STRATEGY LIKAT 2030

„YOU CAN RECOGNIZE A REALLY GOOD IDEA BY THE FACT THAT ITS REALIZATION SEEMS IMPOSSIBLE FROM THE START.“

ALBERT EINSTEIN

Katalysis
Leibniz-Institut für Katalyse
LIKAT

CONTENT

LIST OF ABBREVIATIONS

AAS	Atomic Absorption Spectroscopy
ACA	Institute for Applied Chemistry Berlin Adlershof
ATR	Attenuated Total Reflection: Measurement Techniques of IR Spectroscopy
BET	Brunauer, Emmet and Teller
BMBF	Federal Ministry of Education and Research
CD	Circular dichroism
CE	Capillary electrophoresis
CPMD	Car-Parrinello Molecular Dynamics
DAAD	German Academic Exchange Service
DECHEMA	Society for Chemical Engineering and Biotechnology e.V.
DFG	German Research Foundation
EDX	Energy-Dispersive X-ray Analysis
EELS	Electron-Energy-Loss Spectroscopy
EPR/ESR	Electron Paramagnetic Resonance (EPRor electron spin resonance (ESR)
ERC	European Research Council
ESCA	Electron Spectroscopy for Chemical Analysis
FB	Research Department
GC	Gas Chromatography
GC-MS/LC-MS	Coupling of mass spectrometry with gas or liquid chromatography (GC or LC)
GDCh	Society of German Chemists
HPLC	High-pressure liquid chromatography/ high performance liquid chromatography)
ICP-OES	Inductive Coupled Plasma Optical Emission Spectroscopy
IF	Impact factor
IfOK	Leibniz Institute for Organic Catalysis at the University of Rostock e.V. (originally founded in 1952 as "Institute for Catalysis Research")
IR/FTIR	Infrared Spectroscopy /Fourier Transform IR Spectroscopy
KMU	small and medium-sized enterprises
MoU	Memorandum of Understanding
MPG	Max Planck Society
MS	Mass spectrometry
MV	Mecklenburg-Western Pomerania
NAP	Near Ambient Pressure
NMR	Nuclear Magnetic Resonance, Nuclear Magnetic Resonance Spectroscopy
NWG	Junior Research Group
RFA	X-ray fluorescence analysis
TEM/STEM	Transmission Electron Microscopy/Scanning Transmission Electron Microscopy
TF	Topic Field
TG	Research Group
UV-vis	Spectroscopy using electromagnetic waves of ultraviolet (UV) and visible (VIS) light.

VZÄ	Full-time equivalent
WKM MV	Ministry of Science, Culture, Federal and European Affairs Mecklenburg-Vorpommern
XPS	X-ray Photoelectron Spectroscopy

1. INTODUCTION

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

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

Figure 1. Research task of the LIKAT.

LIKAT conducts *state-of-the-art* catalysis research relevant to society, which is applied to alternative energy technologies as well as to the material and life sciences, in addition to the classical areas of chemistry. For this purpose, the entire range of modern research instruments is made available in one institute. Innovative research approaches are not so much the result of a juxtaposition of individual research areas with outstanding expertise, but rather of interdisciplinary, cross-sectoral responses to relevant research questions. The holistic view of the phenomenon of catalysis enables the institute to make significant contributions to achieving the overarching strategic goal of closing material cycles with its research results.

The *LIKAT 2030 Strategy* formulates clear research goals for the funding period 2023 to 2030, taking into account the available resources. It defines ways to achieve these goals, serves to steer and structure activities & resources along the way, sets priorities and serves to provide transparency & orientation for internal and external stakeholders. Nevertheless, the strategy remains flexible. It is adaptable in order to be able to react to current developments. The *Scientific & Industrial Advisory Board* as well as the *Board of Curators* and the *General Assembly* of the Institute are involved in these changes.

2. POSITION OF LIKAT: KEY POINTS OF STRATEGIC DEVELOPMENT TO DATE

2.1 STRATEGIC DEVELOPMENT – CONTENT & PERSONNEL WISE

[…] To conduct basic and applied research, especially in the field of homogeneous and heterogeneous catalysis, and to promote their technical implementation […]" are the tasks formulated in the statutes of LIKAT. In order to realize them, the guiding principle for the strategic development of LIKAT is ***EVOLUTION INSTEAD OF REVOLUTION***: For the consistent further development of the scientific expertise of the institute, it was and is of central importance to build on the formative strengths of the past. At the time of the last evaluation in 2016, these strengths arose from the combination of fundamentals and applications as well as in the linking of homogeneous and heterogeneous catalysis, which was significantly realized by the merger of the Rostock IfOK with the Berlin ACA in 2006. Thus, LIKAT has a broad competence in catalysis, which includes analytical and spectroscopic expertise as well as extensive know-how in catalyst synthesis and testing. The evaluation of LIKAT by the Senate of the Leibniz Association in 2016 was extremely positive.

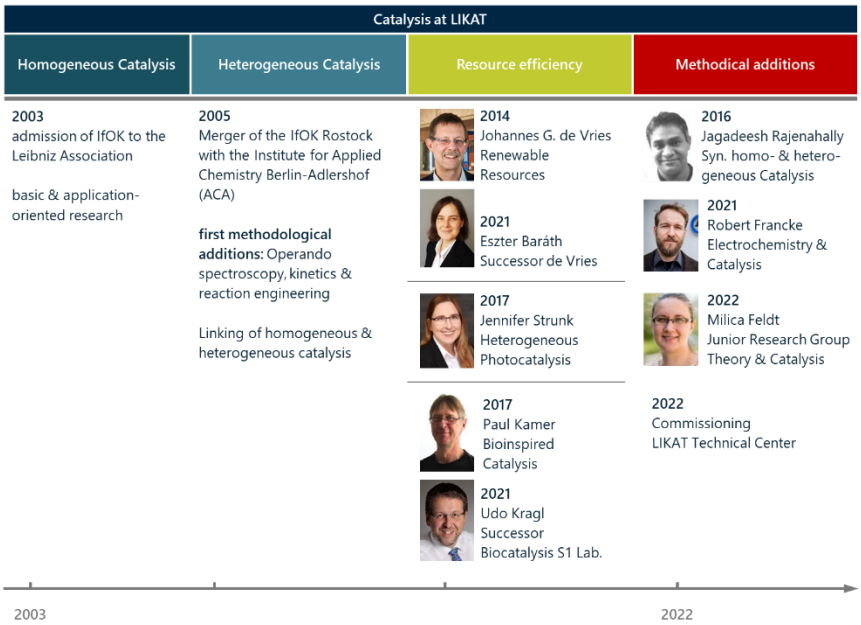


Figure 1. Strategic development of LIKAT within the last 20 years.

Against the background of the shortage of energy and material resources, carbon and phosphorus compounds, and precious metal catalysts, LIKAT formulated the **application of its strengths and expertise to the optimal use of resources** as an overriding goal in its strategy for the period 2016 to 2023. So far, this has been achieved through a targeted combination of internal competencies with external expertise, which has been tapped in the context of new appointments and cooperations at national and international level: The focus was on the material- and energy-efficient utilization of readily available raw materials and commercially little-used renewable or alternative resources, e.g. new catalyst and process developments for the refinement of renewable raw materials as well as CO_2 or carbonates and other Carbon sources with application potential (methane, acetylene). This development was largely due to the realignment of the expiring research department *Process Intensification* into the department of *Catalysis with Renewable Resources* (headed by Prof. Johannes G. de Vries) and the establishment of the new research group *Catalysis with Renewable Resources & Platform Chemicals*.

In its Strategy 2023, LIKAT also formulated that catalysis is an area of chemistry with particularly high application potential in technology, but that this potential is not always effectively exploited. Another strategic goal to achieve improvements in this respect was **the establishment or strengthening of methodological approaches**. The expertise of the **Synergies between Homogeneous & Heterogeneous Catalysis** research group (headed by Prof. Dr. Jagadeesh Rajenahally) established in 2016, for example, complemented the research department of *Catalysis with Renewable Resources* in terms of

methodology. Currently, these activities are being expanded in the research department, which has been operating with an expanded focus since November 2021 under the name *Catalysis with Bioresources* (headed by Dr. Eszter Baráth).

The methodological expansion to include aspects of bio- or bioinspired catalysis took place through the establishment of the research department ***Bioinspired Homo- & Heterogeneous Catalysis*** (headed by Prof. Dr. Paul Kamer) in 2017. The expertise included, among other things, the production of artificial metalloenzymes, proteins functionalized with metal complexes, which are used as catalysts for a number of challenging reactions. A biochemical S1 laboratory was established at LIKAT specifically for this purpose. After Paul Kamer's sudden death in 2021, Prof. Udo Kragl (associate professor at the University of Rostock) took over as head of department.

In 2017, LIKAT again expanded its methodological expertise with the reestablishment of the research department ***Heterogeneous Photocatalysis*** (headed by Prof. Dr. Jennifer Strunk). The research topics of this department include *artificial photosynthesis*, the conversion of CO_2 and H_2O using sunlight to products such as methane and carbon monoxide. One focus is the investigation of the reaction mechanism under high-purity conditions. For this purpose, gas phase photoreactors are operated that are unique in the world. In 2021, the institute established another pioneering method with the research department ***Electrochemistry & Catalysis*** (headed by Prof. Dr. Robert Francke). The ***linking of mechanistic investigations, e.g. operando spectroscopy with kinetics and theory***, pursues the goal of prospective catalyst development for industry. This focus has been strengthened with the definition of *kinetics, theory & mechanisms* as the forward-looking topic *TF 02* in the matrix structure. Furthermore, since January 2022, the junior group *Theory of Homogeneous & Biocatalysis* (headed by Dr. Milica Feldt) strengthens this field.

2.2 PREVIOUS STRUCTURAL STRATEGIC DEVELOPMENT

The steady strategic development in terms of content has been accompanied by the structural expansion of the institute. At the current location on the Südstadtcampus of the University of Rostock, House 1 was occupied in 2005, and its structural expansion was completed in 2009. The second building, House 2, was completed and put into operation in 2014. The total construction costs for both buildings amounted to €38.2 million and provide LIKAT researchers with approximately 2,950 m^2 of laboratory space. The most recent and strategically relevant building expansion is LIKAT's own ***Catalysis2Scale*** transfer technical center, which opened in July 2022 and is closely related to the strengthening of *Reaction Engineering & Implementation*. The technical center allows the institute to consistently expand its value chain from basic research to industrial application. Detailed information on the pilot plant and its use can be found in section 4.9Strategy Catalysis2Scale-Transfer technical Center (p. 23).

2.3 STRATEGIC-ORGANIZATIONAL DEVELOPMENTS TO DATE: THE MATRIX STRUCTURE

As an affiliated institute of the University of Rostock, LIKAT is an organizationally as well as legally independent research institute with the bodies *General Assembly*, *Board of Curators* and *Scientific & Industrial Advisory Board* (Figure 3). Research planning and control are carried out by the *Board*. The scientific director, Prof. Matthias Beller, chairs the board. The board also includes the commercial director and up to three (currently two) additional scientific board members. The basis for the activities of the board are the statutes of the association and the rules of procedure of the institute. As an institute of the Leibniz Association, financing is shared equally by the federal government and the state in which the institute is located.

For a modern organization of the research work, LIKAT has consistently advanced the goal of a holistic view of the phenomenon of catalysis by introducing the matrix structure with *Topics*. The boundaries between the research departments, with research groups as their subunits, have been gradually dissolved, first in the form of three cross-divisional program priorities and, since 2019, in the form of the matrix structure.

Topics are forward-looking research areas that bundle all relevant resources of LIKAT. The research activities of the *Topics* describe the strategic orientation of the scientific work of the Leibniz Institute for Catalysis. A total of seven *Topics* have been identified (Figure 2 vertical). *Topics 01 - 03* are methodologically oriented and *Topics 04 - 07* are materially oriented.

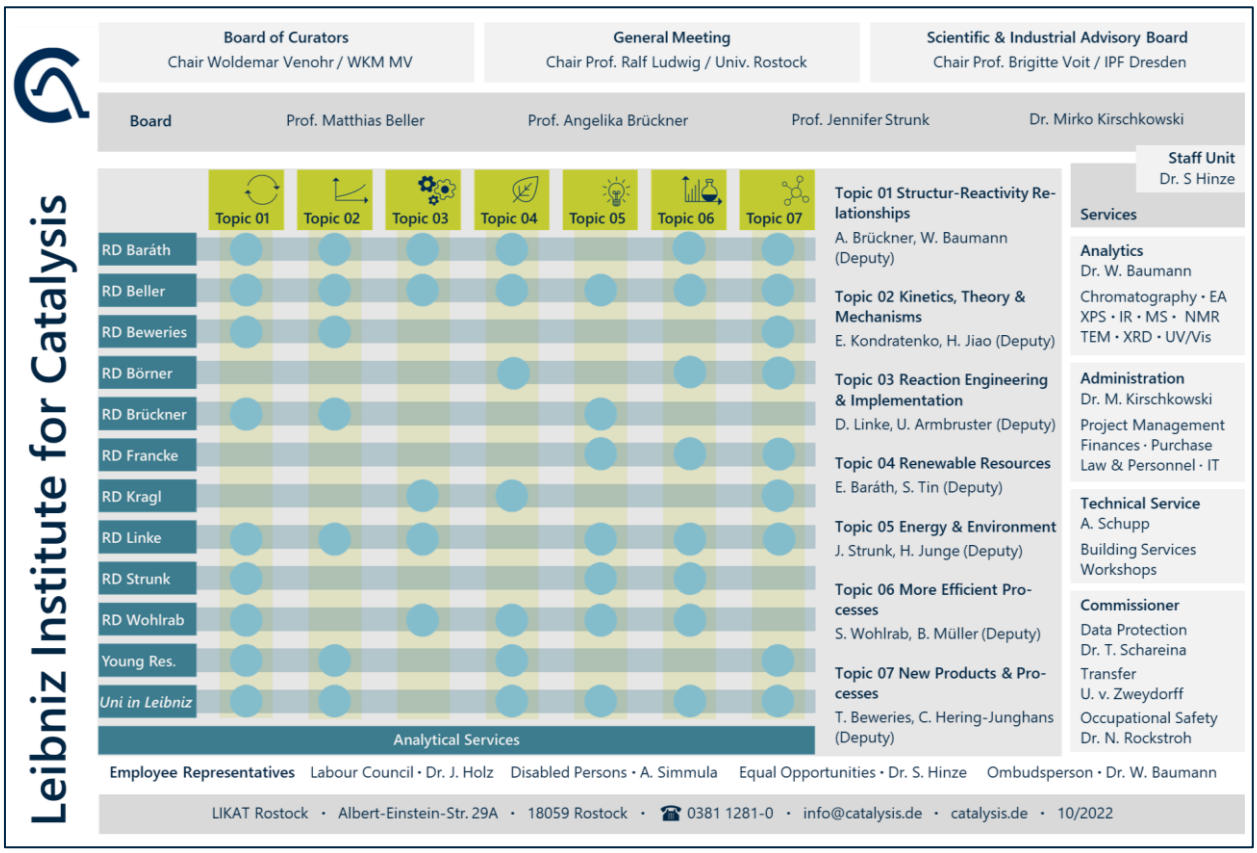


Figure 2. Organization of the research work at LIKAT in the matrix structure.

