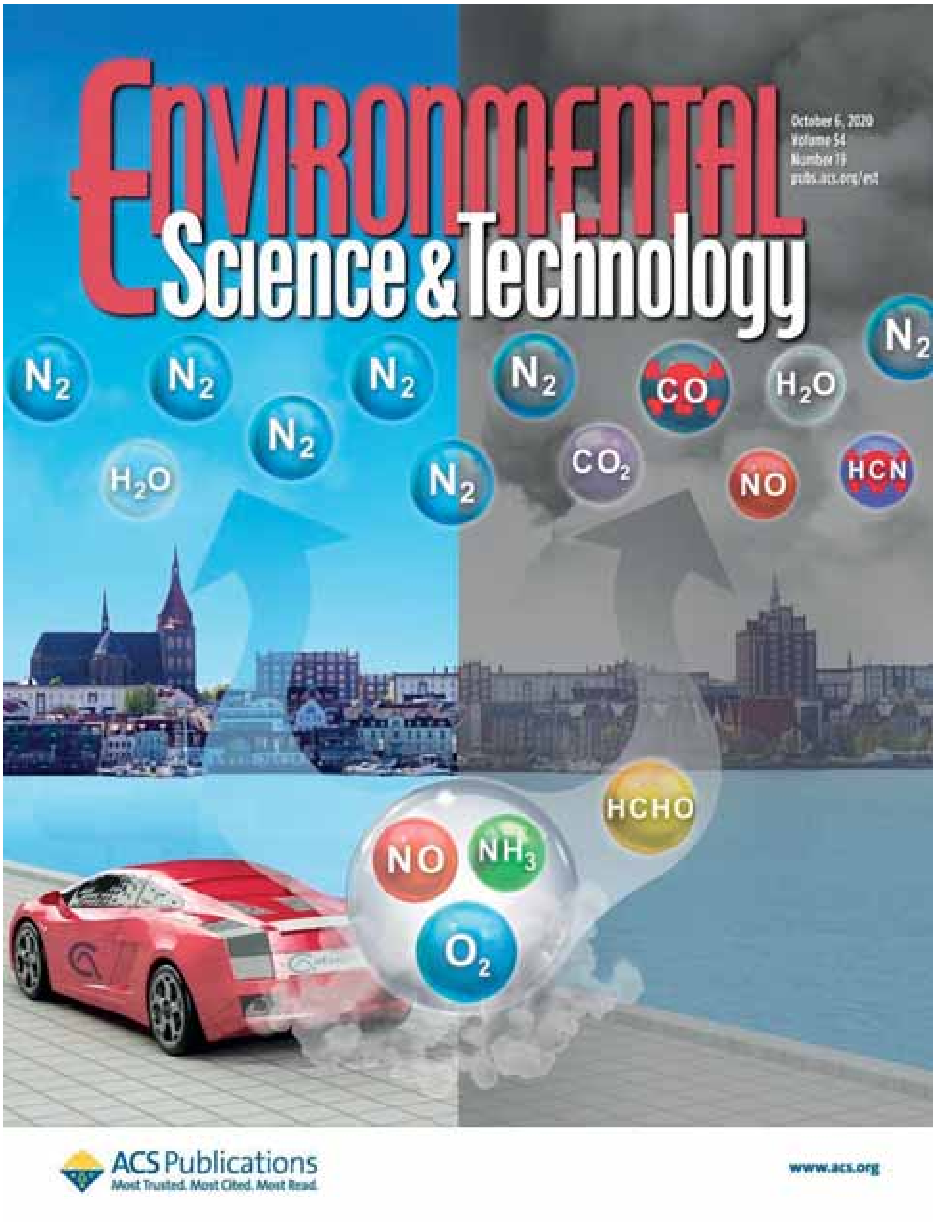

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PROPHECY AND PRODIGY: PROCESS CONCEPTS AND PROCESS DEVELOPMENT IN GAS-SOLID PHOTOCATALYSIS FOR THE REDUCTION OF CO_2

ABSTRACT: In the projects PROPHECY (10/2016 to 01/2020) and PRODIGY (since 02/2020), coordinated by the Department of Heterogeneous Photocatalysis at LIKAT, the five scientific partners (from Berlin, Oldenburg, Karlsruhe) produce nanomaterials and test various reaction environments to be applied in a photocatalytic process to convert CO_2 into valuable products. It is anticipated to use sunlight in an artificial photosynthesis process. In contrast to earlier work, the reaction partner here is not primarily water, but biogenic resources (e.g. methane from biogas).

OBJECTIVE: For such photocatalytic processes to be economically viable even with low yields, products of high value must be produced, such as short-chain alcohols, aldehydes, carboxylic acids or synthesis gas. To this end, three sub-goals are to be achieved: (i) the strategic design of materials that are free of precious metals, absorb visible light and adsorb the reactants, (ii) reliable evidence of product formation from CO_2 and the optimization of the reaction conditions for the new reaction partners, and (iii) a life cycle assessment of the environmental characteristics and costs. LIKAT is particularly involved in sub-goal (ii).

RESULTS: In 2019 and 2020, at LIKAT the prerequisites were established to study adsorption properties of the developed catalysts (BelCat II) and to carry out studies with ^{13}C isotope labeling. In terms of materials, the focus was placed on (ordered) mesoporous titanium oxide, whereby both the introduction of zinc oxide and the creation of a carbon-based shell layer increased the overall product yield. In the case of zinc oxide, in particular the ethane yield was increased. For $SrTiO_3$-based photocatalysts, the highest product concentration was achieved with a Pt cocatalyst, but with Pt-Cu as cocatalyst the competitive H_2 evolution was suppressed. Furthermore, a molecular photocatalyst system was investigated for the formation of CO in an ionic liquid, and product formation from CO_2 was verified.[1]

OUTLOOK: The further studies particularly deal with carbon-based sheet-like and framework materials as metal-free and visible light absorbing alternative photocatalysts. In addition, the work on the photocatalytic dry reforming of methane with carbon dioxide is being expanded. Studies with isotope labeling are planned to follow reaction pathways.

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TOPIC 06

Dr. Sebastian Wohlrab
Dr. Bernd Müller

MORE EFFICIENT PROCESSES

Research within Topic 06 is focused on new collaborations and concepts that can successfully meet future challenges. Economical synthesis routes, promising new starting materials as well as novel attractive processes for industrial applications are the goal.

The design of more efficient processes comprises four different pillars:
(i) *More efficient catalysts*: Targeted ligand design and their synthesis play a prominent role in homogeneous catalysis. This is because even the smallest structural changes can have a drastic effect on the catalytic efficiency of the catalyst. In addition to the synthesis of ligands and complexes for homogeneous catalysis, Topic 06 is dedicated to research on heterogeneous catalysts. One focus is on the development of cost-effective and environmentally friendly alternatives to commercially used catalyst systems. Priority is given to the regenerability of the developed catalysts without losing activity, selectivity and on-stream stability.

(ii) *More efficient process control*: The subject of investigations includes transfers from batch to continuous operation, with the aim of improving various factors such as thermal management, residence time distribution, product separation and ultimately selectivity and yield. Another tool to make thermodynamically and kinetically demanding reactions more efficient is the use of catalytic membrane reactors. By using membranes, thermodynamic equilibria can be shifted or selectivity as well as productivity can be increased.

(iii) *More efficient synthesis routes*: So-called ‘dream reactions’ are attractive reactions that often only exist on paper, for example the production of a complex compound in just one reaction step. However, catalysis opens up the possibility of completely new synthetic routes. One such ‘breakthrough’ is the one-step dicarbonylation of butadiene. After more than 60 years of intensive research worldwide, the reaction could be realized at LIKAT and transferred into application. The targeted adjustment of the H_2:CO ratio of synthesis gas in the catalyzed reforming of methane is another such dream reaction that is the subject of intensive investigation.

(iv) *More efficient use of resources*: The great interest of industry in improving its processes in terms of turnover, selectivity and productivity - even by only a few percentage points - justifies the fourth focus of Topic 06. Behind the primary objectives lies a more efficient use of raw materials and energy, which is of great societal importance for the conservation of our resources. Of great importance is research into carbon extraction from the air and the further processing of airborne CO_2 under mild conditions

RESEARCH GROUPS

Applied Carbonylations Dr. Ralf Jackstell	Reaction Engineering Dr. David Linke
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Micro Reaction Engineering Dr. Norbert Steinfeldt	Oligomerisations Dr. Bernd Müller
High-Throughput Technologies Dr. Uwe Rodemerck	Technology-Oriented Processes Dr. Udo Armbruster
Reaction Mechanisms Prof. Evgenii Kondratenko	Inorganic Functional Materials Dr. Sebastian Wohlrab

EFFICIENT PALLADIUM-CATALYZED CARBONYLATION OF 1,3-DIENES: SELECTIVE SYNTHESIS OF ADIPATES AND OTHER ALIPHATIC DIESTERS

ABSTRACT: Here, we report on a palladium-catalysed process in the presence of 1,2-bis-di-tert-butylphosphin-oxylene (dtbpx) ligands, which allow adipate diester formation from 1,3-butadiene, carbon monoxide, and methanol with 97 % selectivity and 100 % atom-economy under scalable conditions. Under optimal conditions a variety of di-and triesters from 1,2- and 1,3-dienes can be obtained in good to excellent yields.

OBJECTIVE: The dicarbonylation of 1,3-butadiene to adipic acid derivatives offers the potential for a more cost-efficient and environmentally benign industrial process. However, the complex reaction network of regioisomeric carbonylation and isomerization pathways, make a selective and direct transformation particularly difficult. We describe for the first time this 'dream reaction for industry' first time 2019[1] Further on we improved this methodology to an industrial viable level.[2, 3]

RESULTS: Recently, we discovered that a particular bidentate phosphine ligand (HeMaRaPhos) L1 allowed the palladium-catalyzed dicarbonylation of 1,3-butadiene working with high activity in other palladium-catalyzed alkoxycarbonylation reactions too.2 In order to understand the different reactivity of HeMaRaPhos and 1,2-bis-di-tert-butylphosphinoxylene (L2, dtbpx), we re-investigated the reactivity of the latter system in more detail. Notably, L2 is commercially used in the alkoxycarbonylation of ethylene (Lucite α-process)[4] and can be considered as a benchmark ligand for such reactions. In our study, a peculiar solvent effect was discovered, which laid the basis for a new protocol for direct dicarbonylation of 1,3-butadiene and related dienes in the presence of several palladium catalyst systems.

Comparing the kinetic behavior of both catalyst systems, some peculiar differences became apparent (Fig. 1). The one containing dtbpx L2 shows a prolonged induction period (6-8 h), while in the presence of L1 in the first two hours an intermediate is mainly formed, which afterwards rapidly is converted to the desired adipate.

OUTLOOK: The first Pd/dtbpx-catalyzed direct dimethoxycarbonylation of 1,3-butadiene can be presented. Surprisingly, the viability of this industrially relevant process is highly dependent on the ligand, solvent and catalyst system. We believe these findings will provide motivation towards the production of intermediates for bulk polyamides and polyesters produced on multi-million ton-scale.

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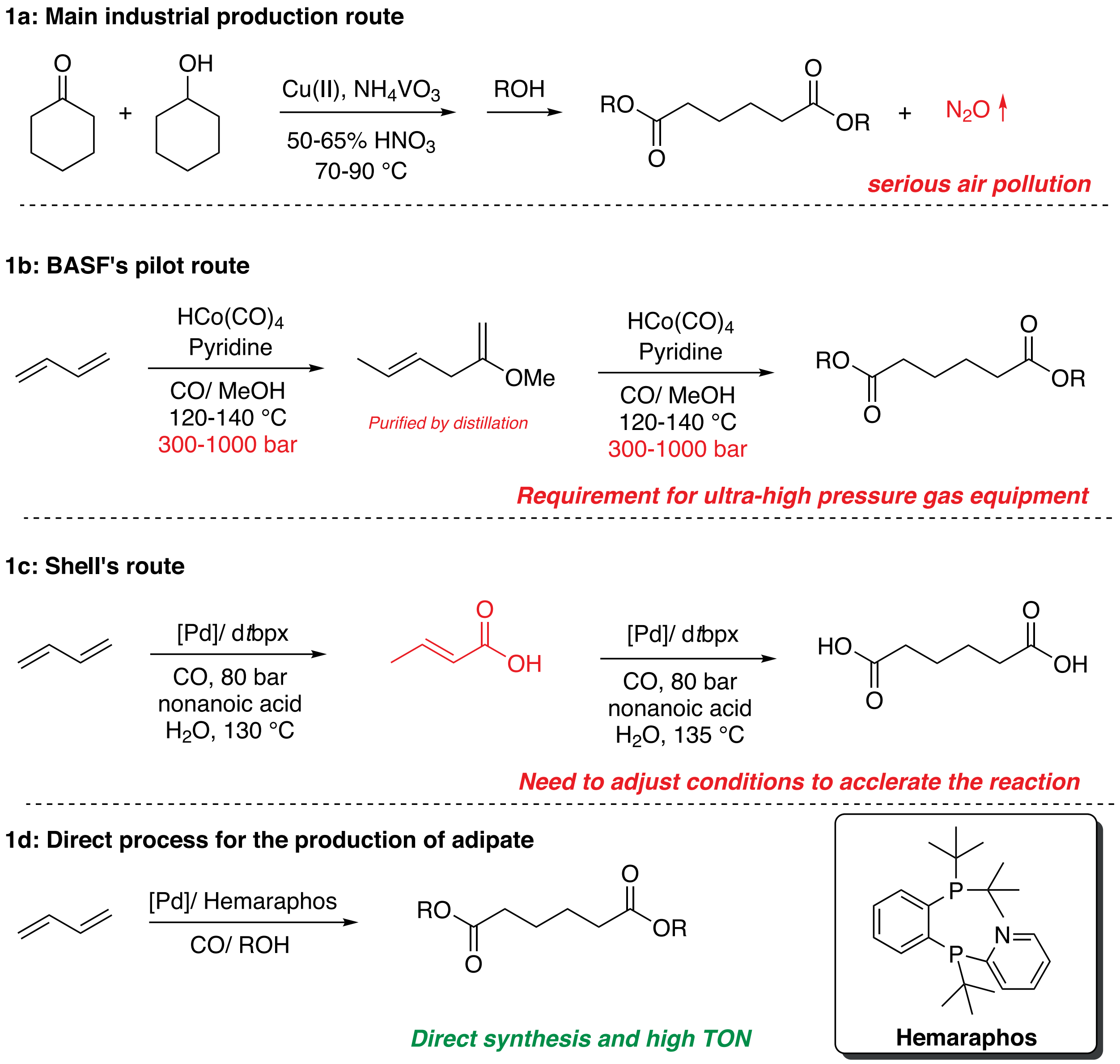


Fig.: Selected processes for making alkyl adipates.

DEVELOPMENT OF A CATALYTIC MEMBRANE REACTOR FOR THE EFFICIENT PRODUCTION OF METHANOL BY THE HYDROGENATION OF CO_2 WITH REGENERATIVE HYDROGEN IN THE GAS PHASE ON A HETEROGENEOUS CATALYST (HYTHANOL ECO_2)

ABSTACT: The background of the project is the concept of hydrogen utilization by an expanded group of users by refining hydrogen within the framework of power-to-X strategies. The primary objective of the joint project is to develop a catalytic membrane reactor for the efficient production of methanol by hydrogenating CO_2, e.g. from flue gas, with regenerative hydrogen in the gas phase on a heterogeneous catalyst.

OBJECTIVE: The core idea of the project is to shift the equilibrium of the methanol synthesis by separating a product in order to increase the yield of the desired product. This allows the reaction to be carried out economically even with expensive starting products such as green hydrogen. Specifically, a catalytic double membrane reactor is developed that allows selective dosing of a reactant (H_2 or CO_2), catalytic conversion and selective removal of a product (H_2O, methanol) to increase the yield of equilibrium-limited methanol synthesis. This increases the production efficiency of this versatile base chemical via the CO_2 route. In order to realize the most efficient synthesis, two substance-selective membranes are used, coupled with an active catalyst in a reactor.

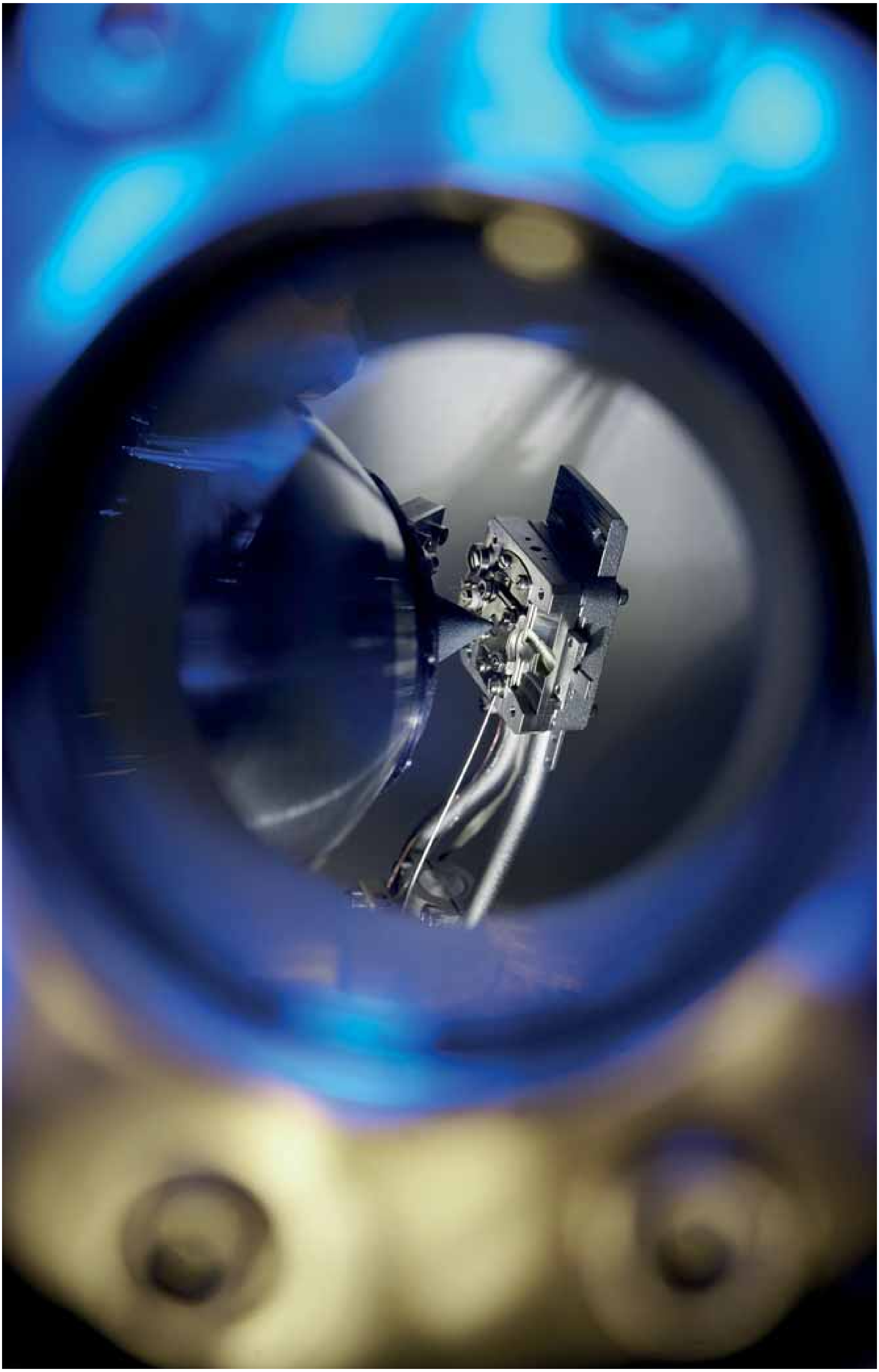
RESULTS: In the project, membranes and membrane-catalyst combinations are to be developed, coupled in terms of process technology, tested under real conditions and checked for practical suitability. The overall process concept should allow the integration of a wide range of CO_2 sources.

Target parameters of the innovative concept are:

- Development of new catalysts and membranes;
- Significant increase in methanol yield compared to CO_2 hydrogenation in a fixed bed reactor;
- Increase of reactor throughput and simultaneous energy savings;
- Realization of at least 3 process steps in one reactor (process intensification) and
- Integration of heat management for waste heat utilization for provided processes (e.g. amine scrubbers).

OUTLOOK: The economic objective is to achieve a process of methanol synthesis based on the use of CO_2 and regenerative hydrogen. The project enables a more variable and intensive H_2 utilization and opens up new utilization routes as well as the possibility of H_2 storage in the form of liquid methanol. Methanol is a value-added product and is conventionally produced from natural gas or coal via syngas. The project aims to make methanol synthesis from renewable sources and CO_2 economically attractive. In addition, there is an enormous savings potential for CO_2-intensive emitters against the background of rising prices for CO_2 certificates in the future and could become an essential aspect for the existence of CO_2-intensive heavy industry in Germany and its social acceptance.

In collaboration with Fraunhofer-Institut für Keramische Technologien und Systeme (IKTS), MUW Screentec GmbH (MUW), DBI Gas- und Umwelttechnik GmbH (DBI -GUT)



TOPIC 07

PD Dr. Torsten Beweries
Dr. Christian Hering-Junghans

NEW PRODUCTS & PROCESSES

Research in Topic 07 is based on LIKAT's long-standing expertise in fundamental and applied areas of homogeneous and heterogeneous catalysis, complemented by new aspects, junior research groups and associated research groups.

This includes aspects of classical homogeneous catalysis, organometallic and coordination chemistry, main group chemistry, photocatalysis, and organocatalysis. This knowledge is complemented by aspects of heterogeneous catalysis.

An illustrative example are transition metal-catalyzed syntheses of fine chemicals, which often find application in the pharmaceutical industry. The development of transition metal complexes with polydentate P-containing ligands plays a central role. Often, a new generation of ligands enables unusual conversions and a significant increase in activity.

Catalysis bears a key role in the valorization of renewable resources and CO_2 chemistry. The production of plant-based platform chemicals or the use of CO_2 hold great potential in terms of climate and resource protection. Catalytic processes are then needed to convert the sustainable platform chemicals into new compounds and materials.