Due to the organization in a matrix, the management of research activities at LIKAT is divided between two positions: All *Topics* are coordinated and managed by speakers and their deputies. At the same time, LIKAT has the historically grown organization of *research groups (TG)* in budgeted *research departments (FB)* as well as *junior research groups (NWG)* and associated university research groups *(Uni in Leibniz)* (Figure 2, horizontal). The *Topics* are worked on by the research groups of the research departments across divisions. A detailed presentation of the matrix structure follows at the end of this section (Figure 3, S. 5). The service departments analytics, technics and administration are equally available to all employees of the institute.

The tasks and roles of the *heads of the research departments* and the *topic speakers* are clearly distributed and complement each other: the *heads of the research departments* is responsible for research, personnel and budget. They decide to what extent the resources of their research groups flow into the *topics*. This makes it clear which resources are available for each topic. *Topic speakers* coordinate and lead the cooperation of the *research groups* of different *research departments* in a *topic* as well as their presentation to the outside.

The organization in a research matrix requires transparent communication and information channels, for example through regular topic field meetings that are open to all employees. This promotes an open communication culture.

This does not affect the granting of research freedom for all scientific employees as a basic principle of work organization at LIKAT (generally 10-20%). Researchers can thus independently develop solutions for existing projects or propose new project topics. *Explorative research groups* set up for this purpose offer the opportunity to explore research ideas and to react flexibly to current problems and challenges.

Topics / Research Departments	Structure-Reactivity Relationships 01 Angelika Brückner Wolfgang Baumann	Kinetic, Theory & Mechanisms 02 Evgenii Kondratenko Haijun Jiao	Reaction Engineering & Implementation 03 David Linke Udo Armbruster	Renewable Raw Materials 04 Eszter Baráth Sergey Tin	Energy & Environment 05 Jennifer Strunk Henrik Junge	More efficient processes 06 Sebastian Wohlrab Bernd Müller	New Products & Processes 07 Torsten Beweries Christian Hering-Junghans
Catalysis with Bioressources Eszter Baráth	Selective Catalytic Synthesis Methods Sergey Tin	Catalysis with Phosphorous Materials Christian Hering-Junghans	Synergy betw. Homogen. & Heterogen. Catalysis Jagedeesh Rajenahally	Sel. Cat. Synthesis Methods Sergey Tin Catalysis with Phosphorous Materials Christian Hering-Junghans		Synergy betw. Homogen. & Heterogen. Catalysis Jagedeesh Rajenahally	Sel. Catal. Synt. Methods Sergey Tin Cat. with Phosphorous Materials Christian Hering-Junghans
Applied Homogeneous Catalysis Matthias Beller	Catalysis for Energy Henrik Junge Redox Reactions Kathrin Junge	Theory of Catalysis Haijun Jiao Synergy betw. Homogen. & heterogen. Catalysis Jagedeesh Rajenahally	Catalysis for Life Sciences Helfried Neumann Applied Carbonylations Ralf Jackstell Catalysis for Energy Henrik Junge	Redox Reactions Kathrin Junge Synergy betw. Homogen. & Heterogen. Catalysis Jagedeesh Rajenahally	Catalysis for Energy Henrik Junge	Redox Reactions Kathrin Junge Catalysis for Life Sciences Helfried Neumann Applied Carbonylations Ralf Jackstell	Redox Reactions Kathrin Junge Catalysis for Life Sciences Helfried Neumann
Modern Concepts in Molecular Catalysis Torsten Beweries	Cat. with Early Trans. Metals Fabian Reiß Cat. with Late Trans. Metals Torsten Beweries Cat. Functionalization Jola Pospech	Cat. with Early Transition Metals Fabian Reiß Mech. in homog. Catalysis Hans-Joachim Drexler					Cat. with Early Trans. Metals Fabian Reiß Cat. with Late Trans. Metals Torsten Beweries Cat. Functionalization Jola Pospech
Hydrogenations & Hydroformylations Armin Börner				Catalysis for Heterocycles Xiao-Feng Wu		Hydrogenations & Hydroformylations Jens Holz	Catalysis for Heterocycles Xiao-Feng Wu Hydrogen. & Hydroformyl. Jens Holz
Catalytic *in situ*-Studies Angelika Brückner	Magn. Res. & X-Ray Methods Jabor Rabeah Opt. Spektr. & Thermoanal. Methods Christoph Kubis	Magn. Res. &X-Ray Methods Jabor Rabeah Opt. Spektr. & Thermoanal. Methods Christoph Kubis			Magn. Res. & X-Ray Methods Jabor Rabeah Opt. Spektr. & Thermoanal. Methods Christoph Kubis		
Electrochemistry & Catalysis Robert Francke					Molecular Electrochemistry Robert Francke	Molecular Electrochemistry Robert Francke Cat.design f. Electrosynth. Bernd Müller	Molecular Electrochemistry Robert Francke Cat.design f. Electrosynth. Bernd Müller
Biocatalysis & Polymer Chemistry Udo Kragl			Polymer Chemistry & Catalysis Esteban Mejia Biocatalysis Udo Kragl	Polymer Chemistry & Catalysis Esteban Mejia Biocatalysis Udo Kragl			Polymer Chemistry & Catalysis Esteban Mejia
Catalyst Discovery & Reaction Engineering David Linke	Reaction Mechanisms Evgenii Kondratenko	Reaction Mechanisms Evgenii Kondratenko	High-Throughput Technologies Uwe Rodemerck Reaction Engineering David Linke		Reaction Mechanisms Evgenii Kondratenko Reaction Engineering David Linke	Reaction Mechanisms Evgenii Kondratenko High-Throughput Technol. Uwe Rodemerck Reaction Engineering David Linke	Reaction Mechanisms Evgenii Kondratenko High-Throughput Technol. Uwe Rodemerck Reaction Engineering David Linke
Heterogeneous Photocatalysis Jennifer Strunk	Structure-Function Correlations Jennifer Strunk				CO_2-Reduction Tim Peppel Micro Reaction Engineering Norbert Steinfeldt	Micro Reaction Engineering Norbert Steinfeldt	
Heterogeneous Catalytic Processes Sebastian Wohlrab	Surface Chemistry in Appl. Catalysis Ali Abdel-Mageed Inorg. Functional Materials Sebastian Wohlrab		Technol. Oriented Processes Udo Armbruster Surface Chem. in appl. Cat. Ali Abdel-Mageed Inorg. Functional Materials Sebastian Wohlrab	Surface Chem. in Appl. Cat. Ali Abdel-Mageed Inorg. Functional Materials Sebastian Wohlrab	Technology Oriented Processes Udo Armbruster	Technology Oriented Processes Udo Armbruster Inorg. Functional Materials Sebastian Wohlrab	
Junior Research Groups	Modern org. Chemistry Osama El-Sepelgy Theory of Homog. & Heterog. Cat. Milica Feldt	Theory of Homog. & Heterog. Cat. Milica Feldt		Modern org. Chemistry Osama El-Sepelgy Theory of Homo. & Heterog. Cat. Milica Feldt			Theory of Homog. & Heterog. Cat. Milica Feldt
„Uni in Leibniz" Associated Groups	Björn Corzilius · Marko Hapke · Axel Schulz	Ralf Ludwig · Klaus Neymeyr		Thomas Werner	Malte Brasholz · Klaus Neymeyr · Wolfram Seidel	Thomas Werner	Marko Hapke · Axel Schulz Thomas Werner
Analytics Wolfgang Baumann	Analytics						

Figure 3. Organization of research work at LIKAT. Detailed matrix structure with topics and the working research groups, junior research groups as well as the associated university research groups (*Uni in Leibniz*, see p. 8). **Status 10/2022**.

3. SCIENTFIC ENVIRONMENT & NETWORKING IN THE SCIENCE SYSTEM

3.1 NATIONAL & INTERNATIONAL SCIENTIFIC ENVIRONMENT OF LIKAT

National environment. Within Germany, various **non-university research institutions**, **competence centers** and **university chairs** conduct excellent catalysis research within the scope of their respective orientation. The *GeCats*[1] *Catalysis Competence Atlas* provides an overview of the research institutions active in catalysis in Germany. As a Leibniz Institute with a focus on applied basic research, we are positioned between *Max Planck Institutes* and university research facilities on the one hand and industry and *Fraunhofer Institutes* on the other. The positioning at the interface of basic research and application is a unique selling point of LIKAT.

International environment. The international catalysis research landscape is just as diverse as that within Germany. Here, we name five selected leading international catalysis research institutions, which overlap in terms of their general orientation and specific focal points, but also show significant differences: The *Catalytic Institute of the Pacific Northwest National Laboratory PNNL* (Washington, USA), the *Merck Center for Catalysis* (Princeton University, USA), the *Institute of Chemical Research of Catalonia ICIQ* (Tarragona, Spain), the *Dalian Institute of Chemical Physics DICP* (Dalian, China) and the *KAUST Catalysis Center KCC* (Thuwal, Saudi Arabia).

Infobox – Unique selling propositions of LIKAT

1. positioning at the interface of basic research and application
2. broad catalytic expertise (homogeneous, heterogeneous, photo-, electro-, partly bio-catalytic) in combination with the necessary analytical and methodological infrastructure
3. synergy effects through flexible cooperation of different subject groups in a matrix structure with subject fields
4. balanced ratio of industrial and public third-party funding
5. *Catalysis2Scale*-Transfer center incl. reaction & process engineering aspects

For 70 years, LIKAT has been exclusively dedicated to researching the phenomenon of catalysis. A central criterion is LIKAT's strategic position at the interface between innovative catalysis research in the basic area and technical application, which makes the institute an essential transfer point. The basic prerequisites for this are the diverse, independent cooperations with private companies that exist at the institute, as well as the processing of application-oriented basic research, which combines far-reaching expertise in homogeneous, heterogeneous and partly biocatalysis, as well as in photocatalysis and electrocatalysis.

In a similar way, the *KAUST Catalysis Center* or the *Dalian Institute of Chemical Physics* combine a comparable range of different expertise under one roof. In comparison, the *Institute of Chemical Research of Catalonia* is more homogeneous. What is unique at LIKAT, however, is the intensive networking of the various catalysis disciplines and research groups due to the organization of its research work: the direct project-oriented collaboration of various research groups, independent of their affiliation to substantive research departments, in the *topic fields of matrix structure*. Research at LIKAT is characterized by flexible structures. The overlapping integration of several research groups in one topic leads to a high scientific level in the treatment of topics and at the same time allows the efficient realization of very complex topics. The use of synergies between the various catalysis disciplines opens up new innovative fields of research in which, for example, aspects of heterogeneous catalysis flow into homogeneous catalysis and vice versa.

At the same time, LIKAT combines long-term technology provision including the corresponding technology platforms as well as the methodologically and analytically necessary infrastructure, which is

1 gecats.org/Kompetenzatlas

special in this range. This special infrastructure of LIKAT constitutes a high-quality catalysis research. This also ensures the existence of a scientific mid-level faculty. The methodological know-how (synthesis techniques, analytical methods, measurement techniques, data processing) is subject to constant updates. Together with about 60 to 70 visiting scientists and postdocs as well as about 100 PhD students per year, LIKAT guarantees a flexible, timely and independent handling of socially and industrially relevant issues. This is supported by the exceptionally intensive cooperation of the Leibniz Institute for Catalysis with the associated university research groups within the framework of *Uni in Leibniz* (p. 8).

Due to its organization and infrastructure, LIKAT is an attractive cooperation partner for academic and industrial partners alike. The balanced relationship and the linking of basic and applied research is another special feature of LIKAT. Other research institutes are increasingly positioning themselves close to industry (*KAUST, DICP, Merck*) or are focusing more on fundamental research into specific catalysis-related issues.

LIKAT is known for its fast and problem-oriented solutions to basic and applied issues in the chemical and pharmaceutical industries, but also in the life sciences and energy supply, as well as in climate and environmental protection. At LIKAT, the holistic view of catalysis from catalyst synthesis to reaction engineering and implementation in industrial applications is in the foreground. This clearly distinguishes LIKAT from other research institutions. The completion of LIKAT's own *Catalysis2Scale* transfer technical center in mid-2022 will allow the testing and transfer of chemical research results into practice in the future (pilot scale).

3.2 NETWORKING OF THE LIKAT IN THE SCIENCE SYSTEM

3.2.1 INSTITUTIONAL COOPERATION WITH UNIVERSITIES & UNI IN LEIBNIZ

In order to use and bundle regional resources in an optimal way, LIKAT signed a far-reaching cooperation agreement with the *University of Rostock* already in summer 2006, which has been continuously extended in the past years and from which LIKAT and the university benefit equally. The contract enables LIKAT to involve research groups of the University of Rostock in the research work of the institute to a high degree: from the natural science institutes, *the interdisciplinary faculty*, the engineering sciences or the medical field. The inter-faculty cooperation allows the establishment of modern, sustainable catalysis research. The cooperation agreement covers, among other things, cooperation in the area of personnel, joint appointments and teaching activities, the joint use of equipment and facilities, the evaluation of research results, and the joint vocational training of chemistry laboratory assistants.

In principle, joint appointment procedures are carried out for scientific leading positions of LIKAT in connection with professorships at the University of Rostock in the field of catalysis, which are subject to the guidelines of the State University Act MV and the appointment regulations of the University of Rostock. In addition to the professors of the institute, habilitated heads of departments and research groups as well as heads of junior research groups are involved in the education of young students and graduates at the University of Rostock with lectures, seminars as well as the supervision of internships and qualification work. In this way, the practical relevance of the education is increased.

The model *Uni in Leibniz* is based on the cooperation agreement of LIKAT with the University of Rostock and includes the concrete professional cooperation of LIKAT with the associated university research groups. The associated professors work at LIKAT on the basis of an honorary agreement. Currently, eight professors of the University of Rostock as well as one professor each of the University of Paderborn and the University of Linz (Austria) are working at LIKAT within the frameworf of *Uni in Leibniz*. The latter are former habilitation students of LIKAT.

The cooperation within the framework of *Uni in Leibniz* was reorganized as an ideas competition at the beginning of 2020. Researchers from the universities can formulate proposals on predefined questions and submit them to LIKAT. The prerequisite is their cooperation with LIKAT staff, for example through the joint supervision of PhD students, for which LIKAT provides resources. Such a competition of ideas promotes the exchange between university and LIKAT and enables the internal start-up financing of high-risk research, which can and should lead to future joint research projects. The predefinition of the research question by LIKAT ensures the research orientation of these cooperations according to the research strategy of the institute.

3.2.2 INSTITUTIONAL INTERNATIONAL COOPERATION

In the paper *Five Points of the Leibniz Strategy 2020*[2], the *Leibniz Association* formulates cooperation with international scientists as one of the five points. International cooperation has long been part of everyday life in science, including at the Leibniz Institute for Catalysis. Research results are obtained and made available across locations and borders, as researchers communicate globally and in real time. International scientific collaborations strengthen LIKAT's competitiveness and innovative capacity. In addition to non-contractual collaborations, LIKAT has Memoranda of Understanding (MoU) with international research institutions and universities. These include the *UK Catalysis Hub* (UK)[3], the *Hanoi University of Science and Technology HUST* (Vietnam), the *Université de Rennes* (France), the *Qilu University of Technology QLUT*, the *Dalian Institute of Chemical Physics DICP* (both China), the *Islamic World Educational, Scientific and Cultural Organization ICESCO*, the *University of Lahore* (Pakistan), and the *Czech Advanced Technology and Research Institute- Regional Centre of Advanced Technologies and Materials CATRIN-RCPTM at Palacky University Olomouc* (Czech Republic). We carefully consider which strategic partnerships we enter into. The prerequisite for this is the suitability and reputation of our partners for the positive influence on the further development of LIKAT research.

LIKAT supports the international mobility of its scientists through various measures. These include temporary laboratory stays abroad, participation in international conferences, workshops and symposia, or the exercise of visiting professorships, especially at foreign universities and colleges.

---

2 https://www.leibniz-gemeinschaft.de/fileadmin/user_upload/Bilder_und_Downloads/Neues/Mediathek/Publikationen/Brosch%C3%BCren/Leibniz-Strategie_2020_web.pdf

3 The UK Catalysis Hub is a consortium of universities involved in catalysis research led by Cardiff, Bath and Manchester (https://ukcatalysishub.co.uk/).

3.2.3 PARTICIPATION IN NATIONAL & INTERNATIONAL NETWORKS & ALLIANCES

Through their activities as reviewers, in networks, committees and international research associations, LIKAT researchers are actively shaping the global research area.

National Networks. National networks relevant to LIKAT include the *Society for Chemical Engineering and Biotechnology (DECHEMA)*,[4a] *the German Catalysis Society (GeCatS)*[4b] and the *Society of German Chemists (GDCh)*.[4c] LIKAT researchers are actively involved in these networks. An example of this is the commitment of the current scientific board members of LIKAT. Matthias Beller was a member of the *GeCats* board from 2008 to 2014. He is also a long-standing chair of the committee that organizes the most important national catalyst meeting (annually in Weimar) on behalf of *GeCats*. Since 2019, Jennifer Strunk has been a co-member of the *GeCatS Strategy Committee* and co-author of the *Roadmap Catalysis* of the *German Catalysis Society*. Angelika Brückner was a commission member from 2014 to 2020 and a member of the *GeCatS steering committee* since 2020. Many LIKAT researchers are also organized and actively involved within the GDCh with its specialist structures and working groups or the *JungChemikerForum* Rostock. Angelika Brückner was elected to the *GDCh board* for the term 2020-2023. During the same period, Jennifer Strunk is a member of the *board of the Sustainable Chemistry Division*.

The *German Academy of Science and Engineering (acatech)* advises politicians and society on issues relating to the future of technology science and technology policy. *acatech* admits its members on the basis of outstanding scientific achievements and high reputation and appointed Matthias Beller as a member of the *German Academy of Science and Engineering* in 2002.

Since 2019, LIKAT has been a partner in the *4chiral*,[4e] network, which comprises nearly 40 partners. Three-quarters of them are small and medium-sized enterprises (SMEs) in eastern German fine chemistry and biotechnology, while the other partners are universities, colleges and research institutes. *4chiral* primarily offers its members a basis for economic activities and research cooperations.

Research Networks. LIKAT is also involved in various national and international research networks. Selected alliances are explained in more detail in the following.

Leibniz ScienceCampi. Together with the *Leibniz Institute for Plasma Science and Technology (INP Greifswald)* and the *Universities of Greifswald and Rostock*, LIKAT initiated the Leibniz ScienceCampus *ComBioCat*.[5] Paul Kamer (former head of research department at LIKAT) was in charge of the application. The positive decision was made in 2019. The institute is coordinating the campus. Since Paul Kamer's sudden death, Jennifer Strunk, speaker of *Topic 05*, has been its spokesperson. The participants are researching the transition from fossil resources to renewable raw materials for the production of chemicals and energy sources. The key technology here is catalysis, including biocatalysis. The LIKAT researchers Esteban Mejía, Johannes G. de Vries, Sebastian Wohlrab, Jennifer Strunk and Henrik Junge are involved (*Topics 01/04/05/07*).

Der Leibniz Science Campus *Phosphorus Research*[6a] under the leadership of the *Leibniz Institute for Baltic Sea Research Warnemünde (IOW)* entered its second funding phase during the reporting period. The central topic is the worldwide decreasing availability of phosphorus, which considerably endangers the supply situation with food and chemical products. Strategies must be developed to use phosphorus much more efficiently than before and to close phosphorus cycles. Here, LIKAT is involved in the work with Matthias Beller, Armin Börner, Christian Hering-Junghans, Dirk Michalik as well as the two

4 (a) dechema.de, (b) gecats.org, (c) gdch.de, (d) acatech.de, (e) 4chiral.de.

5 combiocat.org.

former habilitation students and now associated professors of LIKAT Marko Hapke and Thomas Werner (*Topics 04/07*).

NFDI4Cat [6b] (*Topics 03/07*) The *National Research Data Infrastructure (NFDI)* initiative supports digitization in key scientific areas in order to network important research data from the participating partners and make it widely available. Within this framework, the *NFDI4Cat* consortium is funded as one of nine consortia. LIKAT was in charge of obtaining the funding for the catalysis-related consortium. *NFDI4Cat*, consisting of 16 experienced partners from the fields of homogeneous, heterogeneous, photocatalysis, biocatalysis and electrocatalysis, started its activities at the end of 2020 with Matthias Beller as scientific spokesperson of the consortium. It focuses on catalysis-related sciences, including chemical engineering and process engineering, and brings together the different disciplines of catalysis with regard to data management.

Joint project Research Factory Hydrogen *MV*.[6c] (*Topics 03/05*) The joint project of the three research institutes *Fraunhofer Institute for Large-Scale Structures of Production Technology (IGP, Rostock), Leibniz Institute for Plasma Research and Technology (INP, Greifswald)* and LIKAT researches processes and technologies for CO_2-neutral production cycles on the basis of renewable energies, optimizes them and brings them to application maturity. LIKAT is specifically concerned with PtX transfer: green hydrogen, generated by electrolysis using photovoltaics, is converted with CO_2 to green fuels (so-called *e-fuels*, kerosene), energy storage and basic chemicals (such as MeOH). The carbon dioxide is extracted from the air. The funding will allow investments for the construction of the necessary pilot-scale facilities at LIKAT's *Catalysis2Scale* transfer technical center.

SDG-Graduate Program *RoHan*.[6d] (*Topics 04/07*) The DAAD-funded graduate program *RoHan* is a cooperation between the *University of Rostock*, *LIKAT* and the *Hanoi University of Science and Technology* as well as the *Vietnam National University - University of Science in Hanoi* (Vietnam). It is already in its second funding phase and enables the development and establishment of catalysis technologies and processes through the training of qualified Vietnamese scientists. On the part of LIKAT, Esteban Mejía, Jennifer Strunk, Jola Pospech, Angelika Brückner, Sebastian Wohlrab, Norbert Steinfeldt, David Linke, Sergey Tin, Henrik Junge, Jagadeesh Rajenahally and Osama El-Sepelgy are involved.

Alumni-Network. Within the last years, an effective alumni network has been established and maintained at LIKAT. Alumni are important multipliers and the institute benefits with regard to the transfer of knowledge and research results between the institute and practice as well as in the acquisition of third-party funding and the search for new cooperation partners. Alumni whose employers are in business or science also act as potential cooperation and project partners. Alumni with a corresponding position in society as decision-makers and executives are the link between LIKAT, the public and the economy. They thus build a bridge between theory and practice. An efficient network is equally beneficial for the alumni themselves. Through continuous contact with LIKAT, they are informed about highly topical findings from science. They have the opportunity to competently support or initiate research cooperations with LIKAT and to make current research results economically usable in the context of their work for an industrial employer.

6 (a) science-scampus-rostock.de, (b) nfdi4cat.org, (c) catalysis.de/PtX_Transfer_Research_Factory.pdf, (d) rohan-sdg.com.

3.2.5 INDUSTRY COLLABORATIONS

The strengths of LIKAT include intensive cooperation with the private sector and the high quality of research in the field of industry-relevant fundamental topics. The strategic orientation of LIKAT enables a wide range of business cooperations. A large number of confidential bilateral co-oper-ation projects with industry result in joint patent applications with industrial partners. Never-theless, the institute also works in this area in a highly productive scientific manner. Each year, the institute carries out around 50 bilateral and multilateral projects involving industry. This high number reflects the intensive networking of LIKAT with large and small companies in the private sector, not only throughout Germany but also in Europe and worldwide. Of particular note are cooperations with four companies in the private sector, the nature and scope of which differ from those with other companies. Since 2007, a far-reaching framework agreement has secured LIKAT's co-operation with *Evonik Industries AG*. In 2012/13, longer-term framework agreements were signed with *Henkel AG & Co. KGaA* and *Symrise AG* were signed. The most re-cent addition is the framework agreement with *Apex Ener-gies* for €1.5 million, which was concluded in April 2022. The intensive and long-term co-operations with various companies of the economy allow the LIKAT to realize the central strategic concern of the utilization of the research results. Due to the scientific achievements of the institute's researchers, a total of 10 transfers to industrial pilot scale or directly to industrial production could be realized in the reporting period 2019 to 2021.

Figure 2. Exemplary: Cooperation partners of LIKAT from the private sector.

4. WHERE TO GO: RESEARCH FOR THE CLOSURE OF CIRCULAR FLOWS

4.1 OVERALL SCIENTIFIC CONCEPT OF THE LIKAT

4.1.1 RESEARCH FOR RESOURCE CONSERVATION & CLOSURE OF ORBITAL STREAMS

Earth Overshoot Day marks the theoretical date when humanity has used up all the biological resources that the Earth regenerates over the course of a year.[7] While human life and actions in the early 1970s were still commensurate with available resources, this day has been steadily moving forward ever since.

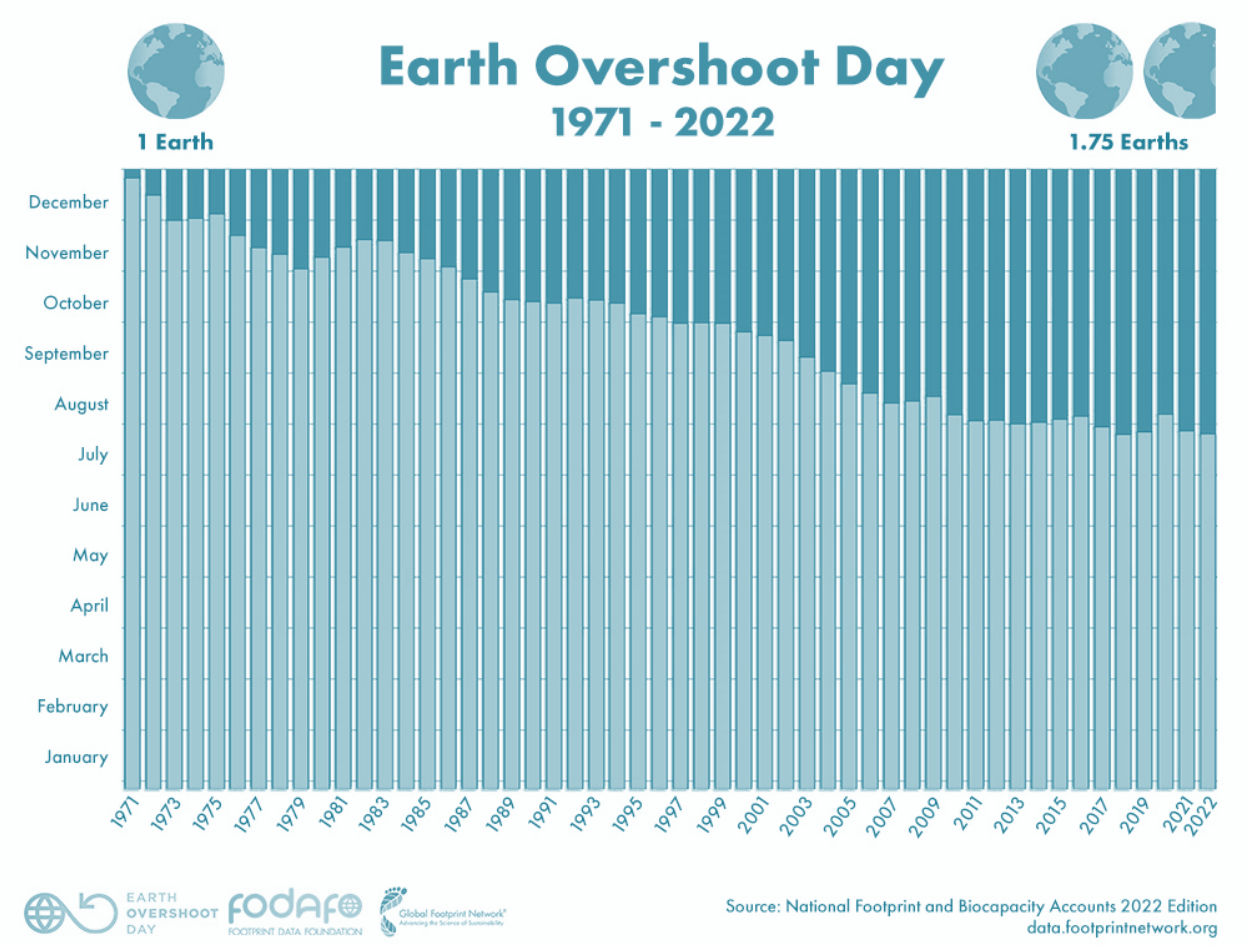


Figure 4. Shift in *Earth Overshoot Day* from 1971 to 2022.

For the current year 2022, *Earth Overshoot Day* falls on July 28 (Figure 5).[7] On average, people worldwide live beyond their means, consuming 170% of the resources that the Earth can provide annually. Broken down to the country level, there is a striking difference between the individual countries (Figure 5).[7] If all people lived as they do in Germany, the annual resources of 2.9 Earths would be required, compared to 2.3 for living conditions in China and 0.7 in India. We therefore bear a great responsibility for better resource use.

7 https://www.overshootday.org/

In order to achieve a balance between the resources produced and consumed, a far-reaching structural change in our society and new, improved technologies are required. The aim is to make the best possible use of existing resources and at the same time to close loops. The European Parliament defines the concept of the circular economy thus: *The circular economy is a model of production and consumption in which existing materials and products are shared, leased, reused, repaired, refurbished and recycled for as long as possible. In this way, the life cycle of products is extended*.[8]

For science, this means developing processes that minimize waste, improve material efficiencies, make the life of products as long as possible, and finally, at the end of their life, return their resources and materials to the economy as much as possible. According to Frans Timmermans, Executive Vice President of the European Green Deal, only 12% of secondary raw materials and resources are recycled.[9]

Figure 5. How many earths?[7]

4.1.2 HOW CAN THE LEIBNIZ INSTITUTE OF CATALYSIS CONTRIBUTE AS A RESEARCH INSTITUTE TO THE CLOSURE OF THE CIRCUITS?

Buzzwords such as resource efficiency, sustainability and circular economy are on everyone's lips. The chemical industry can play a key role in their concrete implementation. This includes the gradual substitution of fossil raw materials and energy sources, the steadily increasing demand for sustainable products on the one hand and production processes on the other. Processes must be designed more flexibly in order to be able to implement various renewable raw materials, energy sources and hitherto little-used secondary material and waste streams from the circular economy. Catalysis is a key technology in this regard. Resource and energy efficiency are inherent properties of catalysis. Catalysts control and accelerate chemical and biochemical processes. They increase yield and avoid by-products by enabling starting materials to react specifically and selectively at the molecular level. Over 85% of all chemical products in our daily lives are produced by catalytic processes.[10] The field of catalysis thus reaches far into society. Research in this field regarding the closure of cycle flows has an effective impact on chemical production and processes. Chemistry is closely linked to almost all industries and is a component of many value chains.[11]

As a Leibniz Institute, LIKAT is dedicated to application-oriented catalysis research for society and its technological implementation. The institute works complementary to other research institutions and has unique selling points (*3.1*, p. 7. These include its 70 years of expertise in applied catalysis research, its position as a link between basic research and applications in the private chemical industry. And last but not least, the Institute's own technical center already mentioned, which allows the Institute's mem-

8 https://www.europarl.europa.eu/news/de/headlines/economy/20151201STO05603/kreislaufwirtschaft-definition-und-vorteile

9 https://ec.europa.eu/commission/presscorner/detail/de/ip_20_420

10 Roadmap of German Catalysis Research - Catalysis a Key Technology for Sustainable Economic Growth, GeCatS, 3rd edition, March **2010**.