In addition to industry-related research projects, basic research accounts for 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, which allows conclusions to be drawn about catalysis-related issues.

In the following, only a few of the multifaceted topics are mentioned as examples.

Intensive research efforts are being made in the field of phosphorus chemistry, also at the boundary between homogeneous and heterogeneous catalysis. This includes the development of new (stereogenic) P-containing ligands, the synthesis of strained P-containing ring systems or P(III)/P(V) redox-based organocatalysis.

Furthermore, it is investigated how inexpensive metal-based and metal-free catalysts for carbonylative coupling reactions can be used for the synthesis of heterocycles or how small bioactive molecules can be produced by established and new methods.

The amine-borane class of compounds holds potential for use as precursors for new B-N materials and is therefore of great interest. Their dehydrocoupling with early and late transition metal complexes or the preparation of linear polyaminoboranes are the subject of intense investigation.

Highly strained metallacycles, such as unsaturated and four-membered Ti-containing ring systems, are challenging compounds to prepare with interesting bonding situations. Based on the synthesis and studies of these compounds, conclusions can be drawn about individual substeps of catalytic mechanisms.

RESEARCH GROUPS

Homogeneous Catalysis for Life Sciences	Dr. Helfried Neumann
Catalysis with Renewable Resources & Platform Chemicals	Dr. Sergey Tin
Organocatalysis	PD Dr. Thomas Werner
High-Throughput Technologies	Dr. Uwe Rodemerck
Reaction Mechanisms	Prof. Evgenii Kondratenko
Reaction Engineering	Dr. David Linke
Catalysis of Late Transition Metals	PD Dr. Torsten Beweries
Catalysis of Early Transition Metals	Dr. Fabian Reiß
Catalysis for Heterocycles	Prof. Xiao-Feng Wu
Asymmetric Hydogenations	Dr. Jens Holz
Bioinspired Catalysis	Prof. Paul Kamer
Catalytic Functionalizations	Dr. Jola Pospech
Small Molecule Activation	Dr. Christian Hering-Junghans
Polymer Chemistry & Catalysis	Dr. habil. Esteban Mejia
Material Design	Prof. Axel Schulz - Univ. of Rostock
Catalytic Cycloadditions	Prof. Marko Hapke - Johannes Kepler Univ. of Linz

P(III)/P(V) REDOX CATALYSIS

ABSTRACT: In this work, the carbon-carbon double bond of unsaturated carbonyl compounds is readily reduced by a phosphetane oxide catalyst. Notably, water is used as the hydrogen source while the P(III)/P(V) redox cycling is realized utilizing a simple organosilane ($PhSiH_3$) or the even less active polymethylhydrosiloxane as the terminal reductant.

BACKGROUND: We have been involved in the development of new catalytic methods based on P(III)/P(V) redox catalysis for some time. In this context, we recently reported the use of a phosphetane oxide as a catalyst in Wittig reactions (Fig. 1a).[1] In the presence of small amounts of this catalyst (1–2 mol %) this reaction can be carried out even at room temperature. It is noteworthy that in some cases hydrogenation of the double bond was observed under the reaction conditions. Initial investigations indicated that water served as the hydrogen source. Based on these observations, a new method for the organocatalyzed reduction of α, β-unsaturated carbonyl compounds should be developed.

RESULTS: A catalyst screening and optimization of the reaction conditions led to a protocol for the efficient organocatalytic reduction of activated alkenes using water as a hydrogen source (Fig. 1b).[2]

The mechanism of the reaction was investigated. It was found that the phosphetane oxide is first reduced to the corresponding phosphetane. This then undergoes a Michael reaction with the substrate to form an ylide, which is hydrolyzed under the reaction conditions to the alkane and the phosphetane oxide. The phosphetane oxide catalyst thus enables the selective reduction of electron-poor alkenes by P(III)/P(V) redox catalysis in the presence of water. Under the optimized conditions, a total of 25 alkenes and two alkynes were hydrogenated to the corresponding alkanes in excellent yields of up to 99 %, tolerating a variety of functional groups that are normally easily reduced. In addition, it was possible to use inexpensive polymethylhydrosiloxane instead of $PhSiH_3$ as the terminal reducing agent and to substitute toluene by the renewable solvent BuOAc.

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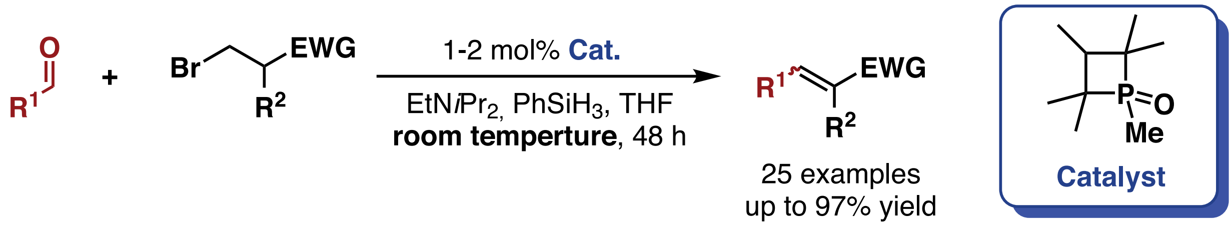
a) Room temperature catalytic Wittig reaction



b) Reduction of activated alkenes by P(III)/P(V) redox catalysis

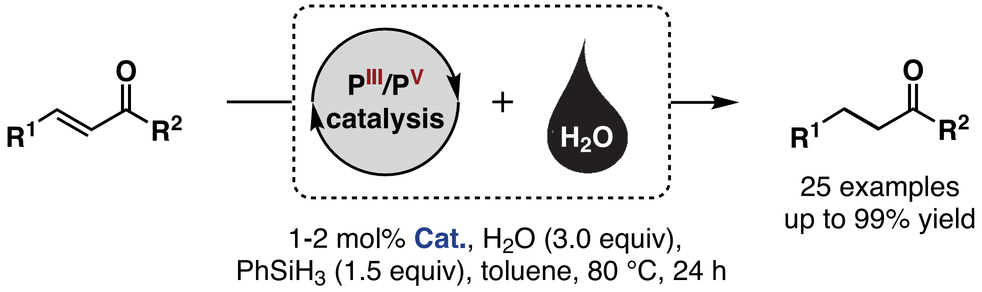


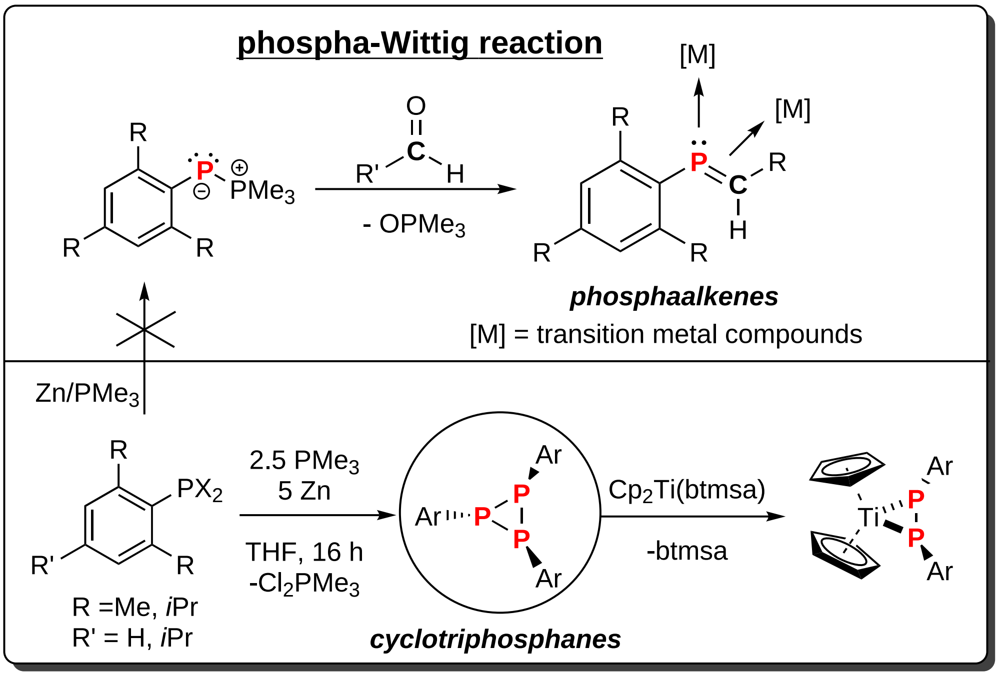
Figure 1. a) Catalytic Wittig reaction at room temperature.[1] b) Reduction of activated alkenes by P(III)/P(V) redox catalysis.[2]

THREE-MEMBERED PHOSPHORUS RING SYSTEMS AS PRECURSORS FOR NOVEL LIGANDS IN TITANOCENE COMPLEXES

ABSTRACT: Phosphaalkenes, systems with a P=C double bond, offer multiple binding sites for transition metals. In the search for new synthetic routes towards phosphaalkenes with small aryl groups on phosphorus, we have discovered a selective synthetic route for strained three-membered phosphorus cycles, $(PAr)_3$, so-called cyclotriphosphanes.

OBJECTIVE: Phosphaalkenes can be obtained in the so-called phospha-Wittig reaction. In this process, phospha-Wittig reagents, ArPPMe (Ar = sterically demanding group), react with aldehydes to form the desired phosphaalkenes, ArP=C(H)R, with concomitant formation of $OPMe_3$. Phosphaalkenes can coordinate metals in many ways, for example via a free electron pair on the phosphorus or via the electron density in the P=C double bond. We now wanted to transfer the concept of the phospha-Wittig reaction to smaller aryl groups on phosphorus, such as the diisopropylphenyl group (dip).

RESULTS: In doing so, we found a selective and scalable access to cyclotriphosphanes, $(PAr)_3$ with aryl substituents (Scheme 1, bottom), which have so far only been described as by-products in the literature.[1] Optimisation of the reaction conditions showed that mixed halides of the type $ArPX_2$ (Ar = Tip, Dip, Mes; X = Cl, Br) represent ideal and easily accessible starting materials. The subsequent reaction with Zn and PMe_3 then yields the three-membered phosphorus rings in excellent yields. These are thermally stable and can be stored indefinitely in an inert atmosphere. In collaboration with Dr. Fabian Reiß, an expert in the field of titanocene chemistry, the P_3-ring systems should be reacted with the complex $Cp_2Ti(btmsa)$ to obtain so-called phosphinidene complexes. In this process, the P_3-ring would be split into individual PAr units and transferred to the titanium centre. Systems of the type $Cp_2Ti{=}PAr$ are unknown to date. If now $(PAr)_3$ and $Cp_2Ti(btmsa)$ are reacted in a 1:3 ratio, we did not find the formation of the phosphinidene com-



Scheme 1. Phospha-Wittig reaction for the preparation of phosphaalkenes (top). Selective route to cyclotriphosphanes and resulting titanocene-diphosphene complexes (bottom).

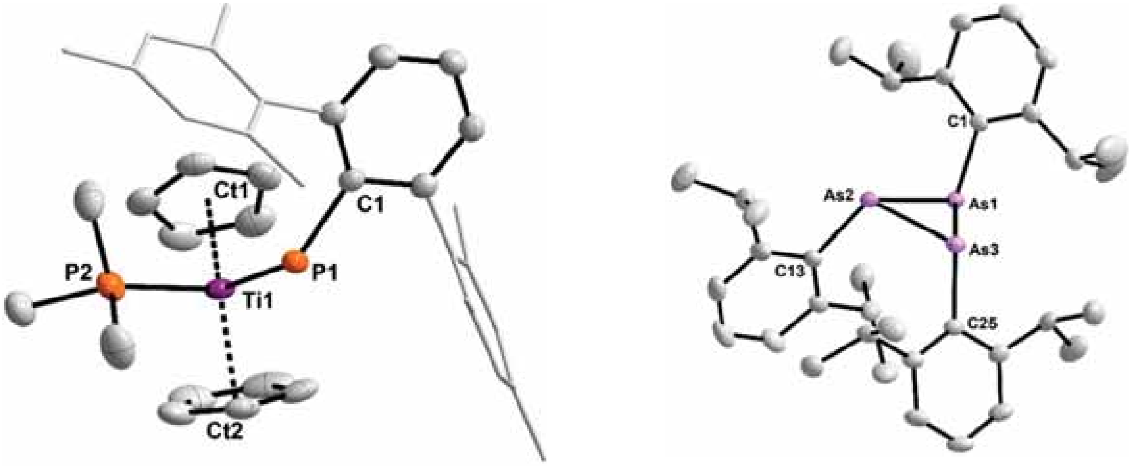


Figure 1. Molecular structure of the first titanocene phosphinidene complex (left) and a cyclotriarsane with dip-substituents.

plexes as expected. Rather, complexes of the type $Cp_2Ti(P_2Ar_2)$ were obtained (Scheme 1), which were isolated in good yields after optimisation. Through close collaboration with Dr. Haijun Jiao, we were able to show by DFT studies that electrons are transferred stepwise from the titanium to the P_3 ring, forming a phosphorus radical, a species with an unpaired electron, on the titanium. In collaboration with Dr. Jabor Rabeah, these radicals could then be detected in the EPR spectrum.

OUTLOOK: In collaboration with the Reiß group, we are currently working on the synthesis of titanocene phosphinidenes,[2] and were able to structurally characterise them for the first time. Furthermore, the synthetic route to the triphosphiranes could be transferred to the analogous arsenic systems.[3] In the future, the chemistry of these strained group 15 ring systems will be expanded with regard to catalytic phosphinidene transfer reactions and the synthesis of functional materials.

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RESEARCH GROUPS

CATALYSIS FOR ENERGY

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Forced by political decisions, intensive work is currently underway in Germany on the development of hydrogen technologies. The group ‘Catalysis for Energy’ has already been working since 2003 on the production of hydrogen from renewable energies and raw materials, the chemical storage of hydrogen and the use of green hydrogen for carbon dioxide utilization by synthesizing energy carriers as well as industrially relevant products (e.g. carbon monoxide, formic acid, methanol). For this purpose, classical hydrogenation/dehydrogenation reactions as well as photocatalytic reactions are applied. To improve these conversions, we combine our methodological expertise in reaction control and product analysis with our experience in the development of active and selective catalysts and photosensitizers. Both organometallic complexes and heterogeneous catalysts, e.g. supported nanoparticles and ‘single atoms’, are used as catalysts. In this respect, non-precious metals also play a crucial role.

Recent highlights were the successful application of one of our catalyst systems in continuous low-temperature hydrogen production from methanol/water over 450 h in a demonstration plant at FAU Erlangen-Nuremberg (Metha-Cycle project, funded by the BMWi) and the start of a project on hydrogen storage in formic acid funded by the state of Mecklenburg-Western Pomerania and the EU.

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APPLIED CARBONYLATIONS

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The research group ‘Applied Carbonylations’ is equally dedicated to basic research (e.g. within the framework of BMBF and EU projects as well as in cooperation with other university institutions and industry) and application-oriented research (cooperation with industry, e.g. Evonik, BASF, Creative Quantum, etc.).

Its research focuses on hydroformulations, alkoxycarbonylations, hydroxycarbonylations and hydroaminomethylations with industrially relevant raw materials (such as olefins, alkynes, carbon dioxide) to industrially relevant products (such as aldehydes, carboxylic acids, esters, amines, alcohols) for applications in polymer chemistry (monomers, plasticizers, etc.).

In order to contribute to the transfer into industrial applications, process-accompanying research is part of our tasks. This includes e.g. the investigation of activity, stability and selectivity behavior of new catalysts in new reactions to known and new products of industrial importance.

Another focus is on the development and testing of new homogeneous and heterogeneous catalysts for carbonylation reactions and CO_2 hydrogenations with known noble metals and alternative catalyst metals such as iron, cobalt, manganese, ruthenium or iridium.

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 serve to validate important process parameters in hydrogenation reactions of carbon monoxide and carbon dioxide.

THEORY OF CATALYSIS

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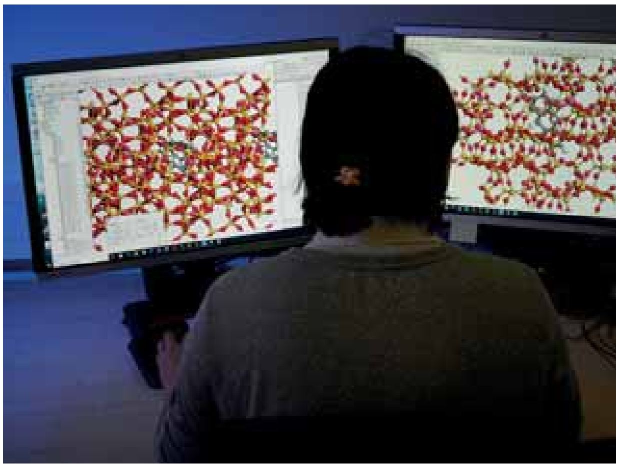
The focus of the research group ‘Theory of Catalysis’ is the computational investigation into physical organic chemistry, organometallic and homogeneous catalysis as well as surface science and heterogeneous catalysis in cooperation with colleagues in our Institute.



In physical organic chemistry and organometallics, we are interested in the structure and stability as well as spectroscopic properties of organic and organometallic molecules.[1, 2] In homogeneous catalysis, we investigate the catalytic activity of transition metal complexes in the hydrogenation, dehydrogenation and transfer hydrogenation reactions of unsaturated compounds,[3-7] carbonylation of alkenes and alkynes.[8, 9] In heterogeneous catalysts, studies are currently being carried out on activation mechanisms of low molecular weight hydrocarbons.[10-13]

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SUSTAINABLE REDOX REACTIONS

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In the research group „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).[1, 2] While the main expertise of the research group originally stems from homogeneous catalysis, heterogeneous systems have also been studied for more than 10 years.[3] The aspect of sustainability plays an important role, which is reflected in the choice of readily available and inexpensive catalyst metals, but also in the establishment of novel catalyst support from industrial waste (e.g. chitosan, chitin). 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. For the synthesis of homogeneous catalysts, Schlenk and glovebox techniques are used. In this respect, especially the synthesis of pincer type complexes is a very efficient concept due to the direct tuning of catalyst properties. The 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 experience with industrial collaborations in various fields (pharmaceuticals, life science, agrochemicals). We are working on application-oriented problems in the field of oxidation and reduction reactions with high flexibility.

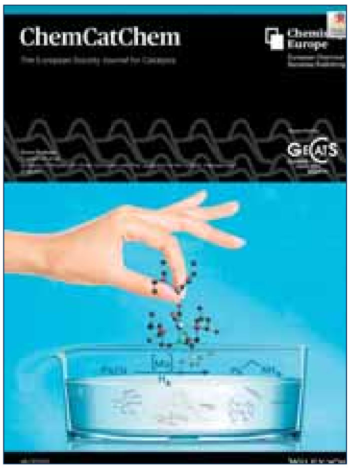

Abb. 1. Cover for the molybdenum catalyzed nitrile hydrogenation.

Abb. 2. Cover for the Cobalt catalyzed reduction of amides.

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CATALYSIS FOR LIFE SCIENCES

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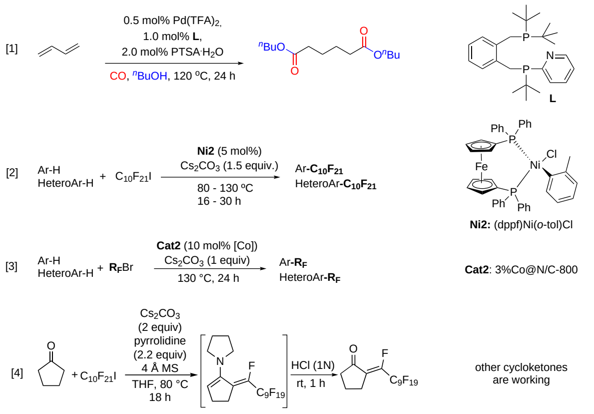
In numerous industrial collaborations, the focus of catalyst development and optimization is on activity, reusability, stability, and synthesis effort.

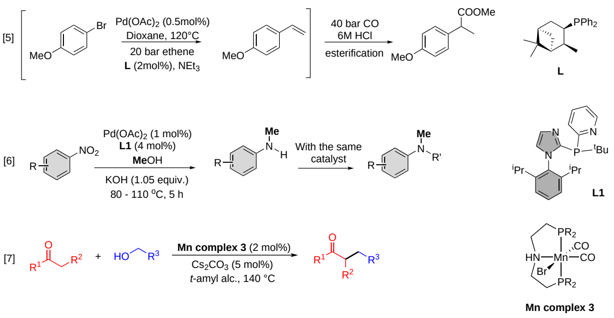
In collaboration with Evonik, homogeneous palladium catalysts are being developed for the methoxycarbonylation of octene mixtures to terminal esters. Based on this, a ‘dream reaction’ in chemistry could be realized with the dicarbonylation of difficult-to-carbonylate 1,3-butadienes to adipic acid esters.[1] The products are used on a ton scale for the production of polymers.

Another focus is on the synthesis of per- and trifluoro alkylated aromatics, which serve as important synthetic building blocks in drug development and agrochemistry. Together with LONZA, different nickel[2]- and cobalt-based[3] catalysts have been developed in this context, which are particularly suitable for electron-rich aromatics or methoxy-substituted arenes. Electron-rich enamines can even be perfluoroalkylated without a catalyst.[4]

Furthermore, classical coupling reactions are investigated. For the preparation of Naproxen® and other profenes, a two-step one-pot synthesis could be developed, consisting of a Heck reaction followed by hydroxycarbonylation.[5]

Methylations of nitrobenzene derivatives to the corresponding methyl anilines using certain catalysts[6] and aldol condensations starting from ketones and alcohols using pincer complexes are also being carried out.[7]





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SYNERGY BETWEEN HOMOGENEOUS & HETEROGENEOUS CATALYSIS

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The group's research focuses on (1) developing low-cost catalysts that combine the activity and selectivity of homogeneous catalysts with the stability and recyclability of heterogeneous catalysts and (2) developing more sustainable processes for fine and bulk chemicals and life science molecules.

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.[2, 3, 4, 5, 9] These materials provide highly active and selective as well as stable and reusable catalysts for amination and hydrogenation reactions. And provide access to essential chemicals.[2, 3, 4, 5, 9]

Fig. 1 shows an example of immobilization of Co-MOF on carbon as well as graphitic encapsulated Co-NPs and SACs generated in subsequent pyrolysis under argon. They are excellent catalysts for reductive amination.[9] This type of catalysts is also used for hydrogenation of (hetero) arenes[3, 5] as well as for the utilization of renewable raw materials.[4] In addition, we develop molecularly defined complexes[1, 8] and *in situ* generated NPs[7] for organic synthesis.

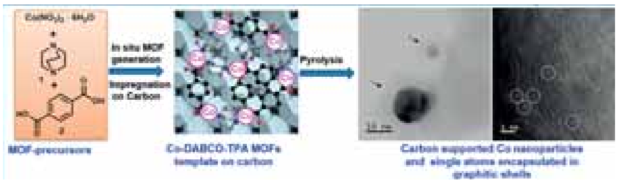

Fig. 1. Preparation of graphitic shell–encapsulated Co nanoparticles supported on carbon by using MOF precursors.

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CATALYSIS WITH LATE TRANSITION METALS

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The research group investigates fundamental aspects of late transition metal catalysed processes based on preparative and mechanistic organometallic chemistry, aiming at an understanding of structure-activity relationships for optimisation of catalytic reactions and developing new transformations. We are focusing on various aspects of activation and transformation of small, partly unreactive molecules such as H_2O, N_2, CO_2, or H_2.

The catalytic formation of bonds between main group elements was widely investigated in recent years, mainly due to the potential of amine borane adducts for hydrogen storage as well as in the context of development of new functional inorganic materials. However, compared to formation of isoelectronic C-C bonds, the synthetic potential of B-N bond formation and B-N compounds in general are much less well investigated. Amine boranes are excellent precursors for the synthesis of new B-N materials. In our group we are working on transition metal complex catalysed dehydrocoupling of amine borane adducts such as ammonia borane and its substituted and functionalised analogues for the synthesis of new oligomeric and polymeric B-N materials.[1] Transition metal catalysts used in this context are based on a variety of different PCP and PNP pincer ligand motifs, which are developed in the group and studied in detail with respect to ligand effects and their coordination chemistry.[2, 3]

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MECHANISMS IN HOMOGENEOUS CATALYSIS

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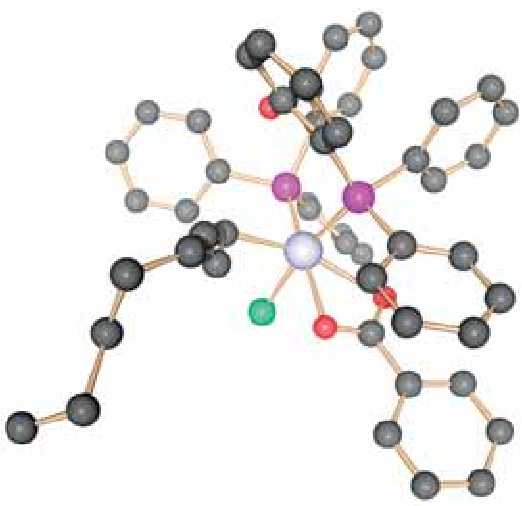
The research group investigates catalyst activation and deactivation phenomena as well as its impact for homogeneously catalysed reactions, aiming at a transfer of this knowledge for improving existing and developing new catalytic transformations. In addition to a method for online registration of gas consumption and development under isobaric conditions,[1] 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. Lately, we have extended our analytical setup with a benchtop 80 MHz $^{31}P/^{1}H$ NMR spectrometer (Magritek), equipped with a flow cell, that will be coupled with already established spectroscopic techniques.

In the area of fundamental research, we focus on the organometallic chemistry of rhodium bis(phosphine) complexes in homogeneous catalysis. Examples include the activation of ammonia using complexes of the type $[Rh(PP)(\mu_2\text{-}OMe)]_2$ (e.g. PP = DIOP), hydrogenation of prochiral olefins, e.g. using the ammonia complex $[Rh(binap)(NH_3)_2]$,[2] as well as studies of catalyst deactivation in propargylic C-H activation. The latter topic is investigated together with the Breit group (Freiburg) as part of a DFG project.[3]

In cooperation with industrial partners (e.g. Hansen & Rosenthal, DSM) we study hydrogenation reactions as well as systems that can replace toxic solvents, e.g. in extraction processes. Lately, for the latter project, transfer of lab process the into the industrial pilot scale was accomplished.



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CATALYSIS OF EARLY TRANSITION METALS

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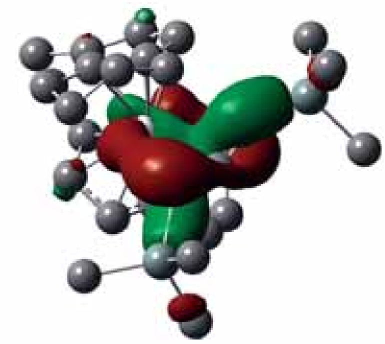
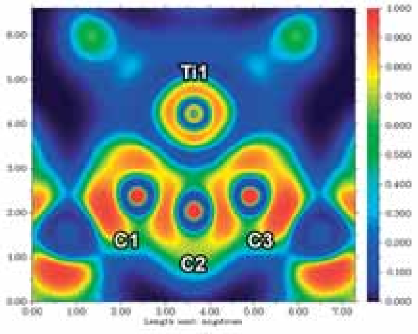
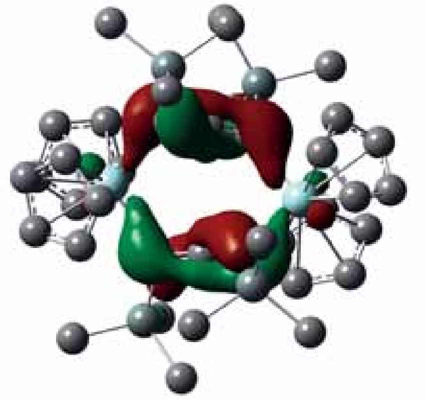
The research group ‘Catalysis of Early Transition Metals’ investigates the fundamentals of catalytic processes occurring at early transition metal complexes. The focus is on the rich chemistry of sandwich complexes of titanium, zirconium and hafnium, so-called metallocenes. This type of compounds allows us to push the borders of experimentally accessible structures and stabilise highly strained unsaturated four-membered ring systems. The synthesis of a suitable organodilithium synthon enables for the first time the preparation of a titanacyclobuta-2,3-diene, which formally corresponds to an organometallic analogue of the highly strained and non-existent cyclobuta-1,2-diene. These highly reactive molecules can be interpreted as intermediates in catalytic C-C coupling processes. The targeted synthesis and analytical characterisation (NMR, SC-XRD, IR, RAMAN, UV/Vis) of such sensitive compounds coupled with quantum mechanical bond theory analyses (DFT, NBO, ELF, CAS) give insights into the structure-activity relationships of this class of compounds.

Over the past two years, quantum mechanical bonding theory analyses as well as mechanistic studies of metallocene catalysed processes have been established in the group. The derived insights allow for a deeper understanding of the activation and transformation of small molecules such as H_2 and CO_2 as well as unsaturated molecules such as nitriles R-C≡N, isonitriles R-N≡C and alkynes R-C≡C-R. These will be used in the future for the development of new group 4 based bimetallic catalyst systems.







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ASYMMETRIC HYDROGENATION

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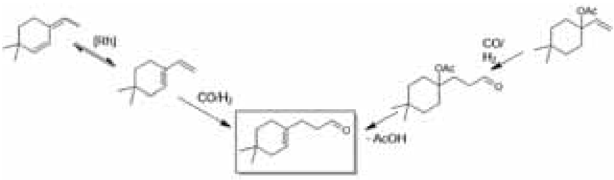
The asymmetric hydrogenation of olefins, ketones, imines or other prochiral compounds is an important method in the production of biologically active agents or intermediates in pharmaceuticals, agrochemicals and fragrance chemistry.

In addition to the development of new hydrogenation catalysts and the search for more effective reaction pathways in various (industrial) collaborations the research group is also dedicated to the investigations of carbonylation reactions.

With FIRMENICH SA (Switzerland), novel pincer compounds for the catalyzed synthesis of flavors and fragrances have been developed. At the same time, a project on regioselective carbonylation was worked on with the same contractual partner and brought to pilot scale.

The rhodium-based catalysts proved successful in the selective hydroformylation of cyclic olefins and dienes towards the desired n-aldehydes (Scheme 1).[1]



Scheme 1. Exemplary representation of the examined Rh-catalyzed hydroformylation of cyclic olefins

With BASF SE, investigations were carried out to elucidate the reaction mechanism of the ruthenium-catalyzed deaminating hydrogenation of an industrially relevant nitrile to the primary alcohol. In this context, the highly developed methods for HP-NMR and *in-situ* FTIR spectroscopy available in the area made fundamental contributions.

After the synthesis of P-stereogenic xantphos ligands and their application in asymmetric reactions[2,3] have been completed, an implementation of this P-chirality in SpanPhos/SpiroPhos compounds is currently taking place.

A successful collaboration was realized with a research group at the University of Chile (Santiago de Chile) in the field of hydrazine-induced reduction of carbonyl compounds.[4]

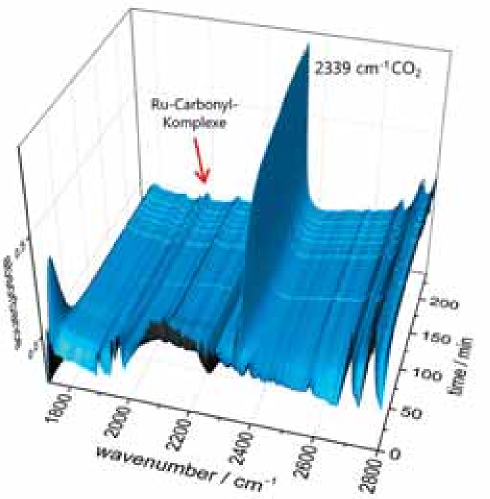


Figure 1. Recorded *in-situ* FTIR spectrum during a deaminative hydrogenation

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CATALYSIS FOR HETEROCYCLES

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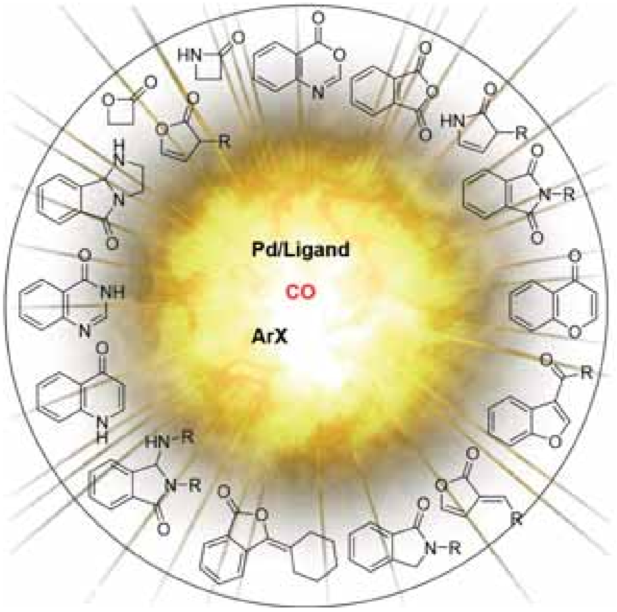
Heterocycles are ring-shaped compounds that have at least one heteroatom in addition to carbon. There is a very extensive class of compounds, as they can differ according to the type and number of heteroatoms, their degree of saturation, their ring size and with regard to the substituents. Thus, about 90 % of all natural products are based on heterocycles. In addition, they find a very wide application in pharmaceuticals, agrochemicals, paints and many more.

Due to this diversity and complexity, the synthesis of heterocycles is one of the most important disciplines in organic chemistry.

The research group 'Catalysis for Heterocycles' is dedicated to the introduction of C1 building blocks via carbonylation reactions.

Our interest is in the development of novel carbonylation reactions for the synthesis of heterocycles using CO (Scheme 1).[1] In this context, flavones, furanones, benzoxazines, etc. were synthesized as examples. Palladium complexes were preferably used as catalysts.



Scheme 1. Carbonylative Synthesis of Heterocycles.

In addition, novel carbonylating transformations with non-noble metals are investigated in the topic group.[2] In particular, 3d transition metals such as Fe, Cu, Co, etc. play a significant role.

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NEW HYDROFORMYLATION CATALYSTS

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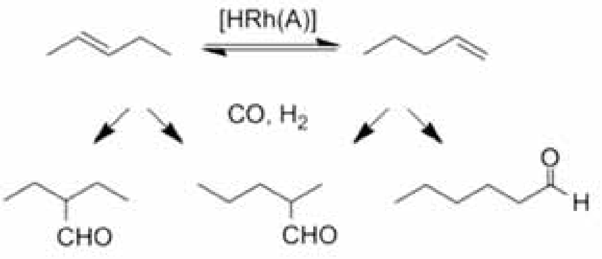
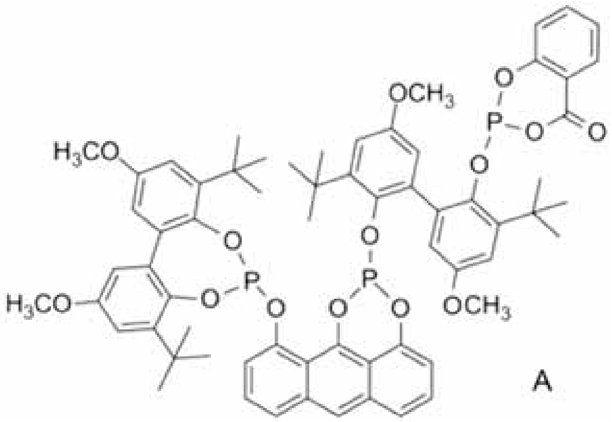
Our work focuses on the *n*-regioselective, rhodium-catalyzed hydroformylation of technically available internal double bond isomeric olefins. This includes the synthesis, preferably patent-free, phosphorus ligands and their testing under industrially relevant conditions. Catalyst stability studies and in situ spectroscopic studies of mechanistic details are performed for selected catalysts with promising properties.

We try to cover as comprehensively as possible the areas of rhodium and phosphorus chemistry and physical chemistry relevant to the catalytic reaction. State-of-the-art management of the pressure experiments with highly effective gas injection and time-dependent gas consumption recording is routinely applied. With respect to *in situ* analysis, we build on the methodology we have developed in recent years for HP infrared and NMR spectroscopic measurements. By means of isotope labeling and chemometric analysis of infrared spectra, detailed information on catalyst structure, reaction kinetics and mass balance of catalytically relevant intermediates can be made accessible. For the use and further development of this know-how, there are internal cooperations with Dr. C. Kubis and PD Dr. W. Baumann, as well as with the working group of Prof. K. Neymeyr from the Institute of Mathematics at the University of Rostock.





A

OPTICAL SPECTROSCOPIC & THERMOANALYTICAL METHODS

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The activities of the research group are focused on the investigation of mechanistic and kinetic aspects of homogeneously and heterogeneously catalyzed reactions under real reaction conditions using *in-situ/operando* spectroscopic methods. A specific aim is to find correlations between structural properties of the catalyst and its performance in the catalytic process. For that purpose, a variety of analytical techniques are used such as FTIR, UV/Vis, and Raman spectroscopy as well as thermal analysis (TG-DSC-MS). The simultaneous coupling of multiple analytical tools allows for the comprehensive study of the catalytic reaction from different viewpoints at the same time. Sophisticated devices such as high-pressure spectroscopic reaction cells are also developed in our group. Scientifically we are especially interested in CO$_2$ valorization reactions, alkene oligomerization and carbonylation reactions. Currently, we work on the establishment of a Raman-profile reactor coupled with an online-GC system for spatially resolved operando studies. In a new BMBF project it is planned to develop FTIR cells for the monitoring of plasma-assisted catalytical CO$_2$ transformations together with the INP Greifswald. In a new PhD program together with the group ‘Numerical Analysis’ we are going to explore the benefits of perturbation experiment designs in combination with an automated chemometric analyses for component identification.

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MAGNETIC RESONANCE & X-RAY METHODS

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The central goal of our research activities is focused on elucidating structure-reactivity relationships and obtaining mechanistic insight in catalysis to provide a solid basis for a rational design of highly active, selective, and stable catalysts, and for improving existing catalytic processes beyond trial-and-error approaches. This requires understanding complex reaction pathways by monitoring catalytic reactions under realistic conditions, normally at elevated pressure and temperature, with real-time online products analysis. For this purpose, our group uses preferentially EPR spectroscopy, also coupled simultaneously with other techniques such as RAMAN, ATR-IR, UV/Vis and synchrotron-based X-ray absorption spectroscopy to widen the extent of achievable information on structural changes and active sites under identical reaction conditions. Currently, we are investigating different catalytic reactions mostly (but not only) related to energy and environmental applications such as preferential CO oxidation, CO_2 hydrogenation and olefin oligomerization on supported metal and metal oxide catalysts, as well as low-temperature NH_3-SCR of NO_x. Enabled by the recent installation of high-end equipment at LIKAT and in cooperation with the Department of Life, Light and Matter at the University of Rostock we are pushing forward our *in situ/operando* studies towards TEM and XPS studies under near-ambient pressure.

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BIONSPIRED CATALYSIS ‘DE NOVO-DESIGN’ OF TRANSITION METALLOENZYMES

Prof. Dr. Paul Kamer
1960-2020

A lab for genetic engineering was established to allow the custom preparation of proteins containing the desired properties. By combining the concepts of biology for selective recognition with those of transition metal catalysis we develop novel, highly selective catalysts for important (asymmetric) catalytic C-C bond forming reactions. Furthermore, the high substrate specificity induced by these enzymes allows conversion of a single substrate present in complex mixtures, like those in biological systems. We have developed methods to introduce phosphine ligands into proteins to introduce non-natural transition metal complexes into proteins. By changing the amino acid sequence and the structure of the catalytic metal complex these catalysts can be optimized towards efficient and selective reactions.

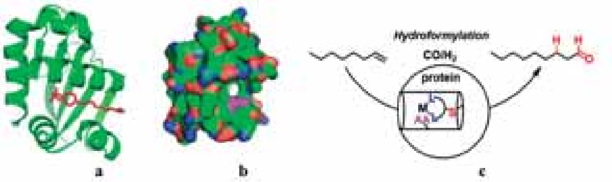

Figure 1. cartoon (a) and space filling structure (b) of SCP-2L used in hydroformylation (c)

We have explored several protein structures such as Photoactive Yellow Protein and Steroid Carrier Protein 2-L. The protein structures have been selected for their substrate binding properties and are applied in several C-C and C-X bond forming reactions[1, 2] and catalytic hydrogenation.[3]

SCP-2L contains a large apolar molecular tunnel and this binding-site can be modified with suitable transition metal complexes. The protein has been modified by mutagenesis to obtain one unique cysteine at the desired position. The protein can be efficiently and selectively modified with phosphines and phosphine-metal complexes. These rhodium phosphine modified SCP-2Ls are efficient linear-selective catalysts in the hydroformylation of long-chain alkenes in water.[4]

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OLIGOMERISATIONS RATIONAL DESIGN OF DIPHOSPHORUS LIGANDS – A ROUTE TO SUPERIOR CATALYSTS

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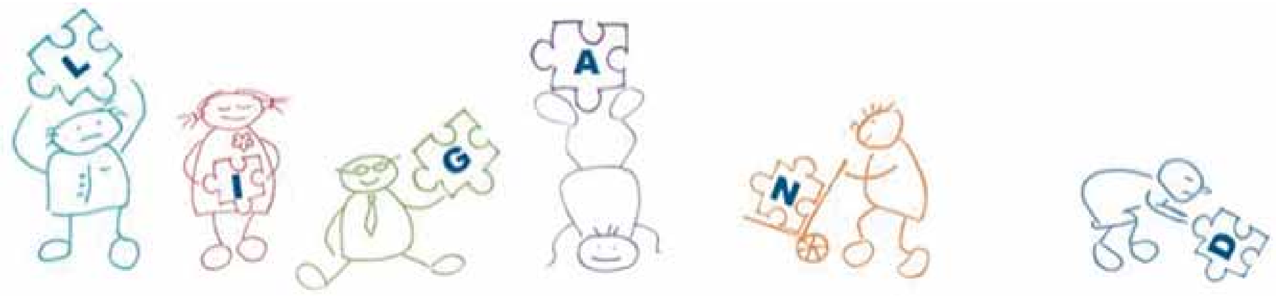
The catalytical features of a transition metal complex is determined by its ligands. By modulation of the ligand both the selectivity and rate of a catalytic reaction can be steered. Essential core competencies for the improvement and new development of homogeneous catalysts are the knowledge about the structure-activity relationship and the ability to synthesize the designed ligands in the lab. Asymmetric catalysts based on rhodium and P-chirogenic phosphine ligands were synthesized.[1] These ligands were used as parts of several transition metal complexes. Ligand effects and kinetics are key issues in these projects.

Also for the catalytic selective oligomerisation of ethylene, innovative ligand design is crucial to achieve progress.[2] The synthesis of custom-made ligands is therefore of key importance.



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CATALYSIS WITH RENEWABLES & PLATFORM CHEMICALS

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In view of the increasing scarcity of fossil resources, research into the conversion of renewable raw materials into basic and fine chemicals is becoming increasingly important. A major role is played by the (homogeneous) catalytic conversion of non-edible plant material such as cellulose, lignin or lignocellulose into a range of platform chemicals such as ethanol, 5-hydroxymethylfurfural (5-HMF) or levulinic acid.

However, the production of valuable chemicals is often accompanied by the formation of undesirable byproducts. These platform chemicals and by-products will be made accessible from waste streams for various applications in the chemical industry.

(1) Methyl levulinate (ML), a side-stream molecule generated during the production of 2,5-furandicarboxylic acid is to be converted into two industrially valuable molecules, methyl acrylate and acetic acid, in only two steps. The first step is well known.[1]

In the second step, which we developed, we succeeded in almost complete conversion of the ML (99 %) with selectivities of 98 % for methyl acrylate and 97 % for acetic acid.[2] Both compounds are easily separable by distillation.[3]

(2) Cleavable adhesives: polyurethanes are used to make adhesive films. Acetals added as additives (5 - 10 %) to bio-based polyurethanes were synthesized in only one step from the platform chemicals glycerol and 5-HMF. Depending on the content of the acetals, the cleavability (and thus degradability) of the adhesives can be adjusted in an acidic environment. This enables many applications where the components are to be recycled at the end of their life. One example is electronic devices in which many different and also expensive materials are bonded together.