11 Roadmap Chemie 2050 - owards a Greenhouse Gas Neutral Chemical Industry in Germany, DECHEMA, October **2019**.

bers, in cooperation with the chemical industry and SMEs, among others, to test research results for their suitability for practical application or to develop them accordingly.

We are convinced that LIKAT can make significant contributions to a circular economy with its research activities. The current research strategy has set the course for this. The integration of the individual research groups into cross-disciplinary research departments complements the content strategy, which is geared towards a holistic view of catalysis research.

To achieve its goals, LIKAT is applying its strengths and expertise more to the closure of material cycles. The following sections explain the resulting concrete research topics and goals of LIKAT for the funding period 2023 to 2030.

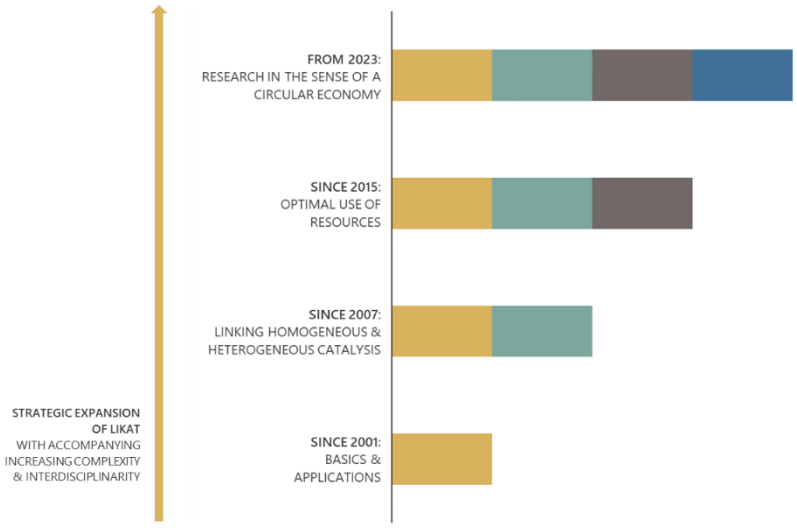


Figure 6. Strategic expansion in terms of content up to the year 2030.

The goal of research under the aspects of the circular economy requires a holistic and yet focused approach to the research activities and the provision of the entire know-how of the institute for the increasingly complex and interdisciplinary research questions. With the definition of the topic fields of the matrix structure, the framework for LIKAT's contribution to the circular economy has already been created: the indispensably close and interdisciplinary cooperation of research groups from different research departments with different expertise. The methodologically oriented topics (*Topic 01 Structure-Reactivity Relationships, Topic 02 Kinetics, Theory & Mechanisms* and *Topic 03 Reaction Engineering & Implementation*) focus on technological solutions. The materially oriented topics (*Topic 04 Renewable Resources, Topic 05 Energy & Environment, Topic 06 More Efficient Processes* and *Topic 07 New Products and Processes*) research and develop efficient processes as well as sustainable and high-quality products.

In this way, a targeted combination of internally available competencies with external expertise is achieved in the context of new appointments and cooperations on a national and international level.

4.1.3 WHICH TOPICS ARE RELEVANT WITH THIS LIKAT?

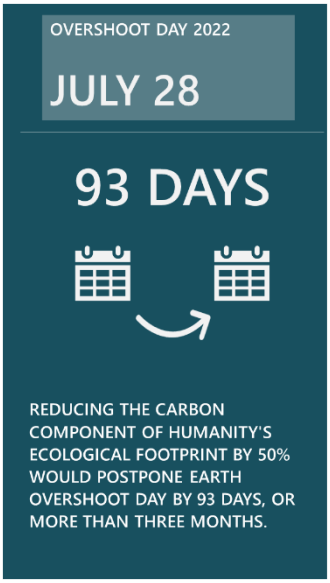


Figure 7[13]

Earth Overshoot Day vom *Global Footprint Network*,[12] an international organization that provides decision makers with tools to enable the human economy to operate within the Earth's ecological limits.[13] One of the solutions is greenhouse gas neutrality (Figure 7). *The German Chemical Industry Association* (*VCI*) commissioned the *study Towards a Greenhouse Gas Neutral Chemical Industry* in Germany by *DECHEMA* and *FutureCamp* which was published in 2019.[11] The paper describes a possible path for the transformation of the German chemical industry toward greenhouse gas neutrality, including both greenhouse gas emissions generated in production itself, from the purchase of electricity and heat, and the carbon content of chemical products as a source of CO_2. As a conclusion, the following additional future research focal points and objectives result for LIKAT in order to effectively contribute to a sustainable economy of the chemical industry with distinctive circular flows, without weighting the order of priority:

- **Climate-neutral or Raw-material-neutral Energy**: the conversion of processes requires a considerable amount of renewable electricity; electricity consumption in the chemical industry amounted to 54 TWh in 2018,[11]
- **Provision of Raw Materials in the Sense of a Circular Economy**: use of previously unused or little-used renewable raw materials, recycling of secondary raw materials and CO_2, use of previously unused material flows for the production of valuable products including the development of suitable process technologies, provision of plastics as feedstock for the production of basic chemicals through improved chemical recycling, recyclable products and material flows for closed material cycles,
- **Cooperation between the Disciplines** process engineering, chemistry & biotechnology or biocatalysis.

Within the coming years, the existing strengths must be applied intensively to the development of closed material cycles in the chemical industry.

As already mentioned above, the granting of research freedom for all scientific staff members as a basic principle of the work organization at LIKAT (generally 10-20%) remains unaffected. Researchers can independently develop solutions for existing projects or propose new project topics.

A future focus is **CO_2 valorization**, the various aspects of which are being worked on in the individual topic fields. At the end of a product's life, chemical combustion or decomposition processes usually emit CO_2 and/or methane. The reintroduction of the greenhouse gas CO_2 into chemical production is to be intensively investigated. In *Topic 05*, the aim is to develop improved absorbents to separate CO_2 directly from the air and convert it into downstream products. In addition, novel approaches to integrated direct air capture of CO_2 with direct catalytic reduction are being pursued. Possible downstream products are carbon monoxide, methane, methanol or higher hydrocarbons in so-called low temperature or more efficient Fischer-Tropsch processes. These thermal processes are to be supplemented by photochemical and electrochemical methods in *Topic 05*. The aim is to develop efficient photo- and electrocatalysts that are also suitable for practical use. *Topic 01* aims to investigate the transferability of structure-reactivity correlations from classical thermal catalysis to alternative methods of energy

12 https://www.footprintnetwork.org/

13 https://www.overshootday.org/solutions/

input by light and current. *Topic 02* will focus on the mechanistic and kinetic studies of homogeneous-, heterogeneous-, electro-, photo- and partially biocatalytic CO_2 conversions to provide fundamental knowledge for catalyst activation and deactivation and rational catalyst design. This will be done by steady-state, transient and spatially resolved analyses of reaction processes, spatially and temporally resolved spectroscopic methods, modeling as well as numerical analysis and DFT calculations. In this context, *Topic 06* will focus in the future on the optimization of methanol and olefin synthesis from CO_2 and direct methane functionalization with the aid of computer-aided data evaluation. In *Topic 07*, new methods for activating and using the small, inert molecule CO_2 are to be researched and developed, e.g. the use of CO_2 as an oxidant or the reductive coupling of CO_2 to oxalates in the presence of green hydrogen as a key step in artificial photosynthesis technologies.

In view of the shortage of fossil raw materials, another focus of future LIKAT research will be on the **use of renewable resources** that are not relevant as food. This includes, on the one hand, the development and optimization of **hydrogen technologies** in connection with **renewable energy** (mainly within the scope of *Topic 05*) and, on the other hand, the utilization of renewable raw materials for the **production of large-scale and fine chemicals**. The latter is to be researched primarily in *Topic 04* in cooperation with *Topic 07*. Research and development of catalytic processes and methods with the aid of the entire methodic spectrum of LIKAT (homogeneous, heterogeneous and biocatalytic) will play a central role. In addition, the electrochemical upgrading of renewable raw materials is to be increasingly investigated. Another focus is the development of new catalytic materials, e.g. for the hydrodeoxygenation (HDO) of oxygenates and the deoxydehydration (DODH) of diols for the sustainable production of chemicals (e.g. phenols and alkenes) from biomass.

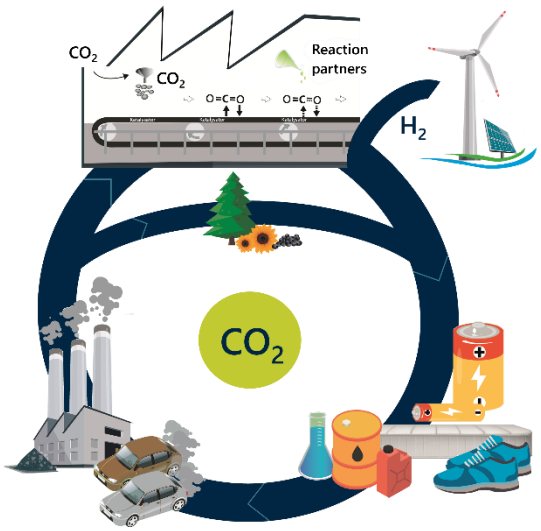


Figure 8. Strategic research activities to close the carbon cycle.

With regard to the development of new and improved hydrogen technologies, the production of hydrogen with the aid of renewable energies, its chemical storage and the use of green hydrogen for the synthesis of liquid energy carriers with the utilization of CO_2 (e.g. formic acid, methanol, formates) are being increasingly researched. The combination of catalytic production and decomposition of liquid energy or hydrogen carriers enables cycles for CO_2-neutral storage and allows the high volumetric energy density of liquid storage media to be exploited compared to that of hydrogen. The goal is to realize at least two demonstrators on a **pilot scale** in the next three years.

For the cost-effective use of renewable resources, the transfer from laboratory to pilot scale is one of the main application hurdles. *Topics 04* and *05* both pursue the central goal of developing new innovative catalysts based on readily available metals and also demonstrating their application on a pilot scale. *Topics 01* and *02* have set themselves the goal of applying their expertise to fundamental findings on catalyst design. Through close cooperation with *Topic 03* in the *Catalysis2Scale* transfer technical center, the scaling up of at least four processes per year to pilot plant maturity is envisaged.

Carbon cycles can also be closed by **efficient recycling processes**. *Topic 07* will therefore conduct more research into the recycling of plastic waste in the future. The aim is to develop new catalytic methods for depolymerization on the one hand and for polymerization of the starting materials thus obtained on the other. Initially, hydrogenating depolymerizations of polyesters, polyamides and polyurethanes will be investigated. The recovery of catalysts plays an important role in this process.

In the sense of a closed **phosphorus cycle,** new resource-saving and atom-economical syntheses of phosphorus-based ligands and reactive low-valent main group compounds are to be developed in *Topic 07*. Phosphates are of particular interest as readily available starting compounds. In addition, approaches for phosphorus recovery or replacement of phosphorus compounds will be investigated.

Reaction Engineering, Implementation & Digitalization. The vision of a circular economy requires far-reaching changes in chemical production: The changing raw material and energy situation, new legal regulations, and a more localized economy necessitate new or significantly modified processes. The overriding goal at LIKAT is to develop the best possible reactor design and operating regime for catalyzed chemical reactions. In the future, it will be necessary to be able to implement these faster than before, i.e. to transfer scientific results from the laboratory to the pilot plant scale more quickly and efficiently and to digitize the development chain from the catalyst to the process. This is done primarily within the framework of *Topic 03* by evaluating various reactor concepts, by means of synergetic development of reactor and process concepts, and by researching process engineering aspects of catalyst synthesis. For this purpose, the possibilities of the *Catalysis2Scale* transfer technical center are to be used intensively.

The following sections 4.2 to 4.8 describe the strategic orientation of the individual topic fields of LIKAT. Section 4.9 sets out the strategic development of the *Catalysis2Scale* transfer technology center.

4.2 STRATEGY TOPIC 01: STRUCTURE-REACTIVITY-RELATIONSHIPS

The need to rapidly convert European industry to renewable energy and raw material sources as well as to resource-saving material cycles, which is intensified by current developments, also requires an adaptation and focus of science and research. In the chemical industry, but also in other technology areas that are essential for Europe, new and improved catalysts are key tools for achieving the desired sustainability goals. One of the basic requirements is a much more efficient and cost-saving design of highly active and selective catalysts that can tolerate a dynamic supply of resources, can also convert inert substrates (CO_2, N_2) and are robust to photo- and electrocatalytic reaction conditions and solvents.

These goals can only be achieved if comprehensive knowledge of the relationship between catalyst structure and mode of action is available. To this end, the strategy of *Topic 01* comprises two main goals, which are to be achieved through flexible cooperation with various *research groups* (TG) and external partners:

1. Establishment of a modern center for *in-situ/operando* microscopy and spectroscopy across research areas: already existing expertise and infra-structures will be used in cooperation with the operative thematic groups and the service area analytics to jointly develop the following focal points: a) new simultaneous couplings to increase the information potential and the relevance of results, e.g. EPR/NMR (with Prof. B. Corzilius, Uni Rostock) and EPR/XAS for heterogeneous catalysis, b) adaptation to industrially relevant and challenging reaction conditions (p20 bar, electric potential, flow reactors, polar solvents), c) higher time resolution (e.g. rapid scan-EPR, ultrafast spectroscopy in cooperation with Rostock University), d) higher spatial resolution (NAP-XPS, NAP-STEM/SEM/EELS), e) automated data acquisition, storage and analysis in combination with machine learning methods, supported by existing activities in *NFDI4Cat* (p. 11). In addition, the use of *in situ* electron microscopy at the new Center for Interdisciplinary Electron Microscopy MV, in which LIKAT is also involved, offers completely new, revolutionary possibilities for catalyst monitoring at the atomic level.
2. Elucidation of catalyst action principles for strategically relevant reactions of a closed-circular economy: in cooperation with other topic fields and research groups, the center generates fundamental

findings on structure-reactivity relationships, which are incorporated into catalyst developments for the following key chemical processes: a) CO_2 valorization incl. hydrotreating of biogenic pyrolysis. Investigations on the transferability of structure-reactivity correlations from classical thermal catalysis to alternative methods of energy input such as light and electricity, b) Hydrotreating biogenic pyrolysis products, c) Photocatalytic synthesis of bioactive compounds as active agents, d) Replacement of noble metal catalysts by non-noble metal catalysts for (transfer) hydrogenations, dehydropolymerizations, cyclizations and deoxygenations.