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(1) HUGS (HUmine as sustainable precursors of environmentally friendly materials and biofuels), funded by Marie Skłodowska-Curie - grant, initiated by Avantium company

ORGANOCATALYSIS

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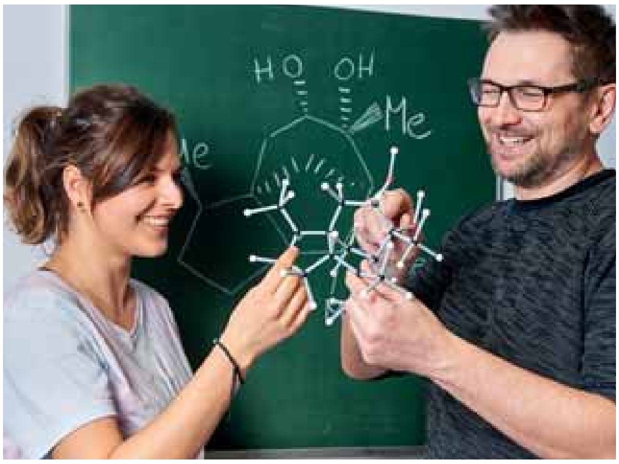
We are engaged in the development and application of sustainable catalytic processes. One aspect of our work is the development and implementation of phosphorus based organocatalysts and synthetic methods such as halogenations, olefinations and reductions using P^{III}/P^{V} redox cycling catalysis. 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_2 as a C1 building, e.g. for the preparation of bio-based carbonates. 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_2 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.



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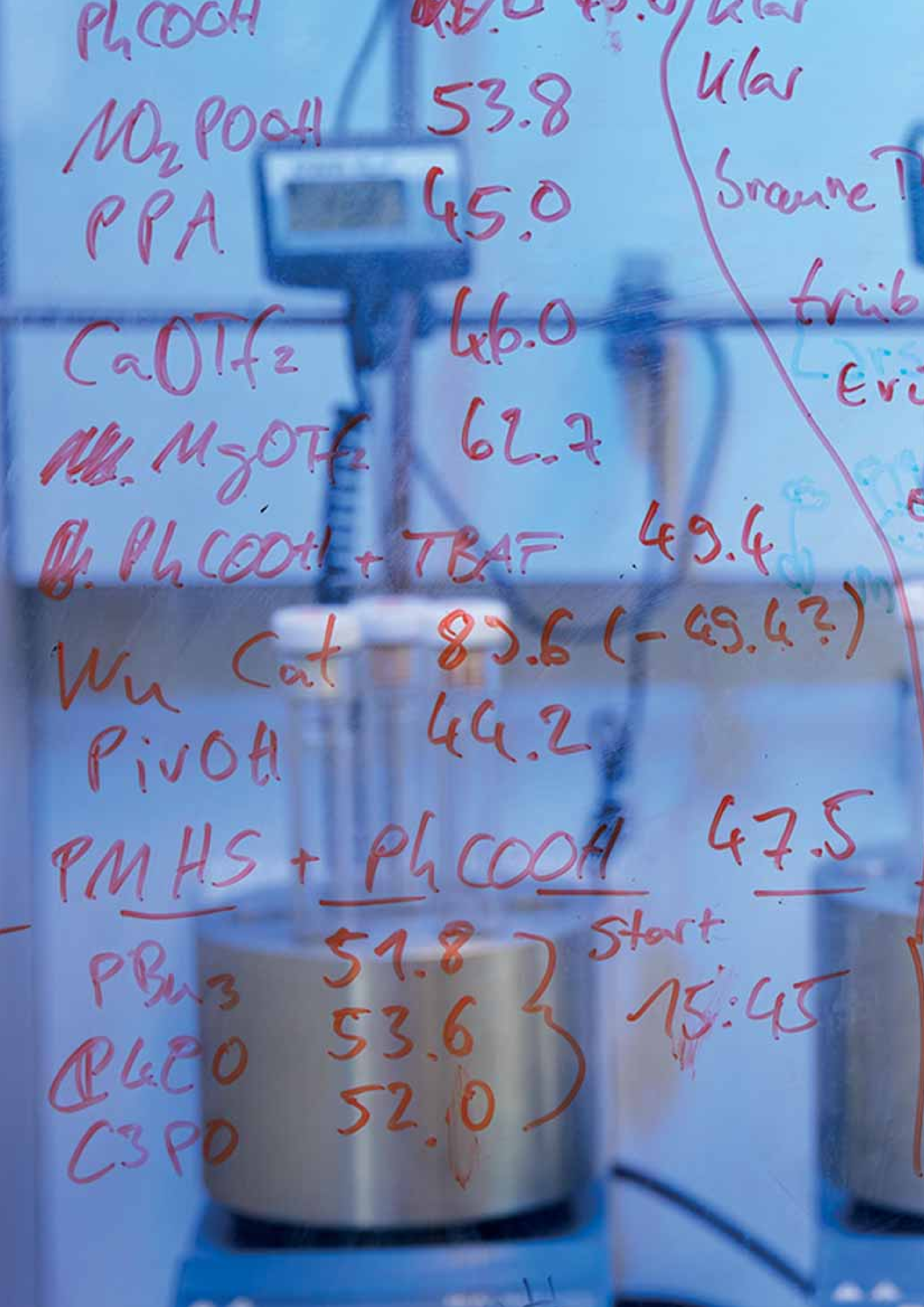
PhCOOH
klar
klar
NO2POOH 53.8
PPA 45.0
braune
CaOTf2 46.0
trüb
MgOTf2 62.7
PhCOOH + TBAF 49.4
Cu Cat 87.6 (-49.4?)
PivOH 44.2
PMHS + PhCOOH 47.5
Start
15:45
PBu3 51.8
Ph3PO 53.6
C3PO 52.0

REACTION MECHANISMS

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Changes in the raw material basis and expanded legal regulations to reduce energy consumption and undesired emissions pose the sustainability challenges for the chemical industry. Against this background, our research activities concentrate on the design of heterogeneous catalysts as well as on the development of reactor concepts for more efficient processes.

Preparation of catalysts with the desired performance obligatory requires the comprehensive understanding of (i) general relationships between activity/selectivity and catalyst architecture, preferably, the structure of active sites and (ii) fundamentals for purposeful creation of such sites. To this end, we combine the synthesis of well-defined bulk and supported materials with advanced mechanistic and kinetic studies based on temporal analysis of products with isotopic tracers, operando time- and spatially resolved spectroscopic studies and catalytic evaluation under industrially relevant conditions.

We study both challenging reactions using alternative raw materials and well-established commercial processes. They include natural gas upgrading, e.g. methane oxidation to C_2-hydrocarbons (ethylene and ethane) or oxidative/non-oxidative dehydrogenation of C_2-C_4 alkanes to the corresponding olefins, carbon dioxide hydrogenation to fuels, lower olefins or methanol and high-temperature ammonia conversion into nitric oxide or hydrogen cyanide.

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Fig.: A photo of setup for high-temperature NH_3 conversion into NO or HCN under industrially relevant conditions.

REACTION ENGINEERING

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The group has been working at the interface between chemistry, engineering, and data science with a special focus on the development and improvement of catalytic gas-phase processes. 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).[1] NFDI4Cat, which started in October 2020, will address creation of machine-interpretable data applying principles that have been recently summarized under the term FAIR (Findable, Accessible, Interoperable, Reusable).[2] Within LIKAT a local system will be developed that assists in producing FAIR data.

Another important part of the work are experimental studies. We use parallel reactors for catalyst development and kinetic studies. We explore reactions related to using alternative raw materials (e.g. bioethanol) or alternative reaction pathways (e.g. CO_2 based fuel production). In the last years, we cooperated with an industrial partner the development of a new fixed-bed process for a 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).

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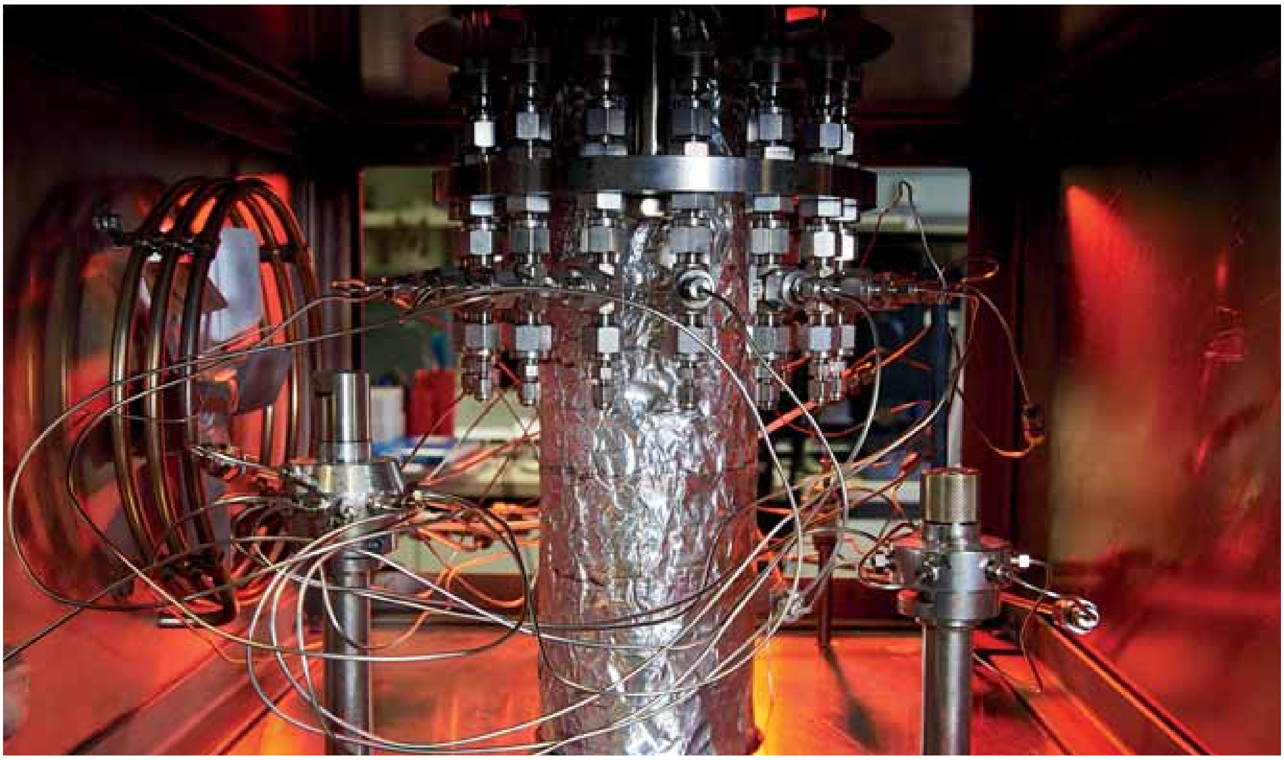
NFDI4Cat



HIGH-THROUGHPUT TECHNOLOGIES

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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 research group Linke)
- 2 synthesis robots, automated calcination apparatus (64 parallel reactor, 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 750 °C and 20 bar)
- Automated apparatus with 8 reactors for temperature-programmed experiments (TPO, TPR, TPD)

Presently, we develop new automated equipment with the aim to understand better the chemistry during synthesis of heterogeneous catalysts. To this end we combine control and data recording for liquid dosing pumps, pH meter, temperature and *in situ* UV/Vis spectroscopy.

The methods and equipment have been successfully applied to the development of catalysts for different reaction types such as dehydrogenation, oxidation, condensation, isomerization, methane reforming, CO_2-based Fischer-Tropsch synthesis and others.

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MIKRO REACTION ENGINEERING

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One focus of the group is the development of photocatalytically active materials. With the help of these materials and sunlight, fine chemicals can be synthesized and pollutants dissolved in water can be effectively eliminated. The photocatalytic performance of these materials depends on their composition, morphology, and electronic properties. Photocatalysts which have been synthesized include titanium dioxides of various compositions, carbon nitrides and metal sulfides. The photocatalysts are mainly tested in a suspension reactor under irradiation with light. The aim of these investigations is to identify active and selective materials and to derive correlations between material and photocatalytic properties.

The group is also involved in the development of continuously operated processes of multiphase reactions (gas/liquid, gas/liquid/solid) for the synthesis of fine chemicals using microstructured reactors. This includes the development of suitable catalysts. The group has a modular PC-based Ehrfeld system equipped with a cartridge reactor 240. This system allows monitoring the catalyst behavior over a long-term period without interrupting the reaction, allowing both catalyst activation and deactivation to be studied in a targeted manner.

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PHOTOCATALYTIC CARBON DIOXIDE REDUCTION

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Studies of the photocatalytic reduction of carbon dioxide face the challenge that the currently achievable yields are very low, so that sophisticated trace gas analysis is required for the reliable characterization of the product distribution. Furthermore, the presence of impurities must be ruled out, since even small amounts, in particular of carbon-containing components, can completely obscure the actual activity of the catalyst.

The core competence of the research group is, therefore, the photocatalytic reaction under conditions of the highest possible purity and accuracy. This is achieved by using components suitable for high vacuum applications. Gas analysis is based on both gas chromatography and mass spectrometry. In 2019, quantitative statements could, thus, be made about the applicability of titanium dioxide for photocatalytic energy storage reactions. Plasmonic systems were also examined. In addition, the focus was on extending the possible reaction conditions. While in the previous years work was carried out exclusively at room temperature and with heterogeneous catalysts, experiments at up to 180 °C and with molecular photocatalysts are now also possible. Moreover, the prerequisites were established to use reactants other than water, e.g., hydrogen or methane, in order to enable further interesting photocatalytic processes (e.g. photo-dry reforming).

The research group ‘Structure-function correlations’ has been under construction since 2019. The research focus will be set on identification of active sites for photocatalytic reactions. Detailed *in situ* studies on ‘single-site’ and ‘single-atom’ catalysts are in progress and will be reported at a later date.

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TECHNOLOGY-ORIENTED PROCESSES

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The research group 'Technology-Oriented Processes' develops heterogeneous catalysts and synthesis routes for the material or energetic use of renewable raw materials and platform chemicals as well as CO_2. Such processes often require high pressure. The long experience of the research group on high pressure reactions (supercritical fluids, hydrogenation) is ideally used in this relation. We aim to design such conversions preferably in continuous processes and to gain knowledge for technical applications at an early stage.

The flexible equipment allows catalyst tests under various reaction conditions, even in larger reactors and with shaped catalysts (tablets). In addition, it is possible to characterize solid catalysts in order to elucidate their mode of action. For this purpose, the research group operates a sorption laboratory in which various methods (BET, TPX-MS coupling) are combined. This expertise is also available to other topic groups in the institute.

Current key topics (BMWi, BMBF projects) are the conversion of sugar-derived platform chemicals such as levulinic acid and the utilization of CO_2. Particularly worth mentioning are methanol synthesis, Fischer-Tropsch synthesis and dry reforming of CO_2 with methane. Experience from current industrial collaborations on ammonia and methanol synthesis and from environmental catalysis (denitrification and desulfurization) can also be used here.

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LIQUID PHASE OXIDATIONS

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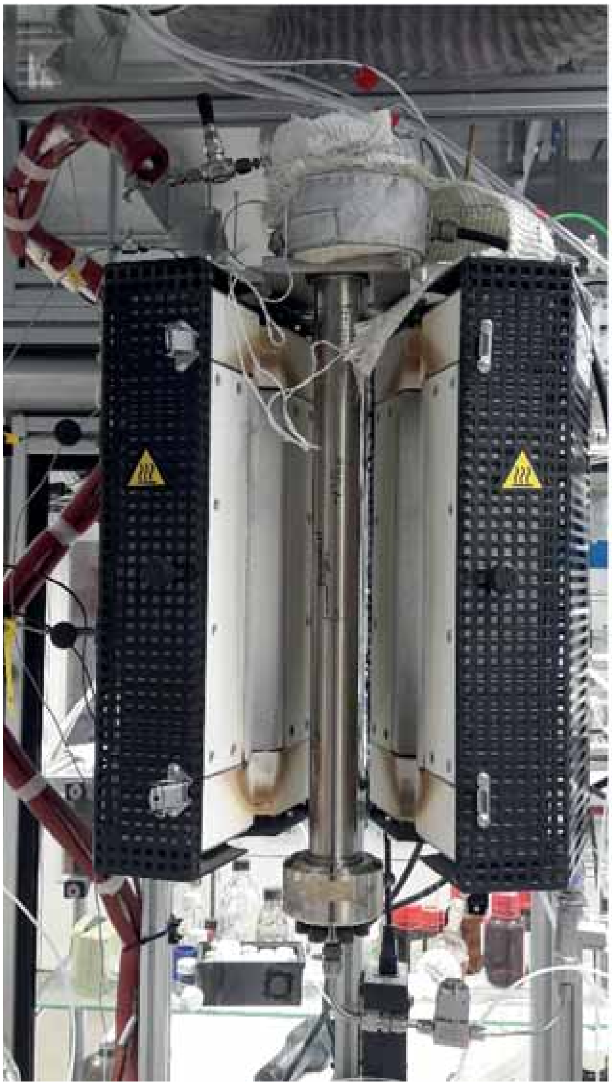
In the research group, innovative material transformations are developed, mainly catalytic oxidations with „green“ oxidants, but also hydrogenations or isomerisations of renewable raw materials to fine chemicals. Terpenes and both fatty acid and sugar derivatives are used as substrates; target products are, for example, flavours and fragrances or building blocks for bio-based polymers. The catalysts used are predominantly heterogeneous supported metal catalysts or oxidic catalysts, and extensive experience exists for their customised synthesis.

The best possible process management is determined for each reaction. Instead of carrying out the reactions almost exclusively in stirred tank reactors or autoclaves, as has been common in fine chemistry up to now, it has been demonstrated that continuous or semi-continuous processes are often the better choice in terms of yield and selectivity of the desired product. Thus, for the first time, syntheses in the gas phase could be successfully used for production of terpenes and diols.

The research group is experienced in many years of co-operations with various industrial partners, and the results of joint research have been utilised in numerous patents and in transfer into industry.



1-Inch titanium tubular reactor with two-stage heating jacket in a set-up for continuous reactions in the liquid phase with analysis of reaction products by an online gas chromatograph.

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INORGANIC FUNCTIONAL MATERIALS

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The research group ‘Inorganic Functional Materials’ focuses on the development of new materials for the catalytic refinement of C1 building blocks. A special focus is on the conception and realization of porous solids. These are used i) for separations,[1] ii) for decoupling of classical multicomponent catalysts[2] or iii) for surface attachment of molecular catalyst species.[3, 4] The materials are applied, for example, in the direct oxidation of methane to oxygenates, for the aromatization of methane or for the catalytic removal of methane traces from exhaust gases. Functionalizations of carbon dioxide to carbonates, methanol or higher hydrocarbons are also an integral part of the research work. In addition to these own topics, the group networks with other researchers in the institute, so that, for example, new photocatalysts for water splitting[5] or highly efficient catalysts for the production of nylon precursors could be realized.[6] In the future, such collaborations will be strengthened by collaborations in the field of ammonia or formic acid synthesis, where new catalytic materials or even processes are to be developed. Furthermore, the planning of catalyst syntheses on a pilot plant scale is taking place. This is essential for future projects with direct relevance to scale-up in order to enable the transfer of laboratory results to applications.

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SMALL MOLECULE ACTIVATION

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Our research group is engaged in the design of novel ligand architectures based on phosphaalkenes. Phosphaalkenes (PA) possess a P=C double bond and offer a variety of attachment possibilities for transition metals (TM) and are predestined to stabilize electron-rich metals. For the formation of the P=C bond, we use the so-called phospha-Wittig reaction, in which phospha-Wittig reagents ArPPMe$_3$ react with aldehydes to give the PAs with cleavage of OPMe$_3$.

In the preparation of ^{Mes}TerPPMe3, ^{Mes}TerP(NEt$_2$)$_2$ is required, which has been successfully applied as a ligand in the gold-catalyzed hydroamination of acetylenes.[1]

In an attempt to use small aryl groups on phosphorus in the phospha-Wittig reaction, a selective route to aryl-substituted triphosphiranes (ArP)$_3$ was found.[2] In addition, we were able to present the analogous arsenic three-membered rings.[3]

Isolable phospha-Wittig reagents ArPPMe$_3$ can be used as phosphinide sources and we have shown that NHC phosphinide adducts are formed with NHCs.[4] NHOs, on the other hand, react (NHO = N-heterocyclic olefins) under C(sp^2)-H activation. Moreover, the reaction of ^{Dip}TerPnPMe$_3$ with (AlCp*)$_4$ succeeded in the preparation of the first base-free pnictaalumene with a Pn=Al double bond.[5]

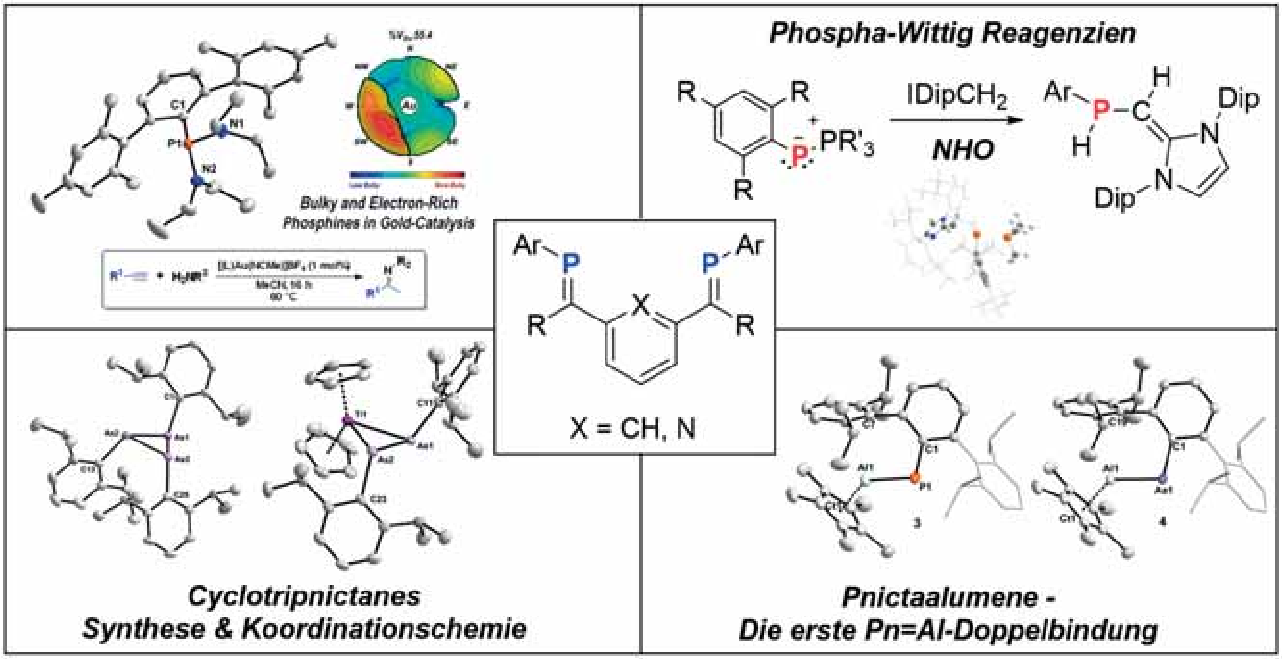

Fig. 1: Overview of the research activities of the Hering-Junghans Group.

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POLYMER CHEMISTRY & CATALYSIS

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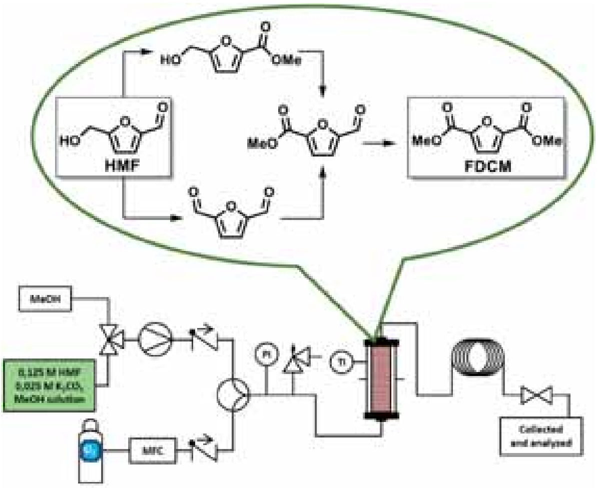
Chemistry, as one of the main players of progress and (arguably) the culprit of most of its evils, has been called to tackle these problems, head-on, for which a 'complete makeover' on the way chemists design their processes and manage their outcomes was necessary. The paradigm shift came with the development 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 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.

Furthermore, the development of 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.



Metal-free catalyst for aerobic oxidation reactions, including heterogeneous carbocatalysts and persistent radical cations are being developed.

Another focus is the synthesis and application of heterogeneous catalysts derived from waste rice husk. An alternative route for the valorization of agricultural rice bio-waste was established, resulting in high added-value products (the catalysts) with potential immediate impact in the chemical industry.

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CATALYTIC FUNCTIONALIZATIONS

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The focus of the junior research group is the development of photochemical, electrochemical and transition metal-catalyzed processes for the targeted synthesis of bioactive molecules. In recent years, the group was engaged in a state-wide research cluster (PePPP) encompassing research groups from the Universities of Greifswald and Rostock to develop a therapeutic platform for the treatment of a hereditary, monogenetic copper storage disease.[1]

In particular, the development and application of new heterocyclic photoredox catalysts enabled the synthesis of a significant number of compounds for individual testing.[2, 3]

Moreover, in a DFG-funded project, the Pospech group concentrates on the targeted synthesis of drug metabolites by photoinduced oxygen atom transfer in the sense of a chemical equivalent to oxygenase enzymes. In close collaboration with in-house research teams in the field of spectroscopy and theoretical chemistry, mechanistic investigations provide an indispensable basis for the optimization of our processes up to translation into process engineering.

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CATALYTIC CYCLOADDITIONS

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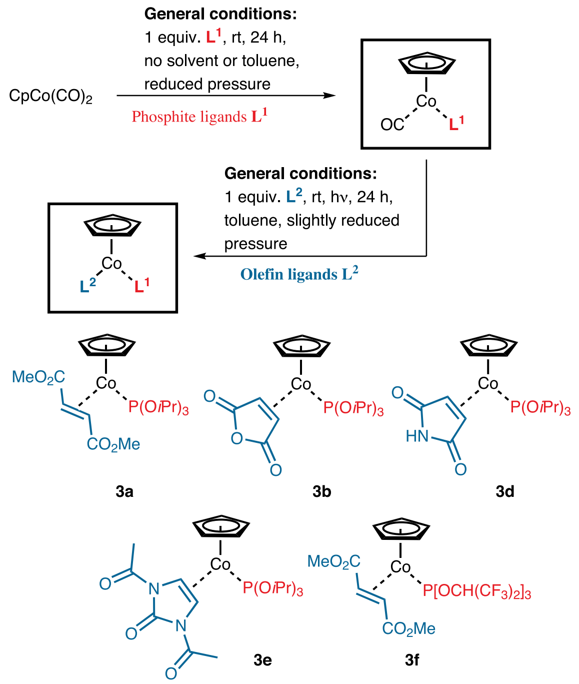
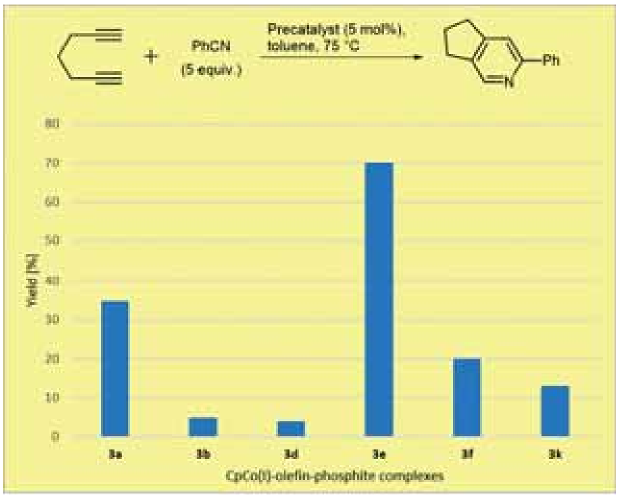
Molecular functionalities with unsaturated groups such as C-C or C-N double and triple bonds can undergo both ‘static’ and ‘dynamic’ interactions with transition metals. In the case of ‘dynamic’ interactions between transition metals and triple bonds of alkynes and nitriles, the transition metal can act as a catalyst for a variety of interesting and atom-economic reactions, among which cycloadditions are most prominent. The systematic construction of molecules with high functionality and complexity by metal-catalyzed cycloaddition reactions starting from alkynes and heteroatom-containing analogues represents an interesting challenge. In this context, the specific preparation and characterization of precatalysts provides the blueprint for the development of new catalyst systems and facilitates the understanding of structure-reactivity relationships.[1] Our focus is on group 9 and neighbouring metals, especially cobalt.[2] The synthesis, characterization and testing of the partially highly reactive catalysts in cyclotrimerizations of new substrates under a variety of conditions is one of our core competences. For the reactions, we use microwave technology, photochemical reactors and increasingly flow chemistry (in cooperation with JKU Linz) in addition to classical conditions.





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POLYMER CHEMISTRY & CATALYSIS

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We are engaged in process development for chemo- and biocatalytic processes. This includes the development of new processes, especially in the field of downstream processing, e.g. with membrane processes, as well as new catalysts and materials. Investigations into scale-up and the optimization of existing processes and procedures with regard to economic and ecological aspects are also the subject of the work. In the field of biocatalysis Dr. Jan von Langermann has habilitated with the concept of *in-situ* product removal, Dr. Robert Francke in the field of electrocatalysis with the concept of membrane separation of polymer-bound mediators. The research activities at LIKAT are characterized by the junior research group of Dr. Esteban Mejia, who is located at the institute and successfully completed his habilitation in December 2020. The main research areas include silicone-based polymers and polyether-based functional materials.

Silicone-based polymers

Silicone polymers, especially polydimethylsiloxane derivatives, are of great importance as adhesives, sealants and insulators. Products that vulcanize at room temperature and mild conditions account for the largest share of the market. Silicone sealants show excellent performance under harsh conditions, are UV, ozone and moisture resistant, and can tolerate high temperatures. In addition, they have excellent adhesion to surfaces of common building materials. New functionalized silicones are being developed for special applications in automotive construction and electronic devices.

Polyether-based functional materials

Together with an industrial partner, new polymerization catalysts and polymers for coatings, sealants and adhesives are being developed. Related process engineering issues are also being addressed for process optimization. In addition to a narrow molecular weight distribution as a key quality criterion, other physicochemical properties such as viscosity are also important target variables for optimizing the process parameters.

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ORGANIC CHEMISTRY

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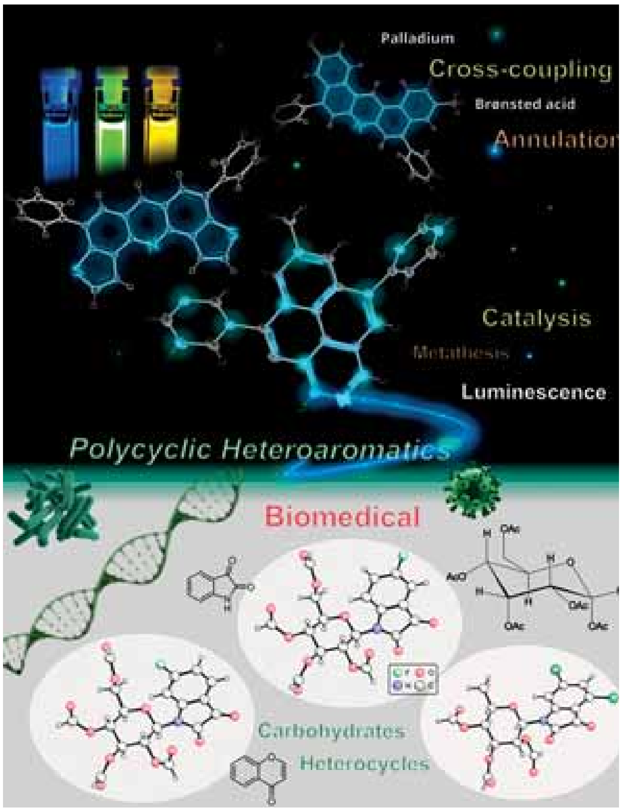
The research group of Prof. Peter Langer focusses on the synthesis and functionalisation of new heterocyclic compounds as well as natural product derivatives. In this regard, we are connecting innovative catalytic reactions with classical organic synthetic chemistry. Core areas are located in the development of new synthetic methodologies and strategies as well as their application in novel cyclisation reactions. Research focuses on the synthesis of biomedicinal and next-generation opto-electronic materials and hence, newly synthesised compounds are comprehensively characterised for their bioactivity and/or physicochemical properties.

The selectivity of Palladium catalysed cross-coupling reactions and the development of novel cyclisation reactions towards several carbazole derivatives and other heterocycles as well as the investigation of new domino-reactions were integral areas of research.

During the last two years, we developed a novel access to several aza-pyrenes, ullazines and acridines which allow the synthesis of analogous heterocyclic derivatives and permits the determination of structure-property-relationships on respective heterocycles in near future.

Another main emphasis of research was the synthesis of functionalised thiadiazoles, chromones and glycolyzed oxindole derivatives exhibiting high activity towards several cancer cell-lines.



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VIBRATIONAL SPECTROSCOPY

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The research activities of the Ludwig group at LIKAT focus on the use of vibrational spectroscopy to study mechanisms of catalytic reactions. This includes high pressure *in situ* IR spectroscopy, development and application of programs for spectra decomposition as well as quantum chemical calculations of spectroscopic properties. The focus is on the identification of catalytically active species and the determination of the kinetics of complex and cluster formation. Recently, spectroelectrochemistry has been added as a method that simultaneously provides information on the structure and charge transfer of reaction partners.

Furthermore, we deal with the investigation of clusters, fluids and interfaces and bridge the gap between experiment and theory with an appropriate spectrum of methods. IR, Raman and NMR spectroscopy are complemented by quantum chemical calculations, and classical molecular dynamics simulations. We would also like to apply this spectrum of methods to the mechanistic understanding of processes in catalysis.

Projects in 2019/2020 include studies of photo- and electrochemical processes in CO_2 reduction, and characterization of metal complexes and hydrogen bonds in ionic and molecular clusters.

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NUMERICAL ANALYSIS

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‘Data Science’ is an interdisciplinary scientific field that develops methods for extracting information from data. The high complexity of chemical reaction systems together with data generating spectroscopic methods represent an ideal field of application. We develop factor-analytical methods of chemometrics for high-resolution spectral series of modern computer-based spectrometers. Such methods allow to determine the number of pure components, the pure spectra and the concentration profiles from high-dimensional spectral data of chemical reaction systems. Numerical method development for chemometric factor analysis is complemented by program implementations. The work with a focus on homogeneous catalysis is carried out at LIKAT in cooperation with the groups of Prof. Brückner (Börner/Kubis) and Profs. Francke and Ludwig.

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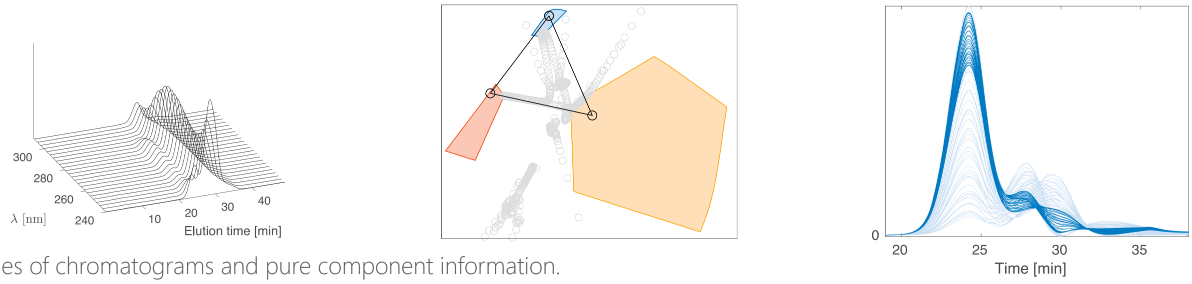
Factor analytical methods often use a bilinear relation in the sense of Lambert-Beer‘s law and start with a singular value decomposition of a matrix of, e.g., IR or UV/Vis measurement data.[2, 5] Routines for curve fitting and modeling complement this.[1, 3, 4] Pure component decompositions are usually not unique. A correct factorization can often be obtained from the set of possible factorizations (Area of Feasible Solutions, AFS[1, 2]). One focus of our work is the identification of ‘relevant’ and thus particularly structure-determining regions in the spectrum series.[2, 5] In the future, these should be a basis for automated decomposition routines. For NMR data, the bilinear relationship is broken. We develop spline-based peak tracking techniques for time series analyses. Peaks are modeled by Lorenz and Gaussian curves and their parameters are represented in the time direction using spline functions. The application to low-field data opens up new fields of application for benchtop NMR instruments.



Series of chromatograms and pure component information.

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MATERIAL DESIGN

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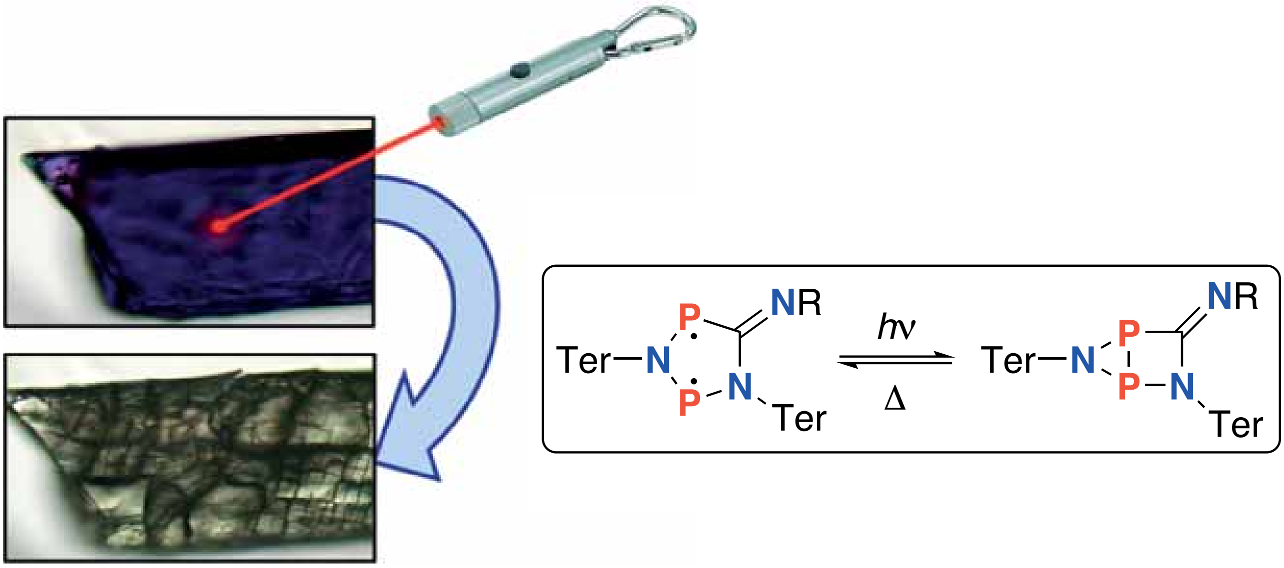
We are involved in the design and application of new materials mainly based on main group element compounds,[1-5] such as silicones for 3D printing or new pnictogen materials (C/N, E/N materials, E = group 15 element) for molecular switches. In addition, we are investigating syntheses in unusual reaction media (e.g. ionic liquids, SO_2, and pure HCN).

In the context of research on new pnictogen materials, new molecular switches based on cyclic biradical compounds have been developed.[1] Molecular switches are molecules that can be reversibly switched between at least two stable states with different physical and chemical properties, which predestines them for use as chemical sensors or molecular machines. The five-membered cyclic biradicals based on group 15 elements proved to be efficient and robust photochemical switches that can be activated by red light (Figure). The fully reversible process was investigated both experimentally (*in situ* NMR techniques, femtosecond spectroscopy) and by sophisticated *ab initio* techniques. Such materials offer the possibility to start and stop the stoichiometric and catalytic activation of small molecules by irradiation.[1]



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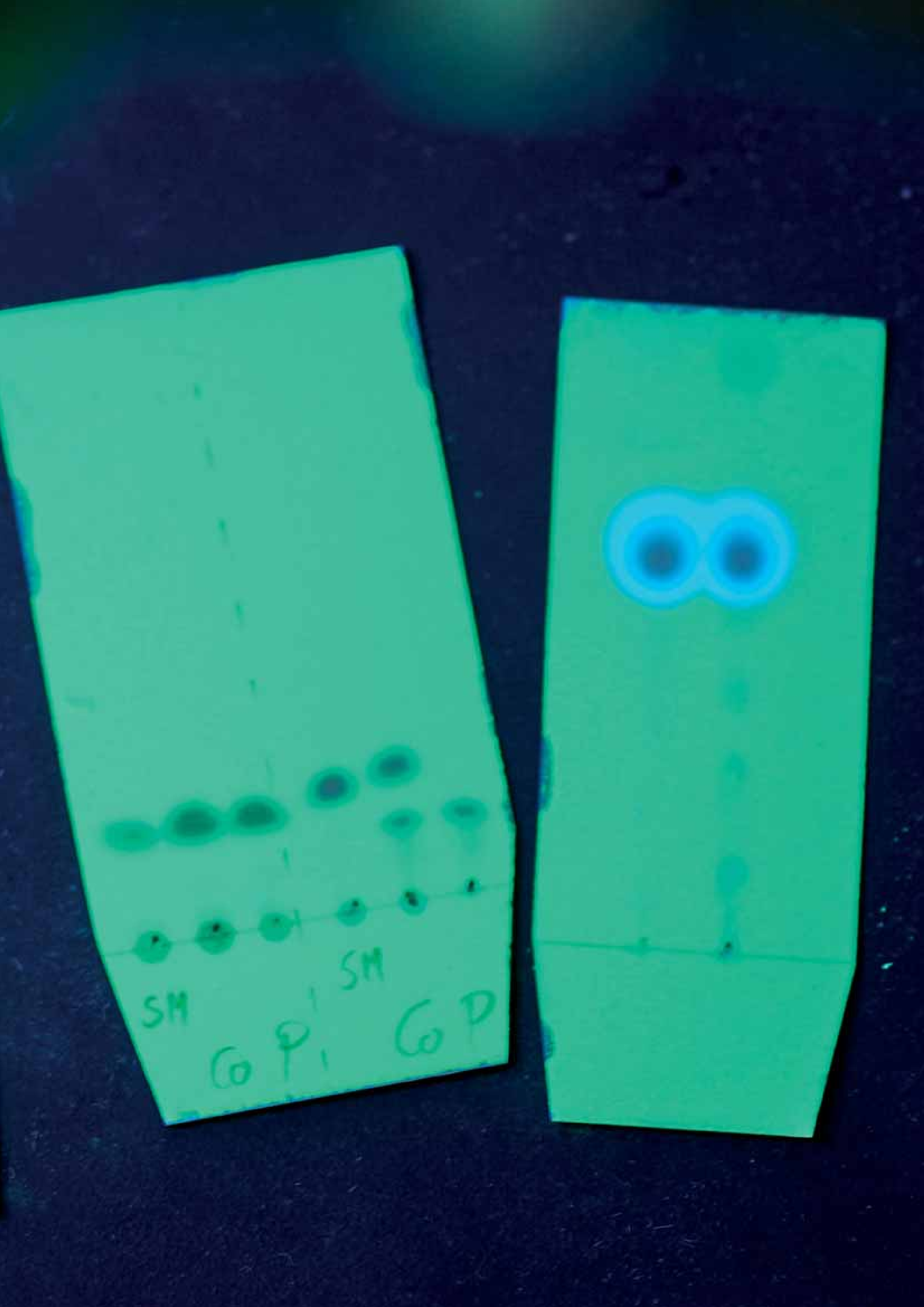
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ANALYTICAL SERVICES

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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.