4.3 STRATEGY TOPIC 02: KINETICS, THEORY & MECHANISMS

A sustainable development of our economy and society also requires a fundamental restructuring of the chemical industry due to changes in the energy and raw material base as well as due to new legal regulations to reduce energy consumption and unwanted emissions. Against this background, the research activities in *Topic 02* focus on the elucidation of the mechanisms and on the gain of the kinetics of heterogeneous, homogeneous, electro-, photo- and biocatalyzed (artificial metal enzymes) reactions with the aim to provide fundamental bases for rational catalyst design and optimal reaction control. To this end, we continue to pursue the strategy of combining the expertise of the research groups in the complementary areas of i) steady-state, transient, and spatially resolved analysis of reactivity sequences, ii) activation and deactivation of catalysts, iii) use of spatially and temporally resolved spectroscopic methods, modeling, and numerical analysis and DFT calculations. Since the beginning of 2022, *Topic 02* is also strengthened by the junior research group *Theory of Homogeneous & Biocatalysis* (Dr. Milica Feldt). Our expertise will be applied to future-oriented reactions: i) CO_2 conversion to carbon monoxide, methane, methanol or higher hydrocarbons (fuels by low temperature or more efficient FT processes), ii) use of non-food biological resources to produce high-value chemical products, iii) storage (e.g. as methanol, formic acid derivatives, NH_3) and production of hydrogen from renewable resources, iv) value addition of bio- and natural gas, v) activation of nitrogen. In the future, *Topic 02* will be expanded to include the study of catalysts for artificial photosynthesis technologies. Work will continue on the development of environmentally friendly, sustainable and cost-effective catalysts for ongoing processes for the production of existing industrial intermediates and platform chemicals.

4.4 STRATEGY TOPIC 03: REACTION ENGINEERING & IMPLEMENTATION

The vision of a circular economy is associated with extensive renewals in chemical production. Current processes are being replaced or significantly modified by new processes due to the changing raw material and energy situation, new legal regulations and a more localized economy. The high demand for new solutions, which should also be available quickly, results in the challenge of being able to implement them faster than before.

Against this background, the strategy of *Topic 03* focuses on the following areas:

1. Faster and more efficient transfer of scientific results from laboratory to pilot plant scale,
2. Digitalization of the development chain from catalyst to process,
3. Development of a more efficient reaction technology for practice-relevant heterogeneous-, homogeneous-, electro- and photocatalyzed reactions.

With regard to reaction technology, the development of the best possible reactor design and operating regime for catalyzed chemical reactions is the overarching development goal. This may include the evaluation of different reactor concepts, but also the synergetic development of reactor and process concepts. In addition to the catalytic reaction, process engineering aspects of catalyst synthesis are also addressed, i.e. the scale-up from laboratory (a few g) to pilot plant (multi-kg) scale.

Digitization of the development chain from catalyst to process is seen as an essential element to accelerate the implementation of new processes and procedures. While techniques such as machine learning and statistical data analysis have been used for years, more effort will be put into capturing as much research data as possible in the future with the long-term goal of enabling a knowledge graph for catalysis. To this end, *Topic 03* is heavily involved in the *NFDI4Cat* project.

In order to realize this vision, research groups from the different research departments as well as the *service department analytics* are working together in *Topic 03* and will also make more intensive use of the possibilities of the new *Catalysis2Scale* transfer technical center in the future.

4.5 STRATEGY TOPIC 04: RENEWABLE RESOURCES

Reducing fossil-based CO_2 emissions is the central goal on the way to a *net-zero carbon* society. This also requires reducing and eventually eliminating the drastic dependence on petroleum as the main source of chemicals. Renewable raw materials that do not compete with food production are available and can serve as an alternative for our bulk and fine chemical needs. Various methods already exist for the production of renewable platform chemicals from biobased resources that can be obtained with high yield and purity by low-cost methods. Therefore, the main goal of *Topic 04* is to develop novel valorization routes to convert these platform chemicals into either new industrially relevanent or already industrially important compounds. In the past years, LIKAT used its very broad spectrum of catalytic processes and methods applied for these conversions (e.g. homogeneous, heterogeneous, biocatalysis, etc.). In the future, the electrochemical upgrading of renewable raw materials or platform chemicals from bio-based waste on the basis of green electricity will be researched. The envisaged routes will not only use bio-based carbon for the conversions, but also aim at reducing or eliminating undesired stoichiometric reagents (e.g. stoichiometric reducing agents or toxic oxidizing agents) that generate significant waste. Likewise, the focus is on the development of new catalytic materials, e.g. for the hydrodeoxygenation (HDO) of oxygenates and the deoxydehydrotization (DODH) of diols for the sustainable production of chemicals (e.g. phenols and alkenes) from biomass. In addition, the methods aim to avoid unwanted solvents and uneconomical synthesis strategies. This will be done in close cooperation with *Topic 07*. The leap from laboratory to industrial scale is still a major hurdle in this field: the transfer of knowledge from the laboratory to an application-relevant scale will therefore be pursued in the future in close collaboration with *Topic 03*. The goal is to bring at least four processes to industrial maturity by 2030.

4.6 STRATEGY TOPIC 05: ENERGY & ENVIRONMENT

The main research objective in *Topic 05* is to gain fundamental and applicable knowledge that enables a circular economy and sustainably secures resources for future generations. The topic field was strengthened in 2021 by Robert Francke with his expertise in the fields of electrochemistry and catalysis. In total, our activities will focus on five main research lines in the future:

1. Development of new and improved hydrogen technologies: The production of hydrogen with the help of renewable energies, its chemical storage and the use of *green* hydrogen for the synthesis of liquid energy carriers with the utilization of carbon dioxide (e.g. formic acid, methanol, alkyl formates), mainly in classical hydrogenation/dehydrogenation reactions. Catalytic studies on NH_3 as a storage medium are also being continued. By combining catalytic production and decomposition of liquid energy or hydrogen carriers, cycles for CO_2-neutral hydrogen storage are enabled and the high volumetric energy density of liquid storage media compared to that of hydrogen is exploited. The central goals in the next three years are the development of new innovative catalysts based on readily available metals and the realization of at least two demonstrators on a pilot plant scale.

2. Use of renewable energies for the chemical production of fine and bulk chemicals, e.g. in electrochemical or photocatalytic processes: Electrochemical reactions can be powered by green electricity, photocatalytic processes ideally directly utilize sunlight energy efficient LED light sources. Strategically, the consideration of processes designed purely for energy storage (water splitting, CO_2 reduction) will be expanded to include selective synthetic reactions. Together with *Topic 03*, the complex interactions of reactor, reaction conditions and catalyst will be considered in order to identify promising chemical processes, such as atom-efficient hydrogenation/dehydrogenation reactions (e.g. alcohols to carbonyl compounds and vice versa), for possible technical implementations (e.g. ethyl acetate from ethanol). Alternatively, the use of plasma reactors powered by renewable electricity will be investigated.
3. Reintroduction of greenhouse gases (CO_2, CH_4) into chemical production: At the end of a product's life, chemical combustion or decomposition processes usually emit CO_2 and/or methane during disposal or recycling. For a complete circular economy, we are investigating thermal, photocatalytic and electrochemical reactions for the recycling of these gases into the value chain, e.g. for the synthesis of fuels, monomers and platform chemicals. The availability and concentration of CO_2, which is at best separated directly from the air with suitable absorbents and converted into downstream products, are essential here. Recently, amino acid-based systems for CO_2 capture have been introduced by researchers at LIKAT (Junge, Beller), which allow the subsequent hydrogenation of the bound carbon dioxide to alternative energy carriers, such as formates, under mild reaction conditions. In the future, even more efficient amino acid analogues, e.g. based on stable carbenes, are to be developed. Together with *TF 03* and *06*, the realization on a pilot plant scale is planned. With regard to photocatalysis, the yields achieved so far are to be increased by at least one to two orders of magnitude by means of systematic test series and derivation of the structural requirements of the reaction on the catalyst (with *Topic 01*). Instead of classical water splitting and CO_2 reduction, photocatalytic dry reforming, e.g. of biogas, comes to the fore.
4. Purification of waste gas streams and waste water: a healthy environment for future generations requires clean drinking water and clean air. We investigate (photo)catalytic processes for the conversion of harmful pollutants in air (e.g. NO_x, volatile organic compounds) and water (e.g. pharmaceuticals, dyes) into harmless end products. In addition to the further development of classical DeNOx catalysts to achieve stricter emission targets in the automotive and power plant sectors, we are researching the development of active, stable photocatalysts and processes that allow the complete mineralization of pharmaceutical residues in water.
5. Establishment and use of electrochemical catalysis: Electrochemistry allows the use of green electrical energy from water, wind and solar energy as the driving force of chemical reactions and thus enables the substitution of chemical oxidizing or reducing agents. Targeted catalyst design can electrify conventional reactions and reveal completely new reaction pathways, which is also attracting much attention in the industrial environment. The aim is therefore the electrification of (industrially) relevant reactions for the production of chemicals. To this end, electrocatalysts are to be developed that can be manufactured from readily available and non-toxic raw materials. The optimization of the electrochemical methods is to be carried out using sustainable components (solvents, conducting salts, electrode materials and separators). Specifically, electrocatalysts for the production of hydrogen by water electrolysis or the development of efficient electrocatalysts for the production of basic chemicals from CO_2 are to be developed and improved.

4.7 STRATEGY TOPIC 06: MORE EFFICIENT PROCESSES

For the coming years, efficient use of resources is the main aspiration of *Topic 06*. The four pillars already mentioned will continue to be instrumental in successfully addressing this core concern in the

future: i). Catalyst design, ii) process control, iii) alternative reaction pathways, and iv) new resources. Ecological synthesis routes, promising new raw materials as well as novel more efficient processes for industrial applications will be addressed here.

1. Efficient ligand design and the development of new, sustainable heterogeneous catalysts (non-toxic, preferably from renewable raw materials) are an important aspect for the development of more resource-efficient processes. New simulation and preparation methods are being established for upscaling on a pilot plant scale to increase TRL levels, e.g. the use of artificial neural networks during catalyst screening or flame spray pyrolysis and extrusion of the resulting catalyst materials as part of catalyst synthesis upscaling.
2. Microprocessing and membrane technology are also to be used in the future for process intensification and thus for reducing the raw material input of continuously controlled, heterogeneously catalyzed reactions. Examples of reactions to be investigated are the synthesis of 1,5-pentanediol from furfural, the hydrogenation of nitro compounds in a flow reactor, or methanol synthesis in a membrane reactor.
3. Resource savings can also be realized by computer-aided data analysis of challenging reactions. The implementation of fast *in situ* spectroscopic methods allows real-time monitoring of the corresponding processes, which enables simultaneous control and optimization. Target reactions are for example: direct methane functionalization, methanol and olefin synthesis from CO_2, dry reforming of methane and CO_2, metathesis and alkane dehydrogenations, as well as feasible synthesis methods for fluorinated derivatives in the field of life sciences.
4. The substitution of stoichiometric oxidizing or reducing agents in selective reductions (e.g. from amides to amines) or oxidations (direct hydroxylations of C-H bonds) by green electrical energy as the driving force of chemical reactions is being pursued in the field of electrocatalysis. New practically relevant CO surrogates (e.g. based on CO_2) are to be established more strongly as a resource for the chemical industry. Further topics for the coming years in *TF 06* are the implementation of new catalytic processes for hydrogen storage and the utilization of little explored renewable raw materials.

In total, it is planned to transfer at least 10 improved processes to an industrial pilot scale in cooperation with *Topic 03* and external industry partners by 2030.

4.8 STRATEGY TOPIC 07: NEW PRODUCTS & PROCESSES

A large part of chemical production is still based on the fossil raw materials coal, crude oil and natural gas. This concerns both the energy demand and the direct and indirect material sources of organic bulk and fine chemicals. Important elements of the strategy of *Topic 07* are the utilization of renewable raw materials, in cooperation with *Topic 04*, as well as intermediates from other material streams for the development of new products and processes. Furthermore, we are concerned with the activation of small, inert molecules by new catalytic concepts. The focus is on new resources, gentle thermo-, photo- and electrocatalytic processes as well as chemistry in flow reactors or new approaches for catalyst recovery:

1. Industrially relevant bulk and fine chemicals (e.g. polyols, methyl acrylate, acetic acid) are to be increasingly produced from bio-based, renewable raw materials in the future. New products from renewable raw materials, which have the potential to replace industrially relevant compounds based on fossil raw materials, are to be developed. Examples are new polyether polyols from 2-methyltetrahydrofuran or HMF-glycerol acetals, which are of interest as additives for degradable polymers.

2. New methods for small molecule activation will be developed. Examples are indirect CO_2 reduction, reductive hydrogenation of CO_2 to oxalates and direct functionalization of N_2 to nitrogen-containing organic compounds, e.g. aniline and aliphatic amines.
3. In the sense of a closed phosphorus cycle, new resource-saving and atom-economical syntheses of phosphorus-based ligands and reactive low-valent main group compounds are to be developed. Phosphates are of particular interest as readily available starting compounds. In addition, approaches for phosphorus recovery or replacement of phosphorus compounds will be investigated.
4. The efficient recycling of plastic waste in the sense of a circular economy requires the development of new methods for depolymerization and polymerization of the starting materials thus obtained. In the future, the focus will be not only on functionalized polymers but also on simple polyolefins that have not been recycled so far and which are to be degraded to monomer building blocks with the aid of mechanochemical or catalytic processes, e.g. by ethenolysis in a tandem metathesis-isomerization sequence.
5. The recovery of catalysts is becoming increasingly important against the background of the scarcity of certain metals. We aim to make contributions to catalyst recycling in homogeneous catalysis, e.g. by using new immobilization concepts. Increasingly, reactions in flow reactors will also play a role.
6. Resource-saving light-mediated syntheses, e.g. selective oxidative coupling of amines with atmospheric oxygen. Metal-free and comparatively inexpensive homogeneous and heterogeneous catalysts are increasingly being used here.

4.9 STRATEGY CATALYSIS2SCALE-TRANSFER TECHNICAL CENTER

Due to the existing close exchange with numerous cooperation partners from industry, LIKAT is very well positioned to implement fundamental scientific developments for the benefit of society even better and more efficiently in practical applications in the future. For this purpose, the institute has essential personnel and technical prerequisites. There is a suitable practice-oriented infrastructure, which is otherwise hardly available at universities and Leibniz research institutions. LIKAT's own *Catalysis2Scale* Transfer Technical Center (Fact Sheet *Catalysis2Scale* Transfer Technology Center, Annex 1) is unique in its orientation and size in northeastern Germany. It serves the testing and transfer of chemical research results from the laboratory to the industrial pilot scale. Thus, it is an essential part of the LIKAT research strategy as well as of the LIKAT transfer guideline (Annex 2). At the same time, the institute offers SMEs and other Leibniz institutions, regionally and supra-regionally, the possibility of joint use of this LIKAT infrastructure for the transfer of relevant research results.