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 (for gas chromatography or X-ray fluorescence analysis) have been replaced by up-to-date devices. In surface and solids' analytics, we now have access to new possibilities:

The University of Rostock and LIKAT jointly managed to get a grant for a high-end electron microscope (funding by DFG within the frame of 'Großgeräteprogramm' – Major Research Instrumentation). This microscope has now been successfully installed and started operation in the 'Interdisziplinäre Fakultät' (Interdisciplinary Faculty of the University). From funds of the European Union, a 'Near Ambient Pressure' photoelectron spectrometer (NAP-XPS) was purchased for LIKAT. This device will allow the inspection of catalyst surfaces under conditions closer to realistic situations than it was possible before, viz. pressure up to 25 mbar and temperature to 1000 °C.

Common feature of both 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'.

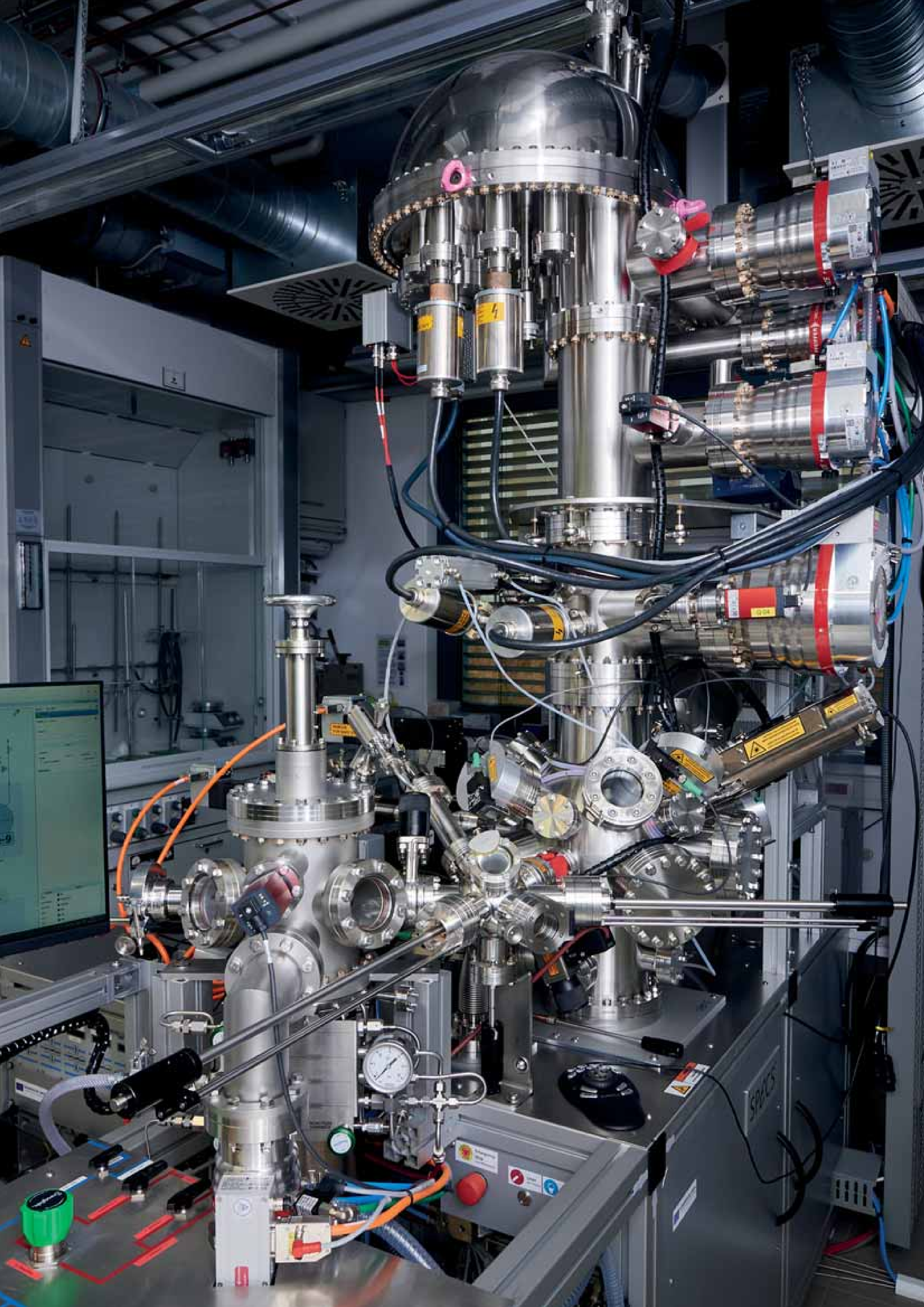
The Analytical Services Department furthermore has a perceptible impact on the publication activity of LIKAT. From time to time, we publish own results, but most of the scientific output results from intensive collaboration with researchers from all LIKAT's departments. Some methods are made available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

Spectroscopic *in situ* studies (on reacting systems) to elucidate the catalyst mode of action are carried out in close cooperation with the respective research groups.

In the research department 'Catalytic *in situ* Studies' further techniques are used, new measurement methods are developed and method couplings are realized, which are specifically used in catalysis research for the elucidation of structure-activity relationships and of reaction mechanisms.

Some large-scale equipment is operated jointly with the Institute of Chemistry of the University of Rostock in order to make optimal use of it.

in situ methods
are extremely valuable for catalysis research, as they allow to observe reacting systems directly, i. e. without sampling. Sampling in combination with external (time-relayed) analytics is normally not suitable to describe the real state of a reaction appropriately. For this reason, both the Research Department 'Catalytic *in situ* Studies' and the Analytical Services deal with this topic intensively.


SPECS

ANALYTICS – METHODS AND EXPERTISE

CHROMATOGRAPHY (GC AND HPLC)

Chromatographic methods allow the separation and analysis of mixtures of substances, such as those produced in chemical reactions, and identification of the individual components, which can also be quantified. Many years of experience are available, especially in the field of analysis of chiral compounds (enantiomer analysis). Analytical methods are being developed for novel separation problems.

ELEMENT ANALYTICS (AAS, ICP-OES, RFA, COMBUSTION ANALYSIS, TITRATION AND PHOTOMETRY INCLUDING DIGESTION METHODS)

Both organic and inorganic materials can be analyzed for their elemental composition. Solids are brought into solution for this purpose, if necessary, by melting or acid digestion, the latter with microwave support.

MASS SPRECTROMETRY, PARTLY WITH CHROMATOGRAPHY COUPLING (GC-MS AND LC-MS)

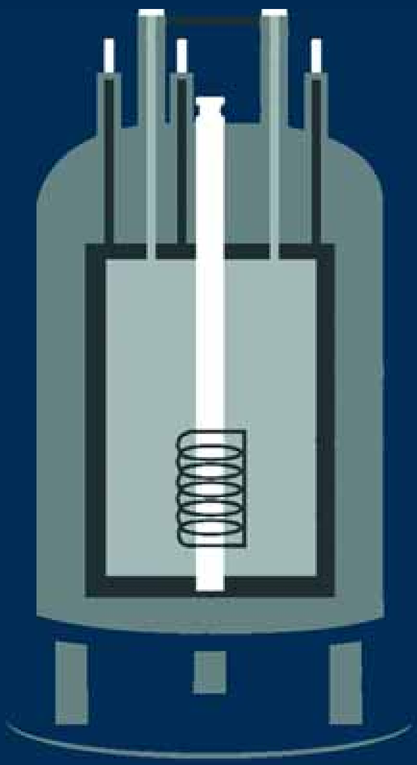
Mass spectrometry (MS) is a method that can be used for the structural elucidation of organic and inorganic compounds, for trace analysis, for the determination of atomic masses and isotope abundances, for the determination of ionization, formation and dissociation energies, for the determination of the elemental composition of organic compounds, and much more.

In the analytical service department, mass spectrometers are operated in coupling with chromatography instruments (‘hyphenated techniques’, GC-MS and LC-MS) and ‘stand-alone’ (with direct inlet).

HIGH-RESOLUTION NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY (NMR)

High-resolution nuclear magnetic resonance (NMR) spectroscopy of liquids and solutions is one of the most important methods for structure elucidation in synthetic chemistry. In addition to this qualitative aspect, nuclear magnetic resonance offers a wide range of possibilities for quantitative determinations and the study of molecular dynamics.

In the field of nuclear magnetic resonance there is a close cooperation with the Institute of Chemistry at the University of Rostock.



CAPILLARY ELECTROPHORESIS (CE)

Capillary electrophoresis is a separation method based on the migration of charged particles through a (liquid) medium in an electric field. Charge, shape and effective size of the ions as well as solvent and strength of the electric field are crucial for the migration speed and separation. The CE manages with very small volumes of only 10 nanoliters.

PHOTOELECTRON SPECTROSCOPY (ESCA, XPS)

Photoelectron spectroscopy (XPS - X-ray Photoelectron Spectroscopy) has been one of the standard methods of surface analysis for decades and is based on the photoelectric effect. Energetic radiation knocks electrons out of the atoms on the surface. Their energy is characteristic of the atoms and their bonding state at or near the sample surface. In recent years, the method has been developed from pure application under ultra-high vacuum conditions to near ambient pressures.

X-RAY DIFFRACTION ON POWDERS AND SINGLE CRYSTALS (XRD)

The diffraction of X-rays at the crystal lattice of single crystals enables the elucidation of crystal structures. In addition to information about the constitution and conformation, statements about the three-dimensional packing in the solid state are also possible.

A main focus is the investigation of catalysts under working conditions, e.g. at elevated temperature and in the presence of different reactive gases (non-ambient, *in situ*). The characterization possibilities of a sample are constantly being developed. One possibility is method coupling (*in-operando*).

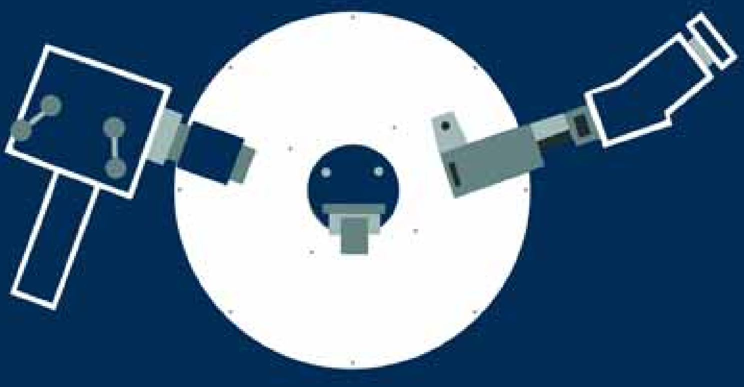
ANALYTICAL ELECTRON MICROSCOPY (CS-CORRECTED STEM) WITH EELS AND EDX

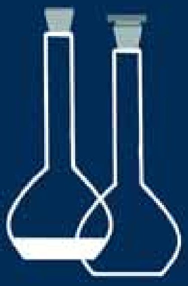
Electron microscopy can be used to visualize structures of samples in the nanometer and subnanometer range.

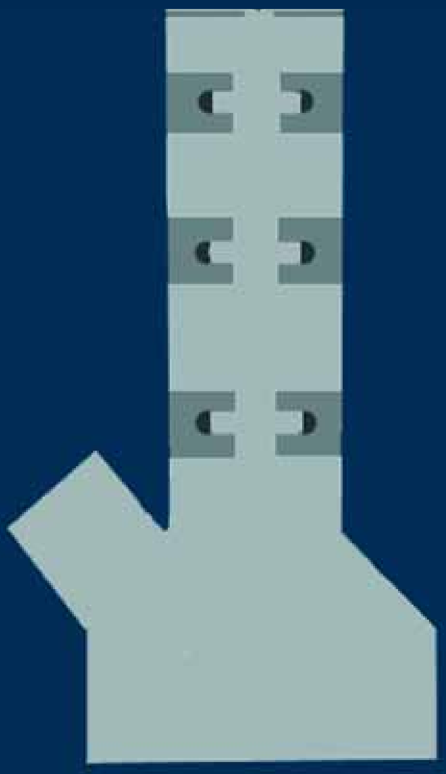
The electron beam can be focused to a very small circular diameter, allowing atomic resolution imaging in scanning transmission mode (STEM). Energy dispersive X-ray spectroscopy (EDXS) enables the high-resolution determination of elemental composition (spatially resolved chemical analysis).

OPTICAL SPECTROSCOPIC METHODS (IR, UV/VIS AND CD/ORD)

These methods work with electromagnetic waves whose propagation essentially follows the laws of classical optics. Spectroscopic use is made primarily of the infrared (thermal radiation), visible and near ultraviolet wavelength ranges.







FROM THE PRESS

‘DREAM REACTION’ – LIKAT/EVONIK ACHIEVES BREAKTHROUGH

Together with partners from Evonik, LIKAT achieved a breakthrough in the production of adipates. Adipates are produced on an annual scale of millions of tons. They serve as starting materials for products such as plasticizers, perfumes, lubricants, active pharmaceutical ingredients and, above all, nylon. For 60 years now, attempts have been made to produce adipates directly from 1,3-butadiene in a single step by means of double carbonylation. The partners have now succeeded in doing just that in the laboratory, laying the foundation for a more environmentally friendly and cost-effective large-scale synthesis route. Due to the particular importance of this innovation, the renowned journal SCIENCE published the results. A joint press release by the partners, issued by LIKAT, appeared in daily newspapers across Germany, and NDR produced a three-minute television report that was broadcast on Nordmagazin.

The difficulty lies in the complexity of the dicarbonylation reaction. Normally, it tends to form numerous by-products (Figure 1). Several challenges arise from the simultaneous introduction of two CO groups in this catalytic process:

- the parallel promotion of two different carbonylation reactions on one diene substrate (which no other research group had previously achieved);
- the selective formation of the linear dicarbonylation product, although the isomerization of the initially formed monocarbonylated intermediate to the terminal olefin is thermodynamically very unfavorable;
- suppression of other side reactions such as telomerization, hydroalkoxylation and (co) polymerization.

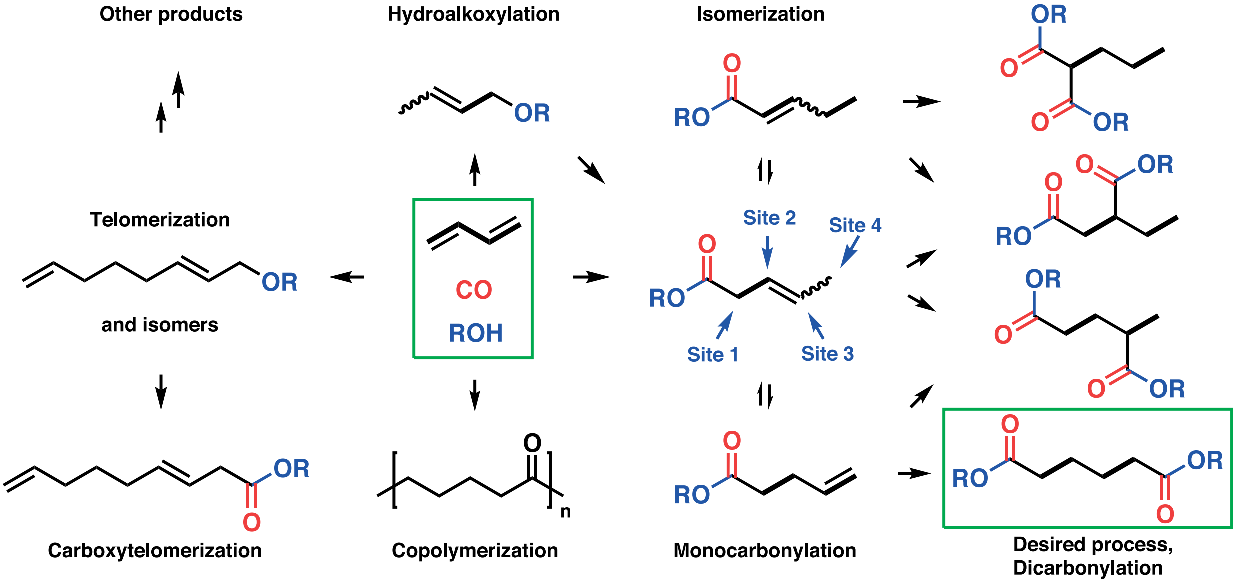


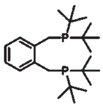
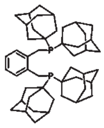
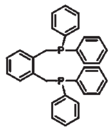
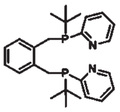
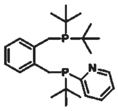
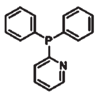
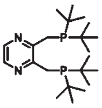
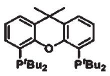
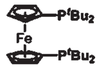
Fig. 1: Complex network of reactions involved in the synthesis of adipate diesters from 1,3-butadiene, carbon monoxide and alcohol.

In the development of a suitable catalyst, palladium complexes with base-modified derivatives of the 1,2-bis[(di-tert-butylphosphino)methyl]benzene ligand (L1, dtbpx) used for the bulk production of methyl methacrylate were chosen. Initial optimization studies with this ligand showed low activity but good selectivity (Table 1). The incorporation of suitable basic groups leads to a significant increase in activity. However, as the direct comparison between L1 and the dual base-modified L4 shows, this is at the expense of selectivity. The solution was to combine both structural elements. The specially developed ligand L5 (HeMaRaphos) combines the excellent selectivity of L1 and the high reactivity of L4.

Complementary studies on the performance and optimization of the catalyst system now enable the direct twofold carbonylation of 1,3-butadiene to adipate diesters with high catalytic productivity (Turnover Number TON > 60,000), large yields (up to 95 %) and outstanding selectivity (> 97 %). The catalyst system can also be transferred to other dienes, thus paving the way for a revolutionary synthetic route for many fine chemical products.

References:

[1] J. Yang, J. Liu, H. Neumann, R. Franke, R. Jackstell, M. Beller, *Science* **2019**, *366*, 1514–1517. Direct synthesis of adipic acid esters via palladiumcatalyzed carbonylation of 1,3-dienes.

Ligand	 **L1**		 **L2**		 **L3**		 **L4**		 **L5**		 **L6**		 **L7**		 **L8**		 **L9**	
Reactivity	X	18%	X	13%	X	0%	–	77%	+	85%	X	0%	X	0%	X	0%	X	0%
Selectivity	+	97%	+	95%	X	0%	–	48%	+	97%	X	0%	X	0%	X	0%	X	0%

+ >80% – 40-80% X <40%

Table 1. Comparison of the different phosphine ligands in terms of reactivity and selectivity.

RADICAL IN THE BLACK BOX

LIKAT Chemists Reveal the Business Secret of a Catalyst

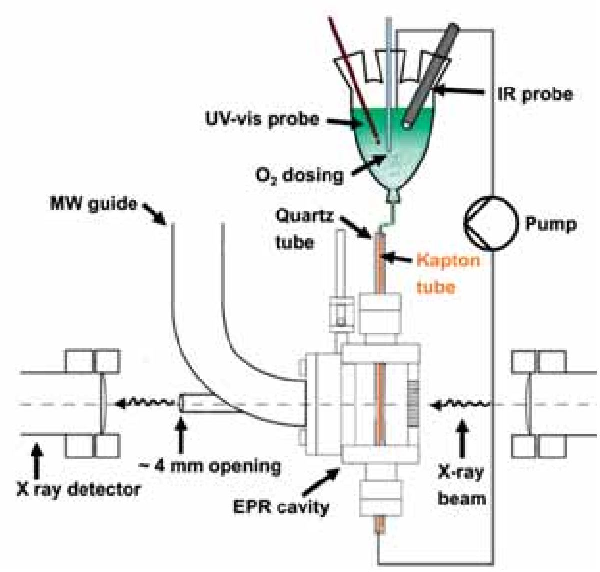
Chemists at the Leibniz Institute for Catalysis in Rostock were able to observe the molecular functioning of the catalyst in a redox reaction and identify important intermediate steps. For this purpose, they coupled, for the first time worldwide, four highly modern measuring methods that work in different wavelength ranges: with infrared, UV and X-ray radiation as well as with microwaves in the magnetic field. In this way, they uncovered the complete catalytic mechanism for the selective oxidation of benzyl alcohol to benzaldehyde. As a basic chemical, benzaldehyde, which smells intensely of bitter almond, is used mainly for perfumes and cosmetics.

Like so often in chemistry, this reaction takes place in a black box. Starting materials, catalyst and solvent are placed in a reaction vessel where they react to form the desired product, benzaldehyde. So far it is clear: The presence of the catalyst makes this process possible or at least accelerates it. But which of its components activate the starting materials, in which order, which reactive intermediates are formed and how they influence the reaction - all this remains in the dark.

‘Green’ Oxidizing Agent

However, this information is essential for a targeted catalyst design. For oxidation to benzaldehyde, the industry usually uses oxidants such as chromate or hypochlorite, which are problematic for the environment and costly to dispose of. For this reason, researchers around the world are experimenting in the laboratory with oxygen, O_2, as a more elegant oxidant. Unfortunately, they are getting only inadequate results in terms of yield. The aim is therefore to improve the catalyst, for which it is best to observe it closely at work, so to speak.

This is the specialty of Prof. Dr. Angelika Brückner, head of the research department ‘Catalytic *in situ* Studies’ and her group leader Dr. Jabor Rabeah. They excite samples with radiation of different energy and wavelength. Specific absorptions of all species involved allow conclusions to be drawn about their properties, such as oxidation states or binding situations, and thus also about their function and role in the chemical process.



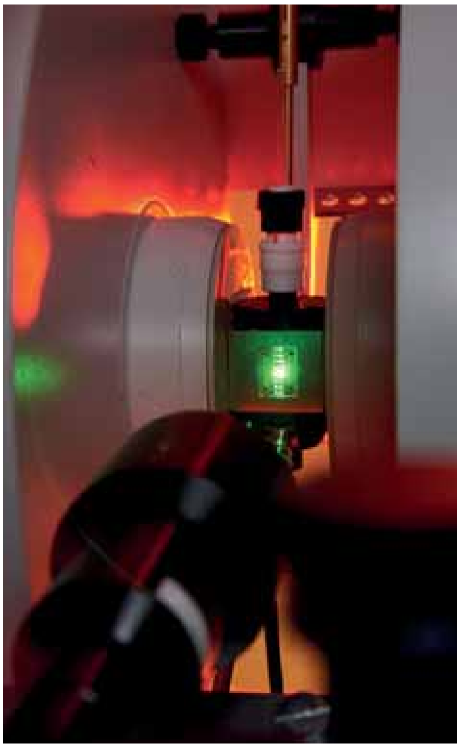


Fig. 1: View into the EPR spectroscope in the research department of Prof. Angelika Brückner.

Highly Complex and Simultaneous

At the heart of the redox reaction under investigation is a copper complex stabilized by an organic ligand, to a certain extent the armor of the catalyst. The catalyst also includes an auxiliary agent, in this case a radical called **Tempo**, a term derived from the acronym of its chemical structure: **Te**tra**m**ethyl**p**iperidinyl**o**xyl.

The catalyst thus consists of three components, plus the starting material and the oxidizing agent O_2. Such a 'complex system', as Brückner and Rabeah say, is best approached using several different methods. The hurdle here was that these measurements had to be made in the same reaction vessel, in the same experiment, i.e. simultaneously. Angelika Brückner: 'Only in this way can we guarantee identical experimental conditions. Carrying out the analyses individually and in sequence always involves certain differences in the reaction conditions, which would make it difficult to compare the results'.

For the parallel measurements, the researchers initially chose infrared and somewhat more energetic UV rays as well as electron paramagnetic resonance (EPR) spectroscopy, which detects unpaired electrons. For example, the role of the excipient Tempo, which has such an unpaired electron - which makes it highly reactive on the one hand and introduces the term 'radical' on the other - had to be clarified.

Cooperation with Soleil, Paris

In fact, the chemists could see during their first measurements that Tempo interferes with the reaction. But in what way? When the reaction starts, some of the copper particles change their valence from Cu-I to Cu-II. Until now, experts have mostly assumed that the Cu-II species forms a compound during the reaction in the form of a so-called dimer and that Tempo is primarily responsible for oxidation of Cu-I to Cu-II.

To clarify these assumptions, the Rostock chemists needed a more precise view of the copper components using a high-energy X-ray beam. For this purpose, they cooperated with the Soleil synchrotron in Paris. First, they acquired a compact EPR spectrometer, which they completed by cleverly modifying the measuring cell with an IR and a UV probe. They also adapted it constructively for the experimental setup at the synchrotron.

Armed with four such ultra-sharp vision aids, the LIKAT researchers at Soleil in Paris were for the first time able to observe one and the same process simultaneously from several perspectives. 'And we were finally able to resolve on what has been controversially discussed in the scientific literature so far', says Dr. Rabeah.

Fig. 2: Laurent Barthe at the Synchrotron Soleil; the entire experimental setup was modified so that it could be introduced into the X-ray beam at the synchrotron in Saint-Aubin (France).

Model Reaction for Future Analyses

They discovered that Tempo does not oxidize itself at all, as previously assumed. Instead, it activates the oxidizing agent oxygen. In addition, they were able to detect the much-discussed dimer. However, they found that it splits back into monomers during the reaction. Prof. Brückner: 'But this has no influence whatsoever on the reactivity of the system. Consequently, this dimer is not important for the reaction.'

With these findings, experts can now further develop and, above all, optimize the oxidation of benzyl alcohol using oxygen. In the long term, this work will lead to replacing the industrial process with an environmentally friendly one. And, as Jabor Rabeah emphasizes, the new coupling technology can also be used for mechanistic analyses of other reactions – right down to metabolic processes in living organisms.

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CASCADE FROM METHANOL TO HYDROGEN

Metha-Cycle Decouples Wind Power from Electricity Demand

For the first time, different sectors were successfully coupled to store hydrogen in methanol: hydrogen generation (electrolysis using renewable energies), hydrogen storage (CO_2 from biogas plants and the green hydrogen are catalytically converted to methanol and released again) and the generation of heat and electricity from hydrogen. The pilot plant has been successfully tested - the follow-up project for upscaling is being planned.

Researchers led by Dr. Henrik Junge, group leader 'Catalysis for Energy Technologies' and Prof. Matthias Beller can produce hydrogen from methanol under mild conditions. Yield and purity are sufficient for use in fuel cells.

They optimized their own process, which they had published in NATURE at the time. The catalytic reaction is at the heart of the MethaCycle project, a research project funded by the German Federal Ministry of Economics with 1.8 million euros for the storage and use of renewable energies. For the first time, wind power, electrolysis and CO_2-based methanol synthesis, as well as the reconversion of methanol into hydrogen, were directly linked to each other and in this way 'decouple the emergence of regenerative energy from its consumption in terms of time'.

It allows companies and municipalities to supply themselves with 'green' electricity independently of wind power generation. As it is well known, electrical energy from wind power is not always generated when it is most needed.

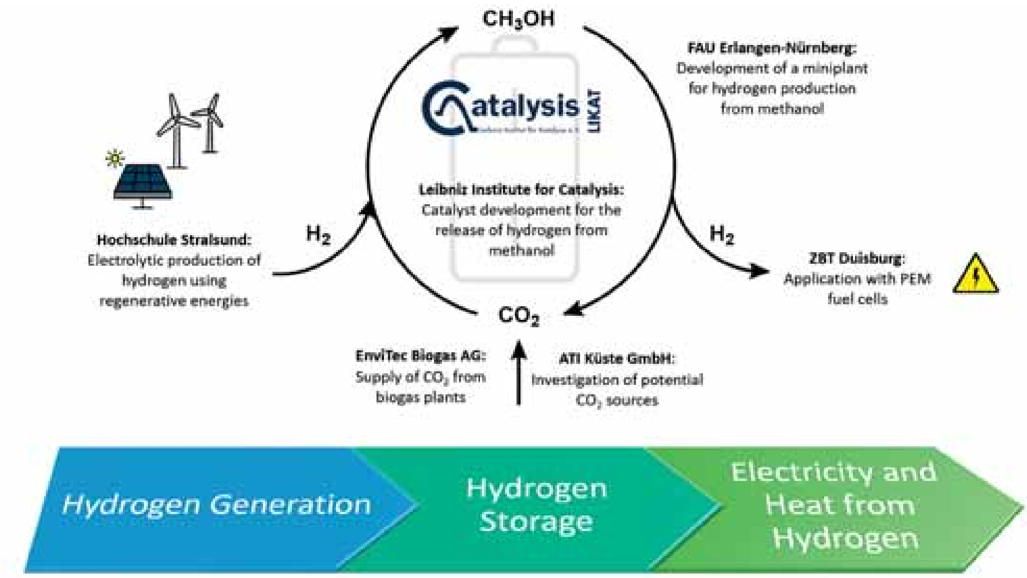

Fig. 1: Sector coupling in the Metha-Cycle project: An interdisciplinary consortium combines for the first time electricity generation from renewable energies, electrolysis, catalytic binding of hydrogen in methanol and subsequent release and conversion of the hydrogen into electricity in fuel cells.

This is where the MethaCycle concept comes in: electricity from renewable energies such as wind and sun is used to generate hydrogen electrolytically from water. This is converted with carbon dioxide (CO_2) into methanol, which acts as a storage medium for hydrogen. 'Methanol, unlike hydrogen, is easy to handle and can be transported over long distances', says Henrik Junge. If required, methanol is converted back into hydrogen and used directly afterwards in a fuel cell to generate electricity.

Since the catalytic release of hydrogen from methanol usually requires high pressure and temperatures of several hundred degrees Celsius, a general

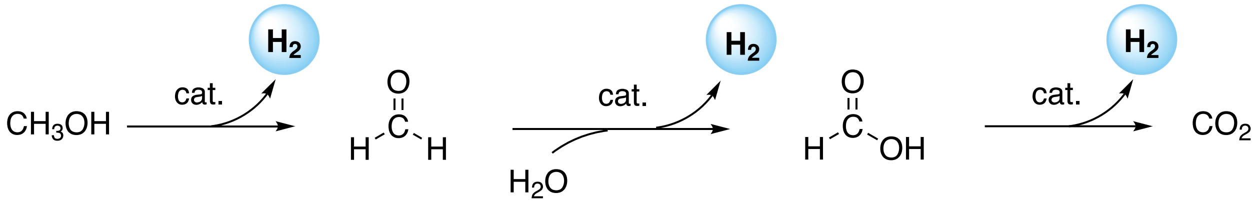

Fig. 2: Cascade reaction - The catalysed release of hydrogen from an aqueous methanol solution takes place in several steps and passes through various intermediates.

application in the context of energy concepts has not been very attractive so far.
Back in 2013, the group led by Henrik Junge and Matthias Beller described in NATURE magazine how a ruthenium catalyst can be used to generate hydrogen and CO_2 from an aqueous methanol solution under mild conditions below one hundred degrees Celsius. However, a constant supply of hydrogen is needed to keep a fuel cell running. The chemical process must provide sufficient hydrogen per time unit in a certain purity.

‘Mechanistic’ Analyses

The mode of operation of the corresponding ruthenium catalyst in the methanol solution was again intensively investigated under mechanistic aspects. It was shown that the release of hydrogen from methanol takes place in three cascade-like steps. After each of the first two steps, a portion of hydrogen and another intermediate are already formed. First, an equivalent of hydrogen and formaldehyde is formed. This is further reacted in the presence of the catalyst, producing another equivalent of hydrogen.

In addition, formic acid is produced in the second step of the cascade. The release of hydrogen from formic acid has been intensively studied at LIKAT for several decades – 20 years ago, it was even possible to obtain hydrogen from formic acid at room temperature. More surprising was the realization that the third step, the release of hydrogen from formic acid, proved to be the slowest and ‘slowed down the entire system’. Hydrogen production comes to a halt, and the system becomes unusable for fuel cell firing.

The solution was a switch to a bicatalytic system. By adding a second, only slightly modified ruthenium catalyst, it was also possible to accelerate the rate-determining last step so that a continuous hydrogen stream can be generated.

In addition, there was a synergetic effect of the system. The combination of both catalysts achieves a better yield than the sum of their individual performances.

This result was integrated into a continuous process in the test plant in the MethaCycle research consortium, which was ultimately able to demonstrate the functional capability of the concept in this way.

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C. H. Schwarz, A. Agapova , H. Junge, M. Haumann, *Catalysis Today* **2020**, *342*, 178-186. Immobilization of a selective Ru-pincer complex for low temperature methanol reforming – material and process improvements.
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THERE IS SOMETHING IN THE AIR

'Carbon Mining': How Chemists at LIKAT Extract Carbon from the Air

For the first time, it has been possible to enrich CO_2 from the air at a catalytic material under normal pressure conditions and moderate temperatures and to induce a reaction right there. The reaction with methanol produces dimethyl carbonate, an ester of carbonic acid that is being discussed as a fuel, among other things, and can replace toxic chemicals in industry.

The research activities led by Dr. Sebastian Wohlrab, head of the department 'Heterogeneous Catalytic Processes', paves the way for two major goals in chemistry: firstly, to 'harvest' carbon dioxide directly from the air and thus reduce the proportion of this greenhouse gas in the atmosphere. The other is to provide carbon for basic chemical processes. The second is to provide carbon for basic chemical processes through 'carbon mining' when fossil carbon carriers - oil, natural gas and coal - are no longer available in sufficient quantities.

Essential Element

Carbon is an essential element, both for the biosphere – in the form of proteins, fats and carbohydrates – and for industrial production. However, with a share in the earth's crust of 0.027 percent, carbon is one of the scarce resources. Access to carbon must be ensured even after fossil raw material sources dry up.

Alternative processes based on renewable raw materials such as wood or agricultural waste are promising.

Vision and Illusion

'However, it is a great illusion to assume that the global economy will be able to cover its carbon needs from renewable raw materials alone', says Sebastian Wohlrab, citing representative statistics.[1] According to these, global plant growth binds 56,400 million metric tons of elemental carbon per year. And only 14 percent of this, i.e. just under 7,900 million metric tons/year, is achieved through plant cultivation, i.e. the food basis of the earth's population. This means that only this amount would be available for the sustainable extraction of raw materials - if the rainforest were not to be completely destroyed.

Almost the same amount of carbon, nearly 7,000 million tons/year, is currently processed into products by the petrochemical industry worldwide. 'So if we want to replace oil and gas with green chemistry without depriving humanity of its food base, the global economy would have to be capable of extreme measures', says Dr. Wohlrab: Either dramatically curb carbon consumption, i.e. the production of goods. Or to double the amount of land used to grow crops, which would be ecologically devastating. 'This highlights how urgently we need to develop other sources of carbon'. One source of that is CO_2 in the atmosphere.

However, the CO_2 content in the air is far too low at 400 ppm for a chemical reaction with effective results. Previous processes for the conversion of carbon dioxide, such as urea synthesis, use highly concentrated CO_2 streams. The esterification of CO_2 has also so far only worked under high pressure in the laboratory.

In fact, Sebastian Wohlrab's field succeeded in 2017 in forming esters at atmospheric pressure – with highly concentrated carbon dioxide.

The scientists successfully mastered the challenge of using CO_2 in extremely low concentrations even from normal room air: Air at atmospheric pressure is passed over a catalytically active material until it is saturated with CO_2.

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[1] a) C.B. Field, M. J. Behrenfeld, J. T. Randerson, P. Falkowski, *Science* **1998**, *281*, 237-240. b) BP Statistical Review of World Energy, 2019, 68th edition. c) FAOSTAT data on land use, 2015.

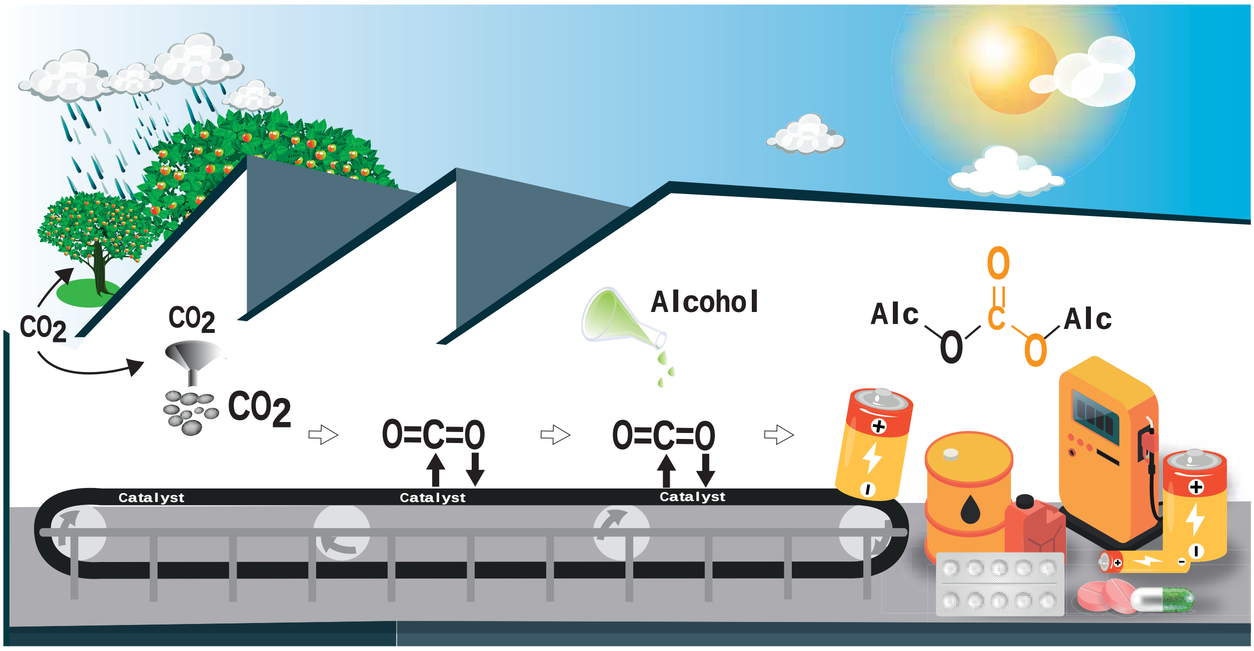


Fig. 1: ‘CO_2 -harvesting’ from the air: The carbon dioxide from the air is enriched on a suitable catalyst and the inert gas is activated. In this way, it can be directly reacted with alcohols to form new products. (Picture: LIKAT)

The catalyst, a powdery mixed oxide, contains basic centers where the acidic CO_2 accumulates. The CO_2-free exhaust air is discharged. Methanol is then added to the saturated catalyst material, whereupon it reacts with the catalytically activated CO_2 at a moderate 90 degrees Celsius to form dimethyl carbonate.

The more than three-and-a-half-hour CO_2 enrichment and conversion with methanol is still far too long for a technical process. However, the product yield is already trend-setting: Three out of four of the adsorbed CO_2 molecules are successfully converted.

The researchers around Wohlrab were able to show that the principle works. They could extract carbon from the air and use a climate gas as a raw material. The task now is to further optimize these results. But other reactions with atmospheric CO_2 will also become possible with this principle.

CONSTRUCTION OF THE ‘ZERO CARBON’ TRANSFER TECHNICAL CENTER

In October 2020, construction work began on the transfer technical center „ZeroCarbon-Catalysis“ at LIKAT. In the future, findings from basic research can be brought to practical maturity under the own roof. With the technical center, LIKAT is expanding its unique selling point: Already, several new laboratory processes, i.e. chemical reactions on a 1 to 100 g scale, are transferred from LIKAT to industry every year, where they are implemented on a pilot scale (kg scale). Successful pilots may lead to new industrial production facilities on a ton scale (1 – 10,000 t).

Small and medium-sized enterprises (SMEs) and non-chemistry-specific user industries usually do not have the technical and financial resources for such scale-ups. Therefore, the pilot plant with piloting directly at LIKAT offers the potential to bring more processes from the laboratory to the application than before.

‘Zero Carbon’ - is the title of the new pilot plant, which is being funded with 10 million euros, half from federal and half from state funds. In the pilot plant, carbon is to be made usable for the chemical industry in a climate-neutral way.

Large quantities of hydrogen are required for the chemical use of renewable raw materials, but since plants (oils and cellulose, for example) contain a lot of oxygen compared to fossil raw materials, this must be removed for further processing by adding hydrogen. Carbon, an essential element for the production of medicines, fuels, paint and cleaning agents, textile fibers, plastics, fertilizers, mostly comes from fossil raw materials.

There are many examples to prove that there are alternatives: Synthesis gas, a mixture of hydrogen and carbon monoxide, is conventionally produced by coal gasification or from crude oil distillates. It could just as easily be produced by reacting methane with carbon dioxide - both of which are produced in biogas plants. The use of biomass analogous to coal gasification would also be a sustainable option. The sustainably produced synthesis gas could then be efficiently converted to methanol or converted to long-chain hydrocarbons, for example for the production of kerosene.

This ‘green chemistry’ requires completely new processes and technologies, for which LIKAT is working on suitable catalysts. Each reaction step within these processes requires a tailor-made catalyst. In the laboratory, the research work is mostly carried out on a very small scale of a few milligrams. Scaling up the process to the ton scale in industry with thousands of tubular reactors and reactor columns up to 20 meters high is a huge step. It is precisely this that the new pilot plant, which will already be operating in the kilogram range, is designed to facilitate. Once a process has proven its practicality in the pilot plants, it has already made it 90 percent of the way to the finished industrial product.

In the future, the Transfer Technicum should lead many more ideas than before from basic research to practical maturity.

The Transfer Technical Center under construction.

RESEARCH DATA TREASURES BECOME AVAILABLE

The BMBF Funds Digitization at LIKAT and the Universities in Rostock and Greifswald (NFDI4Cat)

In June 2020, the *Joint Science Conference* (GWK) of the federal and state governments decided which disciplines will be funded within the framework of the 'National Research Data Infrastructure' (NFDI) project starting in the fall. In this first of three bidding rounds, the Leibniz Institute for Catalysis (LIKAT) in Rostock and the Universities of Rostock and Greifswald will benefit as a significant part of the catalysis-related sciences.

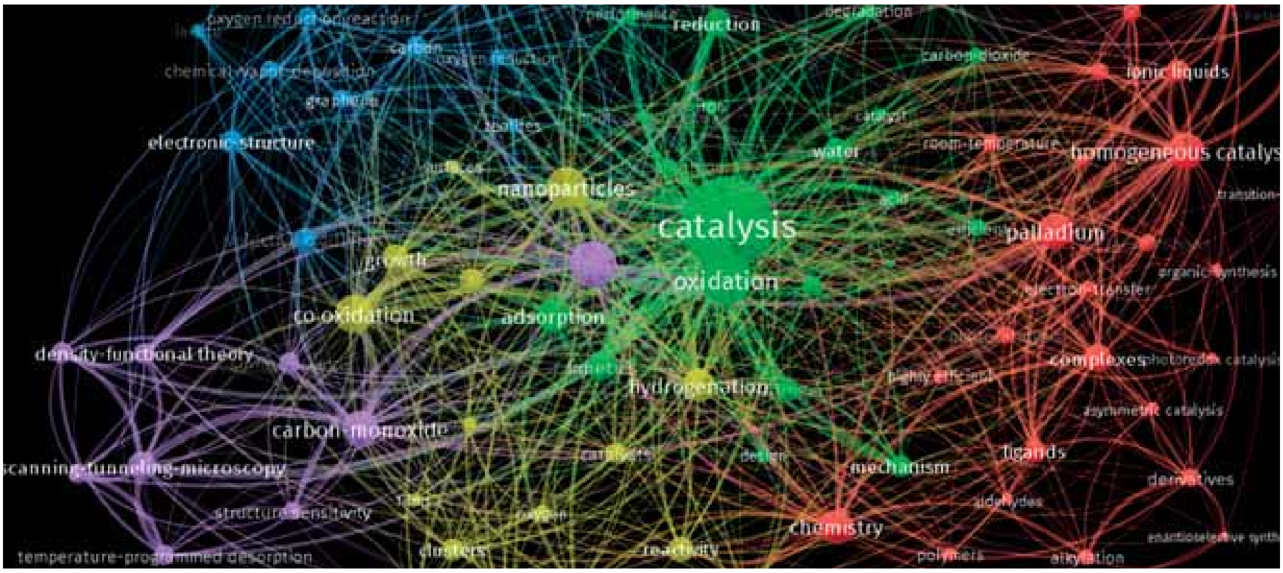
The new project promotes digitization in key scientific areas with the aim of networking important research data from the participating partners and making it more widely available. The current corona crisis clearly demonstrates how essential this is. In this way, researchers can, for example, learn more effectively from the experiences, but also the mistakes, of colleagues from other institutions and thus make better use of their expertise. Instead of putting research data in a drawer at the end of a project, as has been the case in the past, research data will now be pooled, networked and used nationally and, where appropriate, internationally.