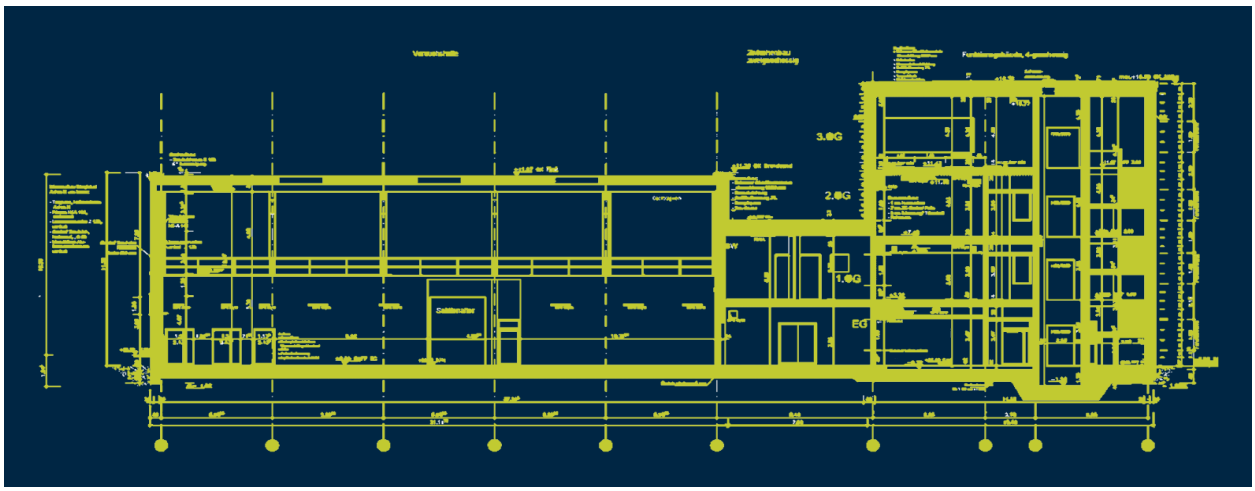
In 2024, LIKAT plans to establish a ***Leibniz Transfer Lab for Sustainable Energy and Transformations (LTLNES)*** as well as a corresponding thematic group that will coordinate and carry out the work in the technical center.

A special focus of the future work of this group will be in the field of renewable energies and technologies for the development of a carbon cycle economy. As an example, a carbon dioxide capture plant will be set up in a first step, where carbon dioxide adsorbed from the atmosphere will be directly converted to renewable chemicals, e-fuels and other valuable materials using green hydrogen.

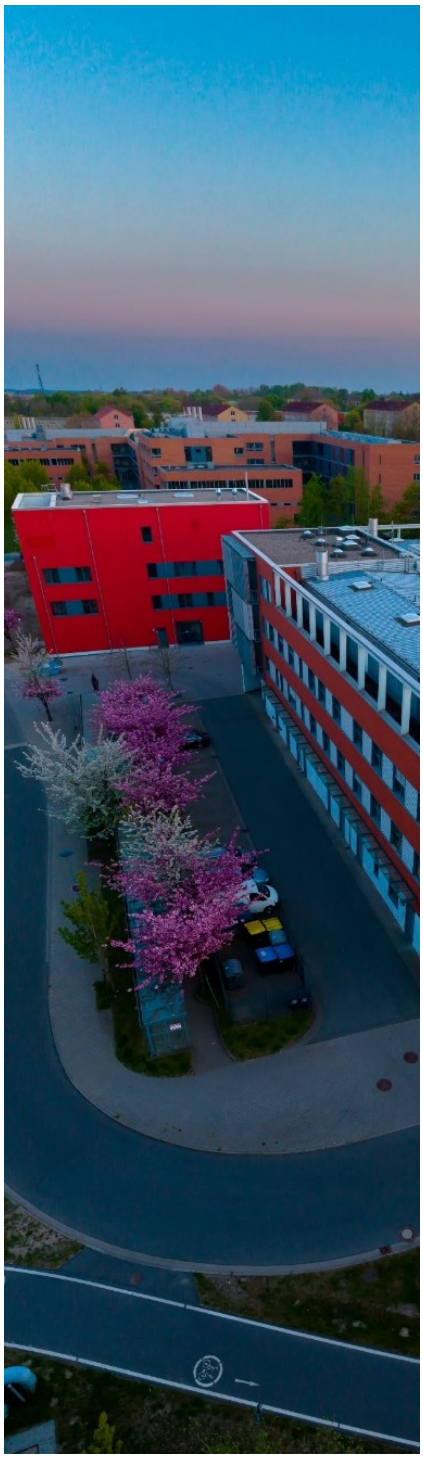
Other examples of development priorities of the Leibniz Transfer Lab:

- Implementation of new storage concepts for renewable energies, e.g. artificial photosynthesis processes,
- Improvement of processes for the production of green hydrogen and its storage,
- Development of more cost-effective CO_2 capture technologies in liquid and solid media,

» Improved catalysts for reverse water gas shift reactions as a key building block of green fuel production,
» Development of low-temperature Fischer-Tropsch syntheses and optimized processing of crude products,
» Low-temperature methanol syntheses and corresponding processes,
» partial automation of the above mentioned plants,
» Preparation line for the production of nano-structured materials and catalysts on a kg scale.



An example of one of the first planned implementations in *LTLNES* is the production of green kerosene, a sustainable aviation fuel based on the use of natural gas or biogas. In order to realize economic production, long-term catalyst tests will be carried out and product samples will be produced on a 100 L scale. The necessary flexible infrastructure is available at LIKAT in the form of the *Catalysis2Scale transfer technical center*. Further projects will be the development of cost-efficient technologies for the production and conversion of green methanol. This can be converted in further steps with the help of catalysts into products with a higher added value, e.g. higher hydrocarbons, long-chain alcohols, polymer monomers, olefins and fuel substitutes.



A current project with our SME partner *APEX* is driving forward the development of a hydrogen battery on a pilot plant scale. The joint project *Research Factory Hydrogen MV* (p. 11) of the three non-university research institutions LIKAT, the *Leibniz Institute for Plasma Research and Technology e.V. (INP)* and the *Fraunhofer Institute for Large Structures in Production Engineering (IGP)* enables investments and measures for the economic operation of the technical center, which is to be powered by renewable energies.

In total, five scientific positions are foreseen (1x E14/3, 4x E13/3). The organizational leader (E14) of *LTLNES* must have a sound chemical expertise in order to plan the future research topics (e.g. material use of H_2 and CO_2) and the strategic orientation of the group. Further tasks include the initiation and organization of projects with existing cooperation partners as well as new partners, especially from the Leibniz Association. An engineering position (E13) is planned to provide technical expertise for the construction of the pilot plants and their operation. Extensive knowledge in engineering and technical design of the facilities is required for the planned work. Both positions will be supported by two additional scientific persons (E13/3). In addition, a Technology Transfer Officer position (E13/3) is planned, whose duties include active administration of the transfer and require knowledge of project management and IP. In addition, the implementation of innovative ideas and development from the laboratory into larger facilities is to be realized by means of three technical positions (E10/3). The specialized tasks involved in operating the *LTLNES* can only be guaranteed by allocating tasks in the technical center and research operations. The tight labor market makes it necessary to stabilize these positions for both scientific and technically experienced personnel. Only in this way can appropriately specialized personnel be found and retained. Material and investment funds are to be used for both the repair and the expansion of the already existing facilities in the pilot plant (e.g. rapid test facility, particle modification & selection). In addition, some of the above-mentioned process developments require specific analytics in order to continuously ensure the high quality of the materials and catalysts produced.

At the same time, the institute offers SMEs as well as other Leibniz institutions, regionally and supra-regionally, the possibility of joint use of this LIKAT infrastructure for the transfer of relevant research results. In order to promote such cooperations, it is planned to organize a transfer workshop for project initiation at least once a year in Rostock and/or Berlin for all interested partners in order to achieve continuous implementations from the entire Leibniz Association. For the year 2023, the workshop *Opportunities of digitalization for a circular economy* is planned.

The aforementioned plans are the subject of an application for a so-called *small strategic institute expansion*, which will be submitted to the Leibniz Association on January 1, 2023. This is a strategic instrument of the Leibniz Association to trigger a permanent need for funds in the budget of the applying institute. The scientific quality of the proposed project, as well as the embedding in the stra-

tegic research planning of LIKAT, was verified by a vote of our *Scientific & Industrial Advisory Board* before the application was submitted, which assessed the project extremely positively.

The *Catalysis2Scale* transfer technical center is a consistent strategic further development of LIKAT as an interface between basic and applied research and thus a central component of its strategy. **Regardless of the outcome of the application** for the small strategic institute expansion, the institute plans for the sustainable operation of the pilot plant:

- The provision of its own financial resources planned for the STB from the core budget (about 420 T€) for the permanent use of the research infrastructure (by reallocating funds released from expiring research areas);
- The registration of the *Catalysis2Scale* transfer technical center as a research infrastructure of the Leibniz Association at the end of 2022 (thus: Making the infrastructure available for use by the entire Leibniz Association);
- The acquisition of public and private third-party funding for the use of the technical center.

5. STRATEGIC ORGANIZATIONAL DEVELOPMENTS

5.1 CONTROL & QUALITY ASSURANCE

The research work at LIKAT is continuously evaluated internally, usually twice a year, by the *Board,* the *General Assembly*, the *Scientific & Industrial Advisory Board* and the *Board of Trustees*. For the assessment of the research results of the institute as a whole and of the individual subject areas, the following performance criteria are used for the evaluation:

Performance criterion	**Formulated objective**
Quality & quantity of publications Number, impact factor, visibility, open access, peer-review	LIKAT publication guidelines (Annex 3) e.g. 50% in journals with IF>5 and 50% of all publications in open access
Transfer work, patent applications, economic applications	LIKAT transfer guideline (Annex 2)
Publicly effective target group oriented science communication	Key figure documentation & communication for events, visitor numbers, press releases, interviews, research infrastructures, dialogue formats (e.g. Leibniz Fragt, Leibniz im Bundestag, Lange Nacht der Wissenschaften), social media, lectures, poster presentations
Acquisition of third-party funds	90 T€ per FTE (scientists, incl. scholarship holders & guests, without PhD students) Importance of the research goal and chances of realization of the project
Networking and cooperation	Key figure documentation & communication
Reconciliation of work and caring responsibilities. Compliance with gender equity including anti-discrimination	Equality plan[14]

5.1.1 QUALITY ASSURANCE THROUGH COMMITTEES

The ***Scientific & Industrial Advisory Board (WIB)*** is, as in all Leibniz Institutes, an important review body, which accompanies the work of LIKAT intensively and critically. The *WIB* consists of at least six members who are not employees of the Institute (Statutes §11(1), Annex 1.3). They are appointed for four years by the *Board of Trustees* on the joint proposal of the *Board* and the *WIB*. The composition of the *WIB* reflects the fields of work of the Institute. The members of the *Advisory Board* have proven expertise in the relevant catalysis disciplines. In September 2022, the *Advisory Board* will comprise a total of ten members, including representatives from industry, universities and other research institutions. The Chair reports to the *Board of Trustees* and the *General Assembly* on the recommendations of the *Advisory Board*.

In 2021, the *Scientific Advisory Board* was renamed the *Science & Industry Advisory Board*. The name more accurately reflects the composition and expertise of the advisory board, which is highly relevant with regard to the transfer work at LIKAT, especially with future pilots in the *Catalysis2Scale* transfer

14 Equality Plan (catalysis.de)

technical center. As an advisory body, the *advisory board* is independent, regularly evaluates LIKAT's scientific performance, research program and program budget, and makes recommendations. In addition, audits play a central role, evaluating not only scientific quality but also strategic development.

The ***Board of Trustees*** is an effective body for ensuring the highest quality research at the Institute. The *Board of Trustees* consists of at least six members, currently (September 2022) nine, representing the federal government, the state of Mecklenburg-Vorpommern, the University of Ros-tock, the private sector, and the scientific community. The board is responsible for the supervision of all essential scientific and economic questions of the institute (statute §8(1)). It determines the guidelines of the Institute's work and supervises the activities of the *Board*. The *Board of Trustees* decides, among other things, on the program budget and medium-term financial planning, the principles for monitoring the success and implementation strategies of the research results, and, in consultation with the *Scientific & Industrial Advisory Board*, the research fields to be worked on and the corresponding work plans.

5.1.2 INTERNAL QUALITY ASSURANCE

The orientation of the research activities at LIKAT are continuously, at least once a year, internally evaluated by the *Board*, the *General Assembly* or the *Scientific & Industrial Advisory Board*. The following performance criteria are used for the assessment of the research results: Scientific quality and efficiency (number and impact factor) of publications, patent applications, invited lectures, acquisition of third-party funding, strategic fit and realization chances of projects, networking and cooperations, promotion of young scientists, teaching, congresses, workshops, expert opinions, external activities, economic applications, support of the compatibility of job and family, and compliance with gender equality and anti-discrimination. Regular monitoring of these criteria ensures the high quality of the research. Particularly successful topics can receive performance-related support through the allocation of central funds.

5.1.3 GOOD SCIENTIFIC PRACTICE

Good scientific practice (GwP) is a system of rules that serves to ensure quality in research. This system contains basic principles that are the same in all countries and scientific disciplines and thus represent ethical standards and the foundations of scientific professionalism. It is based, first and foremost, on honesty towards oneself and others. Violations of the rules of the GwP are scientific misconduct, which will also be punished at LIKAT. The DFG and the major scientific organizations, including the Leibniz Association, have issued recommendations on GwP and on how to deal with scientific misconduct. In accordance with these recommendations, LIKAT has already developed its own set of rules on GwP (Annex 4) since June 2011, which takes into account the specific characteristics and needs of the institute and is binding for all institute members. Compliance with the rules of good scientific practice is ensured at LIKAT by an ombudsperson. In 2019, the last election of the ombudsperson and her deputy took place for a period of four years.

5.1.4 PUBLICATION- & OPEN ACCESS-GUIDELINE

LIKAT has its own guideline for dealing with publications & open access (Annex 3). Against the background of steadily increasing numbers of scientific publications, our main concern is to increase the quality, visibility and influence of publications. Prerequisites for this are a high relevance and quality of the research results, reputation and quality of the publication medium as well as open access (OpenAccess). The LIKAT guideline defines clear goals in this regard, including the publication of >50% of all journal articles in international journals with a high impact factor (>5) and making at least 25% of all journal articles accessible via OpenAccess. In doing so, it points out so-called fake journals and predatory publishing, gives hints and recommendations on different types of OpenAccess as well as on the

participation in transformation contracts, e.g. DEAL. LIKAT encourages its scientists to apply for external funding for OpenAccess publications when applying for projects. In its guidelines, LIKAT defines relevant quality criteria for evaluating publication performance. This guideline is documented and communicated monthly in the management meeting and on the intranet for all employees. LIKAT lists books, book chapters and journal articles in its publication list. Journal articles that have undergone a *peer review* process are identified as such.

5.1.5 ALLOCATION OF FUNDS AS A CONTROL ELEMENT

A more performance-oriented allocation of funds has been introduced at the Institute: The program budget forms the binding basis for the management of funds at the Institute. It has the character of a target agreement, in which guiding, performance and structural targets are agreed upon. In order to carry out scientific work, the following resources are made available to the research areas via different funds on a performance-oriented basis (depending on the nature of the fund as investment, personnel and/or material resources):

- *Investment Fund:* For the allocation of the total investment funds (approx. € 1 million p.a.), the individual research groups submit applications once or twice a year (in urgent cases also unscheduled), which are discussed and decided upon by the Board.
- *Departmental Fund:* The fund is established on the basis of the FTEs financed by the budget and is freely available to the corresponding research groups. In the event of justified additional requirements, the budget is adjusted by the Board.
- *Innovation Fund:* Funds are also available to support basic research and to establish new innovative fields of work. The individual research groups apply annually.
- *LIKAT Community Fund: T*he fund is used to cover temporary employment contracts during pregnancy, parental leave or care for dependents, or in cases of particular social hardship (see p. 35).