This will create a comprehensive 'knowledge repository and data treasure trove' that can also be easily and clearly found and accessed by third parties. The BMBF is funding the development of this national infrastructure for research data with up to 90 million euros. In order to approach this large-scale project, which is initially planned for a decade, in a structured manner, associations of suitable disciplines applied in so-called consortia.

In addition to eight other consortia, the *NFDI4Cat* network, which brings together universities and research institutes in the catalysis-related sciences across Germany, will also receive funding and began its activities on October 1, 2020. In addition to LIKAT, as Europe's leading research institute for applied catalysis, the universities in Rostock and Greifswald will be supported as part of *NFDI4Cat* with approximately 2 million euros for the next 5 years.

Christoph Wulf and Dr. David Linke of the Leibniz Institute for Catalysis, who co-designed the research proposal, say: 'Digitizing our research data helps us, not least, to move more efficiently from basic research to (industrial) applications'.

Catalysis is considered a key technology in curbing pressing problems such as climate change or the scarcity of fossil resources. To return CO_2 and plastics to production or to establish hydrogen technologies for the storage of renewable energies, it requires close networking of various catalysis disciplines and process engineering.



READY FOR ROUTINE OPERATION

An X-ray photoelectron spectrometer called NAP-XPS analyzes the life cycle of catalysts at LIKAT.

They accelerate chemical processes without consuming themselves, is commonly said about catalysts. And yet their effect can diminish over time. What happens on their surface at the atomic level is being investigated by a state-of-the-art device in Rostock: the new X-ray photoelectron spectrometer (XPS) at the Leibniz Institute for Catalysis. It bombards atoms on the surface of a sample with X-rays and dislodges electrons. 'From the energy required to do this, we can tell the character and state of the atom they came from', explains Dr. Stephan Bartling. He led the procurement of the NAP-XPS and prepared the device for routine operation.

New Possibilities for High-End Analytics

Conventional X-ray photoelectron spectrometers only work in an ultrahigh vacuum of 10^{-9} millibars, which is one millionth of normal atmospheric pressure. This is the only way to precisely determine the energy of the photoelectrons released by the X-ray beam, because they must not collide with other particles in the air on their way.

LIKAT has also been conducting research with such an XPS in a high vacuum. But that is not the usual reaction environment for catalysts. 'For certain measurements, you simply need realistic analysis conditions', says Prof. Dr. Angelika Brückner, head of department 'Catalytic *in situ*-studies'. Analyses in the measuring chamber of the new instrument are carried out in the presence of (reactive) gases, hence the name **NAP**: **N**ear **A**mbient **P**ressure. In the future, this high-tech instrument will make it possible to analyze and optimize the function of catalysts in situ, i.e. under conditions close to the reaction.

1.1 Million Euros from EFRE Funds

Catalysis, as Angelika Brückner explains, is 'in the broadest sense a surface phenomenon'. A gas or liquid mixture flows along a porous, often metallic catalyst, for example. This surface contact alone ensures the desired reaction. The atoms on the surface of the catalyst play a role in this process and can sometimes lose their activity in the process, for example through irreversible changes in their oxidation state or through deposits.

Stephan Bartling: 'By studying photoelectrons of the outer atomic layers of a material with the NAP-XPS, we can precisely see what happens to the atoms on the catalyst surface during a reaction'. In a sense, the measurements can be used to map the life cycle of a catalyst.

While most NAP-XP spectrometers are installed at synchrotron sources and have limited availability, the new generation of these instruments can also be used in normal laboratory operation. In northern Germany, the NAP-XPS at LIKAT is the only laboratory instrument; nationwide, there are just under a dozen of these instruments available, and there are perhaps 60 machines in laboratory use worldwide. The Rostock acquisition received 1.1 million euros from the European Regional Development Fund (EFRE), which is primarily intended to expand interdisciplinary cooperation between science and business.

Oxidation of CO in Fuel Cells

One of the first requests for analysis concerned an area that is becoming increasingly popular both regionally and internationally: hydrogen technology, or more precisely, the service life and efficiency of fuel cells. Angelika Brückner explains the problem: hydrogen, the actual fuel for these cells, always contains traces of carbon monoxide, CO, due to the technology. But CO is poison for this technology; it damages the precious metal electrodes. 'As chemists, we remove the CO by oxidizing it to CO_2. To do that, we use oxygen. And the hurdle is to prevent the oxygen from oxidizing the hydrogen at the same time'. That's what the fuel cell needs as fuel, after all.

To solve the problem, laboratories around the world are experimenting with different catalysts. At

LIKAT, one of the catalysts is a copper-containing catalyst based on cerium oxide, a rare-earth metal oxide known for its strong oxidizing power. Put simply, in this case the ceria donates the oxygen for the oxidation of CO, reducing it itself and making it inactive. To prevent this, it must at the same time recapture gaseous oxygen before it can tamper with the hydrogen.

This means the surface atoms of a good catalyst (in this case cerium) must change their oxidation state quickly and reversibly. 'With our new device', says Dr. Bartling, 'we were able to observe very nicely how this ‚redox swing' works at different temperatures and gas compositions'.

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https://doi.org/10.1021/acscatal.0c01580

Further papers for publication of the new findings, including in Nature Chemistry, are in progress.

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In charge of the method
X-ray photoelectron spectroscopy (XPS)
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Dr. Stephan Bartling prepares the new NAP-XPS for a measurement.

LIKAT IN NUMBERS

in Mio. €

20.2 I 24.6

2019 I 2020

Budget

12.8 I 13.06

Basic Funding

7.11 I 6.99

External Funding

3.17 I 2.95

thereof

Industrial Funding

3.94 I 4.04

thereof Public Funding

0.3 I 4.5

Construction Investment

4 I 6

Bachelor

8 I 7

Master

37 I 24

Doctorates

1 I 1

Habilitations

129 I 135

2019 I 2020

Scientists

102 I 90

PhD Students

83 I 84

Science Supporting Staff

16 I 21

2019 I 2020

Patents

284 I 240

2019 I 2020

Publications

54 I 68

thereof OA

128 I 119

thereof IP > 5

1 I 1

Books

11 I 3

Book Chapters

EQUAL OPPORTUNITIES & GENDER EQUALITY AT LIKAT

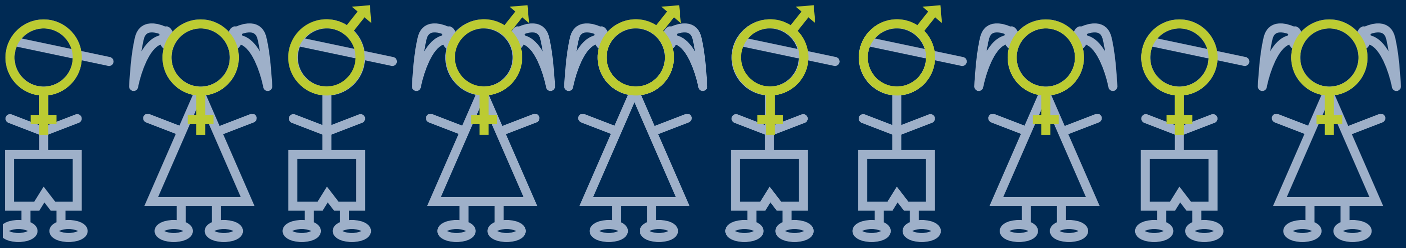
LIKAT explicitly acknowledges its responsibility to actively promote equal opportunities and gender equality and has anchored this in its statutes in 2012. Equality in this context means not only enabling equal opportunities for the genders, but moreover bringing about balanced gender proportions through binding measures.

LIKAT's Equal Opportunity Officer and her deputy have been elected every four years since 2006. Measures for a good work-life balance, such as the company agreement on flexitime or dual-career measures, are essential lived components of working life at the institute. In the Corona pandemic with its school and daycare closures, particularly young parents were challenged in 2019 and 2020. With its research work, the institute is involved in important projects and committed to its partners. LIKAT is therefore maintaining its laboratory operations as far as possible, naturally in compliance with the necessary health protection measures. From the beginning, the Executive Board granted all employees the greatest possible flexibility in addition to the company-agreed flexitime, so that they can fulfill their family care obligations. Where desired and possible, employees work on a mobile basis.

LIKAT also set up a so-called *come-back fund* to help employees reconcile work and family life. It was set up specifically to provide security for employees in temporary employment during pregnancy, parental leave or nursing leave and is now a fixed component of the institute's budget. The fund offers employees planning security and binds them more closely to the institute than before.

Currently, about one third of all employees at LIKAT are women. Since 2019, the administrative management has been filled by a female commercial director, who forms a dual leadership together with the scientific director of the institute as part of the executive board. The board is now 60% women, a proportion that LIKAT aims to preserve. In contrast, women are significantly underrepresented in the management of the research departments and research groups. We want to change this in the long term, e.g. by actively recruiting new female staff.

The success of gender equality work at LIKAT is constantly monitored. At least once a year, we publish gender-specific statistics. In the regular evaluations by the Leibniz association, the status of our gender equality measures, among other things, is a major factor in determining whether we remain in the association and thus whether we receive further funding. LIKAT also regularly undergoes an external audit by the TEQ certificate. In 2020, we were awarded the certificate for the fourth time in a row.



Topics Research Departments	Structur-Reactivity Relationsships 01 Angelika Brückner Wolfgang Baumann	Kinetics, Theory & Mechanisms 02 Evgenii Kondratenko Haijun Jiao	Reaction Engineering & Implementation 03 David Linke Udo Armbruster	Renewable Resources 04 Johannes de Vries Thomas Werner	Energy & Environment 05 Jennifer Strunk Henrik Junge	More Efficient Processes 06 Sebastian Wohlrab Bernd Müller	New Products & Processes 07 Torsten Beweries Christian Hering-Junghans
Applied Homogeneous Catalysis Matthias Beller	**Redox Reactions** Kathrin Junge	**Theory of Catalysis** Haijun Jiao	**Applied Carbonylations** Ralf Jackstell **Catalysis for Life Science** Helfried Neumann	**Redox Reactions** Kathrin Junge **Synergy hom. & heterog. Catal.** Jagadeesh Rajenahally	**Catalysis for Energy** Henrik Junge	**Applied Carbonylations** Ralf Jackstell **Catalysis for Life Sciences** Helfried Neumann	**Catalysis for Life Sciences** Helfried Neumann
Biocatalysis & Renewable Resources Johannes de Vries	**Catalysis with Renewable Resources** Sergey Tin **Bioinspired Catalysis** komm. Johannes G. de Vries		**Synergy hom. & heterog. Catal.** Jagadeesh Rajenahally	**Catalysis with Renewable Resources** Sergey Tin **Bioinspired Catalysis** provis. Johannes G. de Vries		**Rational Ligand Design** Bernd Müller	**Catalysis with Renewable Resources** Sergey Tin **Bioinspired Catalysis** provis. Johannes G. de Vries
Heterogeneous Catalytic Processes Sebastian Wohlrab	**Inorganic Functional Materials** Sebastian Wohlrab **Technology Oriented Processes** Udo Armbruster		**Liquid Phase Oxidations** Angela Köckritz **Technology Oriented Processes** Udo Armbruster **Inorganic Functional Materials** Sebastian Wohlrab	**Liquid Phase Oxidations** Angela Köckritz **Inorganic Functional Materials** Sebastian Wohlrab	**Technology Oriented Processes** Udo Armbruster	**Technology Oriented Processes** Udo Armbruster **Inorganic Functional Materials** Sebastian Wohlrab	
Catalytic in situ Studies Angelika Brückner	**Optical Spectroscopy** Christoph Kubis **Magnetic Resonance & X-Ray Methods** Jabor Rabeah	**Optical Spectroscopy** Christoph Kubis **Magnetic Resonance & X-Ray Methods** Jabor Rabeah			**Magnetic Resonance & X-Ray Methods** Jabor Rabeah	**Optical Spectroscopy** Christoph Kubis	
Catalyst Discovery & Reaction Engineering David Linke	**Reaction Mechanisms** Evgenii Kondratenko	**Reaction Mechanisms** Evgenii Kondratenko	**Reaction Engineering** David Linke **High-Throughput Technologies** Uwe Rodemerck		**Reaction Engineering** David Linke **Reaction Mechanisms** Evgenii Kondratenko	**Reaction Engineering** David Linke **High-Throughput Technologies** Uwe Rodemerck **Reaction Mechanisms** Evgenii Kondratenko	**Reaction Engineering** David Linke **High-Throughput Technologies** Uwe Rodemerck **Reaction Mechanisms** Evgenii Kondratenko
Heterogeneous Photocatalysis Jennifer Strunk	**Structure-Function Relationships** Jennifer Strunk				**Photocatalytic CO_2-Reductions** Tim Peppel **Micro Reaction Engineering** Norbert Steinfeldt	**Micro Reaction Engineering** Norbert Steinfeldt	
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Electrochemistry & Catalysis Robert Francke					**Catal. Design for Electrosynth.** Bernd Müller **Molecular Electrochemistry** Robert Francke		
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Analytical Services Wolfgang Baumann	**Analytics**						

Stand: Mai 2021

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The Leibniz Institute for Catalysis (LIKAT Rostock) is a member of the Leibniz Association and has the legal form of a registered association (e.V.). It is an „An-Institut" of the University of Rostock, which means that LIKAT is connected to the university, but organizationally and legally independent of it. The bodies of LIKAT are the *General Meeting*, the *Board of Curators*, and the *Scientific Advisory Board*. Funding is shared equally between the federal government and the state. In terms of the specialist subject matter, at host-state level the responsibility lies with the Ministry for Education, Science and Culture; at national level it lies with the Federal Ministry for Education and Research (BMBF).

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Prof. Norbert Stoll, Vice Chair, *University of Rostock*
Prof. Ulrich Bathmann, *IOW Rostock*
Prof. Uwe Bornscheuer, *University of Greifswald*
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Prof. Reinhard Schomäcker, *TU Berlin*
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TOPIC SPEAKERS:

Topic 01	Prof. Prof. Angelika Brückner & PD Wolfgang Baumann
Topic 02	Prof. Evgenii Kondratenko & Prof. Haijun Jiao
Topic 03	Dr. David Linke & Dr. Udo Armbruster
Topic 04	Prof. Johannes G. de Vries & Dr. Thomas Werner
Topic 05	Prof. Jennifer Strunk & Dr. Henrik Junge
Topic 06	Dr. Sebastian Wohlrab & Dr. Bernd Müller
Topic 07	PD Dr. Torsten Beweries & Dr. Christian Hering-Junghans

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Prof. Prof. Peter Langer, *University of Rostock*
Prof. Ralf Ludwig, *University of Rostock*
Prof. Klaus Neymeyr, *University of Rostock*
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PD Dr. Torsten Beweries
Prof. Armin Börner
Prof. Prof. Angelika Brückner
Prof. Paul Kamer
Dr. David Linke
Prof. Jennifer Strunk
Prof. Johannes G. de Vries
Dr. Sebastian Wohlrab

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Dr. Barbara Heller, Administration
Andreas Schupp, Technical Services
Dr. Sandra Hinze, Staff Unit

EMPLOYEE REPRESENTATION:

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DEGREES

2019

Habilitations

Sawall, Mathias (Neymeyr)

Doctorates

Adomeit, Sven (Brückner), Al Barakat Almasalma, Ahmad (Kragl), Anke, Felix (Beweries), Cibura, Niklas (extern) (Strunk), Dietrich, Annika (Kragl), Dilla, Martin (extern) (Strunk), El Ouahabi, Fatima (de Vries), Farrar Tobar, Ronald Alvaro (de Vries), Flader, Anika (Langer), Garbe, Marcel (Beller), Ha, Quan (Kragl), Hancker, Sören (Beller), Hertrich, Max (Beller), Janke, Julia (Langer), Janke, Sophie (Langer), Konrath, Robert (extern) (Kamer), Kortewille, Bianca (extern) (Strunk), Kreft, Steffi (Beller), Murugesan, Kathiravan (Beller), Ohlendorf, Lars (Langer), Oubaassine, Saadia (extern) (Wohlrab), Petrosyan, Andranik (NG Pospech), Prymak, Iuliia (Wohlrab), Rumpel, Katharina (Börner), Sang, Rui (Beller), Scharnagl, Florian (Beller), Schröder, Henning (Neymeyr), Seeburg, Dominik (Wohlrab), Sivasankaran, Ramesh Poonchi (Brückner), Steinlechner, Christoph (Beller), Täufer, Amely (Börner), Wei, Zhihong (Beller), Wozniak, Bartosz (de Vries), Yin, Zhiping (Börner), Zhang, Shaoke (Beller), Zhang, Yaoyuan (extern) (Linke), Zhou, Wei (Beller)

Master

Hünemörder, Paul (Kragl), Jannsen, Nora (extern) (Beweries), Khsara, Bahaa Eddin (Brückner), Lindenau, Kevin (Beweries), Moritz, Jan-Ole (Kamer), Schmidt, Christoph (Wohlrab), Schöll, Christopher (NG Pospech), Zander, Edgar (Schulz)

Bachelor

Lambrecht, Sina (Strunk), Leidecker, Benedict (Börner), Romischke, Johanna (de Vries), Wellnitz, Tim (NG Hering-Junghans),

2020

Habilitations

Mejia, Esteban (Kragl)

Doctorates

Agapova, Anastasiya (Beller), Behrens, Stephan (Börner), Brunzel, Tom (Wohlrab), Chen, Bo (Börner), Grauke, Reni (Brückner), Han, Shanlei (extern) (Linke), Hasche, Patrick (Beweries), Hu, Yuya (de Vries), Keller, Sonja (Brückner), Kloß, Svenja (Börner), Leischner, Thomas (Beller), Leval, Alexander (Beller), Longwitz, Lars (de Vries), Papa, Veronica (Beller), Piehl, Patrick (Beller), Salazar, Abel (Kragl), Schneekönig, Jacob (Beller), Schumann, André (NG Hering-Junghans), Senthamarai, Thirusangumurugan (Beller), Stadler, Bernhard (de Vries), Wang, Hai (Börner), Xu, Jianxing (Börner), Yang, Ji (Beller), Zhao, Dan (extern) (Linke)

Master

Kell, Lukas (de Vries), Mayer, Thea (NG Pospech), Neitzel, Gordon (Beller), Schafhausen, Niklas (Kragl), Siewert, Jan-Erik (NG Hering-Junghans), Singer, Christian (Strunk), Zahednia, Mathab (Brückner)

Bachelor

Brandt, Sina (de Vries), Fokken, Wilko (Kragl), Knuth, Cornelius Leonardt (Kragl), Rippke, Mirko (Beweries), Schlapp, Janina (Kragl), Seifert, Jenny (Beller),


Licht

PUBLICATIONS 2019

[1] S. Abbas, K. Ayub, M. Sohail, ***S. Ali***, R. Ludwig, ***M. A. Nadeem***, S. Muhammad, *J. Mol. Struct.* **2019**, *1175*, 439-444, Synthesis, X-ray crystal structure and spin polarized DFT study of high spin Mn based metal-organic framework.

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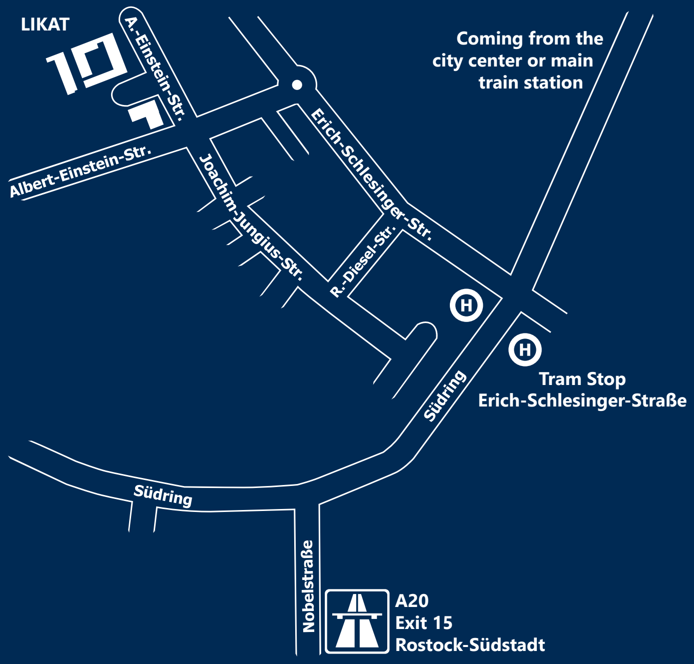
DIRECTIONS:

BY CAR

Coming from the A 20, take exit no. 15 SÜDSTADT in the direction of ZENTRUM and you will reach NOBELSTRASSE. From NOBELSTRASSE, turn right onto SÜDRING and continue to follow the signs for the city centre. At the next major intersection, turn left into ERICH-SCHLESINGER-STRASSE.
At the roundabout take the second exit into ALBERT-EINSTEIN-STRASSE. Follow this road for approx. 150 metres and then take the first turning on the right. After about 50 metres you will see LIKAT on your left.

BY PUBLIC TRANSPORTATION

From the main railway station, take tram line 5 in the direction of SÜDBLICK or line 6 in the direction of CAMPUS SÜDSTADT and get off at the ERICH-SCHLESINGER-STRASSE stop. Cross the street and walk along ERICH-SCHLESINGER-STRASSE to LIKAT. Follow ERICH-SCHLESINGER-STRASSE and turn left at the roundabout into ALBERT-EINSTEIN-STRASSE. After approx. 150 metres, take the first turning on the right. After about 50 metres you will see LIKAT on your left.



Leibniz
Association

Catalysis
Leibniz-Institut für Katalyse
LIKAT