5.1.6 QUALITY MANAGEMENT OF RESEARCH INFRASTRUCTURES

The *operando* measurement techniques developed over many years in the research department *Catalytic in situ Studies* (Head: Angelika Brückner) are research infra-structures assigned to *Topic 01*. They are used throughout the institute and in cooperation with other institutions in Germany and abroad. This involves the simultaneous coupling of several *operando* techniques in the same experiment, for which LIKAT has developed highly complex apparatus over many years, providing comprehensive knowledge of the relationship between the structure and mode of action of catalysts. These *operando* techniques belong to the core competences of the research department *Catalytic in situ Studies*, are based on its long-standing expertise and are documented by numerous publications in high-ranking peer-reviewed journals. In addition, there are clear measures for quality management of the infrastructure:

- Selection procedure at LIKAT for the use of the infrastructure: review and preliminary discussion of the project by the research department and research group heads, e.g. in the context of joint projects, adjustments, coordination and advice if necessary,
- Use of the infrastructure and evaluation of the research data received are carried out exclusively by highly qualified personnel,
- Research work is subject to the LIKAT rules of good scientific practice.

5.1.7 RESEARCH DATA MANAGEMENT & OPEN DATA

Different catalysis expertise, reaction engineering and data science are represented in LIKAT. Based on experience in data management in heterogeneous catalysis, the challenges of cross-disciplinary research data management are addressed, solutions are tested on a local level and introduced into net-

works, such as *NFDI4Cat* (p. 11). LIKAT is currently working on various fields of catalysis research as a benchmark: classical heterogeneously catalyzed processes, homogeneously catalyzed hydrogenations and carbonylations, and photocatalytic reactions. The integration of the various catalysis disciplines and the associated analytical methods is considered the greatest challenge of digitization. Currently, an *Electronic Lab Notebook/Laboratory Information Management System (ELN/LIMS)* is being evaluated, which will be iteratively optimized and extended in the coming years. The experience gained within LIKAT will be incorporated into *NFDI4Cat* in order to integrate data from all sub-disciplines of catalysis research and to develop common concepts, vocabularies and ontologies on this basis. In this way, integrated data sets will be created that will enable further data-based research approaches and will generate considerable added value for the institute in the future.

5.2 COOPERATIVE RELATIONSHIPS WITH THIRD PARTIES

Every year, LIKAT works on about 100 publicly and privately funded third-party projects. In order to keep these contractual relationships, which vary in type and scope, manageable and controllable with reasonable effort, the institute has model contracts that contribute to favorable framework conditions and create freedom for science. In addition to the scientific review criteria for research cooperations and third-party funded projects, the administrative structure of cooperative relationships with third parties is also clearly regulated:

- Contract design and project management are controlled and accompanied by the service department of administration,
- Contractual assurance of the project-related full costs at standard market conditions,
- Patenting and transfer of project results are to be contractually secured in accordance with LIKAT's transfer guideline; contractual arrangements that entail the gratuitous use of research results are excluded,
- The publication of project results must be contractually secured in accordance with LIKAT's publication and open access guidelines,
- Contractual agreements with third parties concern LIKAT as a whole and follow the rules of good scientific practice.

The institute strives to maintain a balanced relationship between public and private third-party funding while maintaining a high level of scientific quality. The increasing complexity of research and societal challenges makes large collaborative projects increasingly necessary. National and international cooperations are therefore of great importance. The large number of industrial projects, which on the one hand represent a criterion of success for LIKAT, and on the other hand often have a duration of only one year, make the institute dependent on short-term project research. To counter this, we rely on long-term framework agreements and on the diversification of industrial funds.

5.3 TRANSFER

5.3.1 KNOWLEDGE & TECHNOLOGY TRANSFER AT LIKAT

LIKAT understands knowledge and technology transfer (KTT) as all activities that serve to process scientific findings and technologies in a target group-oriented manner and to transfer them to the non-academic world. At the same time, the dialogue with society, politics and industry enables the adaptation of own research to societal problems. The target groups of the KTT at LIKAT include actors from the economy, municipal and regional initiatives, regional and supra-regional transfer-relevant networks (e.g. alumni, see p. 11), politicians at various levels (municipal, state, federal), the level of policy preparation, ministries, the media, interested members of the public, students and schoolchildren.

Infobox - Transfer at LIKAT

A transfer (Überführung) is defined as the transfer of a process from laboratory scale in the chemical or pharmaceutical industry or other relevant branches of industry to pilot scale, small-scale production or large-scale production with the aid of a catalyst developed at LIKAT. If LIKAT scientists are actively involved in the process design in a pilot or multi-100 kg plant via a scientific project, this is also defined as a transfer; the same applies to the development/design of prototypes.

With regard to **technology transfer**, the LIKAT guideline (Annex 2) formulates the transfer of at least three catalysts or catalytic processes to industrial pilot scale per year as a concrete goal for the employees of the institute. In this context, the *Catalysis2Scale* transfer technical center plant plays a central role (see p 23)pr. Cooperations with industry players are an essential part of the research work at LIKAT. As a rule, the results of such cooperative projects are initially patented throughout Europe. In order to benefit from the expertise and infrastructure of the partners and to be able to transfer research results quickly, the patents are preferably filed jointly with the industrial partners. Individual advice on questions of intellectual property rights is provided by the transfer officer. In the context of **knowledge transfer**, it is important to ensure the transfer of knowledge to the public, to provide a scientifically sound basis for decision-making, and at the same time to create an awareness of the scientific process and the sense and social benefits of investing in research. The focus of LIKAT's science communication and public relations work is on socially relevant issues, e.g. the application of catalysis in the environmental, energy or health sectors, in a target group-oriented manner and in appropriate formats. This is supported, for example, by articles that are not subject to the *peer-review* process, by the training or supervision of qualification work of students, doctoral and post-doctoral researchers at LIKAT, and by employees of the institute who belong to various external bodies and committees. In addition, there is the institute's website (catalysis.de), press relations (press releases and interviews), selected social media and portals (*Twitter, LinkedIn*), LIKAT's biennial report and the biannual journal *Leibniz-Nordost*, which is published by the four Leibniz institutes in MV and the *Research Institute for Farm Animal Biology (FBN)* and presents current socially relevant research work of the institutes in a popular scientific way. LIKAT also regularly participates in series of events for the public, e.g. *Open Science Night, Rostocks Eleven, Girls Day, Virtual LabDay, Leibniz Asks, Leibniz in the Bundestag* and *Leibniz Book a Scientist*. We offer guided tours of the institutes, internships for school students and participate in the *Jugend forscht* competition with a special prize. The success of the transfer work at LIKAT is monitored by traceable and evaluable quantitative **indicators**, which are recorded and communicated. These include the number of collaborative projects with industry, transfers, patents and intellectual property rights, events and visitor numbers, radio and television interviews, international collaborations, publications outside the *peer review* process, press releases, and our media response (print, online, radio, television) and Twitter (tweets and reach). The development of qualitative indicators for the evaluation of KTT at LIKAT is planned. The prerequisite for this is a reasonable effort of the survey in relation to human and monetary resources, accompanied by the statutory research mandate.

6. STRATEGIC PERSONNEL DEVELOPMENTS

Only with well-trained and motivated employees can the Leibniz Institute for Catalysis fulfill its statutory mission and make an active contribution to solving the challenges facing society as a whole. In order to attract researchers from all over the world, the institute aims to offer not only excellent research conditions but also a prudent human resources strategy with effective framework conditions that promote science. Among other things, it is involved in the regional network [Rostock thinks 365°] together with the University of Rostock, non-university research institutes, the Hanseatic City of Rostock and other stakeholders to jointly market Rostock as a science location and to develop a genuine welcoming culture for international researchers.

6.1 SCIENTIFIC & ADMINISTRATIVE MANAGEMENT POSITIONS

In the international competition for top-class scientists, working conditions, employment prospects and personnel development measures play an important role. The recruitment of qualified personnel on the basis of earning opportunities in accordance with the TV-L and the new professors' pay scale is proving difficult despite very good working and research conditions. LIKAT makes use of any leeway that these possibilities allow. In addition, we would like to offer all employees resilient occupational perspectives and the best possible conditions for individual life and career planning, taking into account the compatibility of work and welfare obligations. The corresponding measures include:

- Filling senior scientific positions in conjunction with professorships at the University of Rostock via joint appointments (in accordance with the cooperation agreement),
- Support of dual career couples,
- Support for new international employees in dealing with authorities, childcare, enrollment, etc.

The standards of the Leibniz Association are binding for the appointment of **scientific and administrative management positions** at LIKAT.[15] The appointment of board members is the responsibility of the *Board of Trustees* of LIKAT (Statutes §8(2e)), which is therefore involved in the selection process at an early stage. In addition, the *Scientific & Industrial Advisory Board* and the *General Assembly* are involved in the selection process when filling scientific positions at the *Board* and heads of research department level. In this way, the broad professional expertise, the many years of experience and, last but not least, the networks of experts in the fields of science, industry, science management and public administration are used for the benefit of the strategic further development of the Institute. The positions are advertised in accordance with the present research strategy and filled by the applicant with the best possible qualifications (internal or external). The selection is made by a search committee. The procedure always follows clear and transparent rules:

- public, international advertisement in national and international print and electronic media, journals such as Nature and Science as well as international job portals,
- direct search through targeted approach of candidates in Germany and abroad, invitation to scientific presentations at LIKAT,
- clear description of the expected scientific profile and other key qualifications (acquisition of third-party funding, networking, etc.),
- complete documentation of the entire procedure for the purpose of transparency and quality assurance.

15 Standards for filling scientific management positions in the Leibniz Association, **2016**; Standards for filling administrative management positions in the Leibniz Association, **2018**.

Leading positions in connection with a professorship are filled in joint consultation procedures with the University of Rostock (see also p. 8).

In general, targeted subject-specific external recruitment is sought for management positions. However, the retention of key technologies and expertise is essential for the further positive development of LIKAT. For this reason, the heads of the corresponding research groups is partly secured by internal personnel development. Such positions are initially filled for two years on a temporary basis. After a positive internal evaluation, the position will be made permanent.

6.2 EQUAL OPPORTUNITIES & GENDER EQUALITY

LIKAT explicitly acknowledges its responsibility to actively promote equal opportunities and gender equality and has anchored this in its statutes in 2012 (§2(4)). In this context, equality does not only mean enabling equal opportunities for the sexes, but also the achievement of gender balance through binding rules and measures that are clearly formulated in the equality plan[16] regularly reviewed and, if necessary, adjusted. The overarching goal is to increase the proportion of women in areas where women are underrepresented and to improve training and working conditions for all employees with caring responsibilities. The goals and measures for gender equality drawn up by the Institute's management in cooperation with the Equal Opportunities Officer and her representatives are based on the statistical data collection and evaluation of LIKAT's employee structure. The equal opportunity representative and her deputy have been elected at LIKAT every four years since 2006.

LIKAT strives to increase the proportion of women, especially at the middle leading levels. In this context, the cascade model is a key steering element: In 2019, LIKAT again committed to setting flexible target quotas for the proportion of women at each level by 2025 in line with the cascade model of the DFG's research-oriented equality standards (Table 1). The targets agreed upon there provide for ambitious increases in the proportion of female management personnel at the institute, since the majority of positions that become vacant are filled by women. Only by filling these positions with female staff will it be possible to maintain the current quotas. LIKAT also sees it as a major challenge to maintain the quotas achieved at board level.

16 https://www.catalysis.de/fileadmin/user_upload/MAIN-dateien/2021_1221_Gleichstellungsplan_LIKAT_2022-2025_dt.pdf

Table 1. LIKAT cascade model (as of 2019)-formulated flexible target rates by 2025 according to pay levels or management levels.

Pay grades	Women's quota 31.12.2019	Target quota 2025	Forecast of positions that can be filled by 2025 (as of 2019)
Level 5: W3/C4	0%	0%	0
Level 4: W2/C3	66%	66%	1
Level 3: E15/W1	13%	25%	2
Level 2: E14	18%	19%	6
Level 1: E13	31%	35%	40
Management levels			
1st level: Executive Board	60%	60%	2 (currently women)
2nd level: Division management	22%	22%	1 (currently women)
3rd level: topic management, junior research groups, coordinators & staff management	31%	35%	40

The measures laid down in the Equal Opportunity Plan to achieve this goal cover various aspects, including recruitment procedures from job advertisement to selection as well as personnel development and recruitment, e.g. measures to train future female leading persons within LIKAT, active recruitment of external female scientists. LIKAT continues to promote the professional development of women on various levels with a focus on the promotion of employees and doctoral candidates. LIKAT does not have special support programs for female habilitation candidates and professors. However, as a Leibniz Institute and affiliated institute of the University of Rostock, which was again awarded the *audit familiengerechte hochschule* certificate in 2019, LIKAT has an excellent infrastructure for support programs at its disposal. Measures taken by LIKAT to reconcile work and caring responsibilities include the LIKAT company agreement on the regulation of flexible working hours, which serves to make working hours at LIKAT more flexible, *dual-career* measures and the LIKAT *Community Fund* (see infobox).

Infobox – LIKAT-Community Fund

The LIKAT-Community-Fund is an established instrument for the protection of employees in temporary employment during pregnancy, parental or nursing leave or in cases of special social hardship. It is an integral part of the institute's budget and offers employees and scholarship holders planning security and binds them more closely to the institute than before.

The success of gender equality work at LIKAT is constantly monitored. Gender-specific statistics are compiled and communicated at least once a year. In the regular evaluations by the Leibniz Association, the status of the gender equality measures, among other things, is a key factor in determining whether the institute remains in the Association and thus whether it receives further funding. In addition, LIKAT is subject to an external audit by the TEQ certificate.[17] In 2020, LIKAT received the certificate for the fourth time in a row. In the future, it will be necessary to further expand the aspects of diversity.

LIKAT would like to make excellent women at LIKAT visible and create new role models. For many years, LIKAT has been taking various measures to awaken and promote the interest of schoolgirls and girls in the natural sciences. These include guided tours for school classes, internships for school students, support for *Jugend forscht*, including the awarding of a special prize, the institute's participation in the annual Rostock *Open Science Night* and *Girls Day*.

17 https://www.total-e-quality.de/

6.3 DOCTORAL & POST-DOCTORAL STAFF

Fundamental for an excellent education at LIKAT is the *Leibniz Guideline Career Development*.[18] Targets and procedures tailored to the institute are summarized in the binding *guideline for the promotion of young scientists at LIKAT* (Annex 5). The guideline addresses doctoral students and staff with a doctorate, i.e. postdocs and staff aiming at a qualification in the form of a habilitation, and regulates relevant topics such as employment relationships, structured career paths, good scientific supervision and support measures.

The Leibniz Institute for Catalysis, like all non-university research institutions, does not have its own doctoral or habilitation rights.[19] Qualification measures for young scientists are carried out in cooperation with the University of Rostock. The doctoral and habilitation regulations of the Faculty of Mathematics and Natural Sciences of the University of Rostock are authoritative. For the communication with the University of Rostock and for advising the students, LIKAT appoints a doctoral representative. The interests of the PhD students and PostDocs are safeguarded and represented at LIKAT by the annually elected PhD & PostDoc representation, which usually consists of three persons.

The quality assurance of the training of young scientists is a central concern of LIKAT. In the course of the new strategic orientation of research at LIKAT, the promotion of young scientists aims at a thematic and personal diversification. Young scientists should be encouraged to engage in international and interdisciplinary exchange and supported in building up networks. The conditions at the institute are ideal for implementing both basic research and application-oriented projects. Thus, the future alumni can optimally prepare for a career in business or science. The promotion and qualification of young scientists at LIKAT serves on the one hand the LIKAT-internal junior staff and on the other hand an international scientific career of the LIKAT graduates.

LIKAT accompanies the career paths of its graduates beyond the promotion. As already mentioned, our main concern is to work on application-related projects in bilateral cooperations with industry or in interdisciplinary publicly funded joint projects, such as the *Leibniz ScienceCampi Phosphorus Research Rostock* or *ComBioCat*. In this way, future alumni can build up a network at an early stage and optimally prepare for a career in industry or science. This is supported by the ***LIKAT alumni network*** (p. 11), which has been established and intensively maintained at the institute over the past years.

6.4 SCIENCE SUPPORT STAFF

A prerequisite for excellence in research, including at LIKAT, is a well-trained and motivated workforce, both in the scientific and in the science support areas. Especially against this background, LIKAT strives for very good working conditions and professional perspectives for employees in the science-supporting areas.

6.4.1 PROFESSIONAL QUALIFICATION OF SCIENCE SUPPORT STAFF

The Institute supports all individual qualification efforts of employees in the science-supporting areas, if the planned qualification is to be regarded as further training in the overriding interest of the Institute and the work processes in the Institute remain unaffected. In individual further education agreements, financial framework conditions (participation of LIKAT in the costs of 50 to 100%, depending on the type and scope of the training) as well as release and further education phases are contractually secured. The spectrum of supported qualification measures ranges from courses in the IT and secretarial

18 Leibniz- Guideline Career Development, **2020**.

19 https://www.mathnat.uni-rostock.de/studium/promotion-habilitation/promotion, https://www.mathnat.uni-rostock.de/studium/promotion-habilitation/habilitation

fields to the acquisition of a trainer's certificate or master craftsman training to distance learning. LIKAT itself organizes further training in the linguistic field (e.g. English courses for employees in the service departments) or courses that are necessary for dealing with new software programs. Depending on their needs, colleagues are given time and financial support to attend courses offered by the University of Rostock or the Fraunhofer Institute for Computer Graphics in Rostock.

6.4.2 TRAINEES

In order to be able to work at a high level in a future-oriented manner, it is essential to recruit very good specialists also in the science-supporting area and to bind them to LIKAT. According to the principle of the Leibniz Association *x plus 1*, LIKAT trains together with the University of Rostock in a joint training program for chemical laboratory assistants. The joint training initiative was anchored by an extension of the cooperation agreement between LIKAT and the University of Rostock, which has been in place since 2006. The dual training of chemical laboratory assistants is carried out in close cooperation with the vocational school, the educational institutions, the Rostock Chamber of Industry and Commerce and the local Federal Employment Agency. The training takes place in the laboratories of LIKAT and the chemistry department of the University of Rostock. Both partners, LIKAT and the University of Rostock, are, depending on the financial situation, striving to offer their trainees employment after they have completed their vocational training.

In order to enable more young people to get an apprenticeship and to prevent a lack of skilled workers in all science supporting service areas established at LIKAT, LIKAT offers apprenticeships in its service areas technology and administration. The training takes place according to demand in order to be able to offer employment after completion of the training.

7. CHALLENGES, GOALS & MEASURES

7.1 STRENGTHS, WEAKNESSES, OPPORTUNITIES & THREATS

In the course of strategy development, a so-called SWOT analysis was conducted, summarizing strengths & weaknesses as well as risks & opportunities for LIKAT in the coming years (Figure 9). LIKAT's **strengths** include our reputation and visibility, our expertise and research metrics, our staff, and our networks and international collaborations.

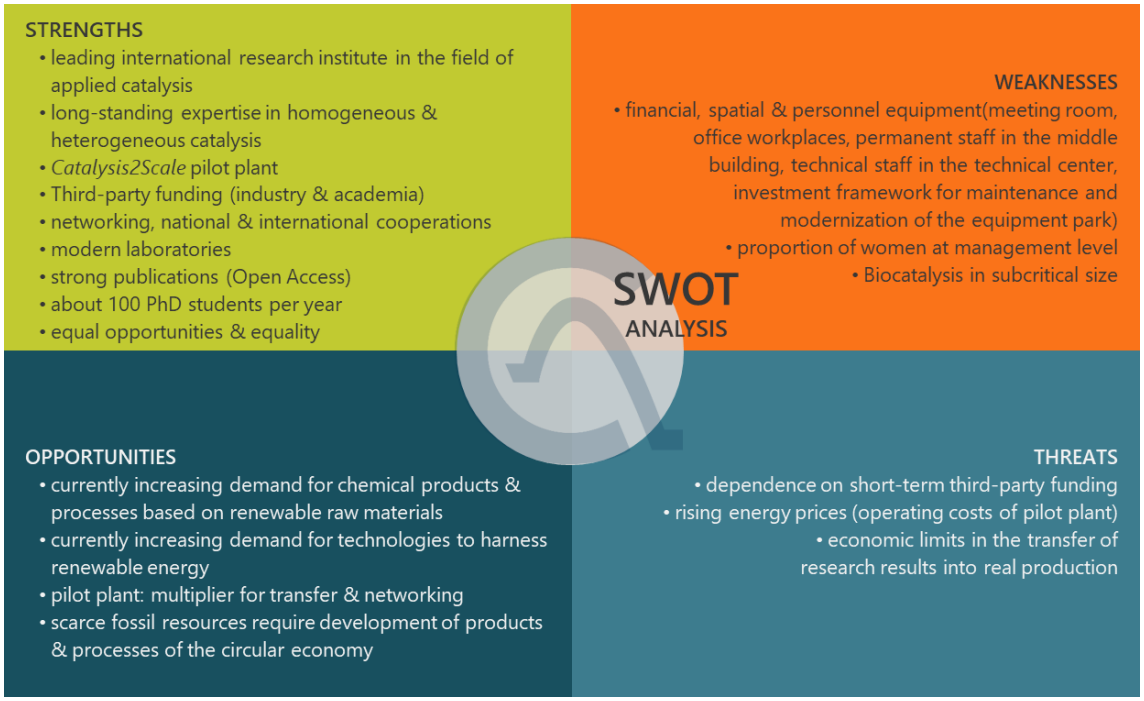


Figure 9. SWOT analysis of the Leibniz Institute for Catalysis (Status: 2021).

Our greatest challenge in the coming years is to maintain our position as a world-leading institution in the field of catalysis, to develop it effectively, and thus to remain competitive in the future. An essential prerequisite for this is high-quality, relevant and innovative catalysis research. We set ourselves ambitious goals for this:

- high scientific output: >2.3 publications per FTE in science and year (including all PhD students and postdocs),
- High quality and visibility of the scientific output: >50% of the annual LIKAT publications in influential journals (IF>5) and >25% in *peer-reviewed* open access journals,
- High third-party funding: >90 T€ per FTE in science and year (incl. scholarship holders and guests; PhD students excluded),
- increase total third-party funding from DFG and EU grants to 30% of the total third-party funding budget,
- Increase transfer services through own technical center: at least three transfers of research results to pilot or industrial scale per year,
- Expansion of structured and transparent career planning for doctoral and post-doctoral students,
- Equal opportunities and equality: Expansion of institutionalized measures (e.g. for reconciling work and care obligations) with regard to anti-discrimination and diversity.

On the research side, the overall objective of LIKAT is to promote the closure of cycle flows of chemical and catalytic processes and products (*4.1OVERALL SCIENTIFIC CONCEPT OF* THE LIKAT). For this pur-

pose, expertise and methods of the entire institute are made available. Important strategic decisions have already been made, such as the establishment of the matrix structure for cross-disciplinary activities with the best possible energy effects or the construction of the institute's own *Catalysis2Scale* transfer technical center. This presents opportunities and risks in equal measure.

On the side of **opportunities**, with fossil resources in short supply, there is a clear need for research into greenhouse gas neutrality and the closing of cycles in sectors relevant to chemistry and catalysis. Currently, the demand for chemical products and processes based on renewable raw materials and technologies for the utilization of renewable energy is increasing. The completed technical center allows increased cooperation with the private sector of the chemical industry and especially with SMEs.

The **threats** associated with the strategic goal relate to dependence on short-term third-party funding. Public third-party funded projects usually have a duration of three, ideally four years. Collaborations with the private sector are much shorter-term, usually one year or even only a few months. The development of alternative technologies and their conversion from existing processes designed on a fossil resource infrastructure requires at least 10 to 15 years, as well as intensive long-term research and development and corresponding long-term investment.[11] Moreover, such conversions can only take effect if they are economically viable. There is thus a risk that limits will arise in the transfer of research results to real production.

LIKAT counters these risks with the following measures:

- Increased research coordination, identification and application for long-term public collaborative projects that allow researchers the necessary time freedom, e.g. *NFDI4cat* (p. 11), *Research Factory* (p. 11),
- long-term framework agreements with the private sector,
- medium-term selective strengthening of research activities through the establishment of junior research groups, potential areas of work are Renewable Resources, Catalysis & Energy and possibly Biocatalysis for Material Cycles.

4. , p. 13) highly qualified and motivated staff with a high level of commitment is required to implement the research projects. At the same time, suitable framework conditions, i.e. the financial, spatial and instrumental equipment of LIKAT, form the necessary foundation to be able to meet the growing scientific and organizational requirements. In this context, the Institute is critical of the adequacy of the material and personnel resources on the basis of the resources promised by the funding agencies ("medium-term financial planning") for the years 2023 to 2026 and thus sees this as a **weakness**.

In the following it is explained from the point of view of the institute that for the realization of the strategic work planning an increase of the budget becomes necessary particularly with regard to the infrastructure and the basic financed personnel master for institute-spreading tasks.

7.1.1 THE FINANCIAL ENDOWMENT

As an institute of the Leibniz Association, LIKAT is financed equally by the federal and state governments. The Ministry of Science, Culture, Federal and European Affairs (WKM MV) is responsible for the funding of LIKAT in Mecklenburg-Vorpommern, while the Federal Ministry of Education and Research (BMBF) is responsible for the funding of LIKAT in Germany. The institute had a total budget of 27 million € in 2021. This includes, among other things, institutional funding, third-party funding and the funds for the construction of the *Catalysis2Scale* transfer technical center (€ 5.0 million).

The broad research orientation of LIKAT, knowledge-oriented basic research and research approaches up to application, will continue to be the mission in the future. However, it can only be fulfilled if the institute attracts extensive public and industrial third-party funding in addition to the basic funding from the federal and state governments. In 2021, the total of third-party funds amounted to € 8.16 million and thus 39% of the total budget. This means the acquisition of 89.6 T€ per scientific FTE (91.05 FTE, incl. scholarship holders, stipendiates and guests; however, doctoral students are excluded from this). We are aware of the current critical situation. For example, the BMBF website states that "*Although the amount of the BMBF's total budget for 2023 is increasing compared to 2022. Nevertheless, the financial leeway is limited, for example, by the debt brake or the financing of security and energy policy measures in connection with Russia's attack on Ukraine.*"[20] Regardless of this, we are increasing our previous target of 70 T€ to 90 T€ per FTE (including fellows and guests; excluding PhD students). This is because research on closing circular flows with the help of the technical center as a core element of the *LIKAT 2030 strategy* is indispensable. Third-party funding is particularly strong in the area of bilateral cooperation with industry, which is directly linked to transfer to society (2021: 33% of all third-party funding). With the availability of LIKAT's own technical center, it is a clear goal to sustainably increase the share of funding from industry to 50% of the total third-party budget by 2030. In the area of public project funding, the last evaluation in February 2016 formulated the goal of increasing the sum of third-party funding from DFG and EU grants to 25% of the total thirdparty budget. This share was 25% in 2021 and is to be increased to 30% in the future.

The existing budget is just sufficient for the immediate maintenance of LIKAT research, but not for the modernization and implementation of new research fields. According to our estimation, investments of at least 2 million € will be necessary in the following years, especially for the establishment of *Topic 03 Reaction Engineering & Implementation* using the technical center. The current price increases for electricity and district heating far exceed the financial possibilities of the institute.

20 The BMBF budget: What will change in 2023? - BMBF

The strategic measures of LIKAT to secure its financial resources include:

- Application for a *Small Strategic Institute Expansion* for the sustainable, widely self-sufficient use of the *Catalysis2Scale Transfer Technical Center* in January 2023: for detailed information, see *4.9Strategy Catalysis2Scale-Transfer technical Center*, p. 23).
- Energy saving measures: In mid-2022, the *Board* decided to identify effective energy-saving measures. Significant savings potential has the reduction of the ventilation or the refrigeration systems of the LIKAT houses under strict consideration of occupational safety due to the time-restricted access to the laboratories (Monday-Friday from 07:00 to 20:00 and Saturday from 08:00 to 18:00). The measures will be regularly reviewed in the future and adjusted if necessary.

7.1.2 THE SPATIAL & APPARATIVE EQUIPMENT

The Leibniz Institute for Catalysis is located in Rostock on the Südstadt-Campus of the University of Rostock in close proximity to the institutes for chemistry, physics and biology as well as the engineering sciences and the computer center. As explained in section *2.2* (p. 3) the institute has been successively expanded structurally since 2005. The latest addition is the completion of the technical center in mid-2022, which currently provides researchers with approx. 3,150 m^2 of laboratory space.

The laboratories were each equipped to the latest technical standards and their equipment corresponds to that of a modern research institute. Very limited construction funds for all four construction phases always made it necessary to focus on well-equipped scientific workplaces in the sense of operational research. In contrast, the number of available office workstations is insufficient and a meeting and lecture room of appropriate size is missing. Currently, LIKAT has a seminar room with an area of about 115 m^2, which allows seating for a maximum of 100 people when used for lectures. With approx. 300 employees, there are no rooms available for full meetings.

Table 2. Devices of the Analytics service area at LIKAT (as of 07/2022).

Methode	Geräte	Anschaffung
NMR (Hochauflösung)	3 (Bruker)	3 x 2017
MS	2 (Thermo Finnigan MAT, Waters)	2005, 2018
GC-MS	2 (Agilent)	2018, 2022
LC-MS	1 (Agilent)	2014
GC	7 (Agilent)	2000-2020
HPLC	2 (Agilent) 1 GPC (Agilent/PSS)	2007, 2013 2016
Röntgendiffrakto-metrie	2 Einkristall (STOE, Bruker) 3 Pulver (STOE, Panalytical)	2005-2011 1995-2015
Elektronen-spektroskopie	1 XPS (Thermo VG) 1 NAP-XPS (SPECS)	2013 (Modernisierung) 2020
Elektronenmikro-skopie	1 TEM (JEOL) dazu: EDX-Spektrometer (JEOL) dazu: EELS-Spektrometer (Gatan)	2010 2020 2016
IR	1 (Bruker)	2007
Kapillarelektrophorese	1 (Agilent)	2014
UV/CD-ORD	3 (Perkin-Elmer, Jasco)	1992-1994
Elementaranalyse	1 CHNS (Leco) 1 AAS (Analytik Jena) 1 ICP-OES (Varian) 1 RFA (Panalytical)	2007 2018 2009 2019

Competitive catalysis research requires both adequate equipment (e.g. continuous and pressure apparatus, gloveboxes, in-house developed equipment for *operando* spectroscopy and kinetic investigations) and the corresponding large-scale analytical equipment. In the research laboratories and in the analytical service department (Table 2), the institute has (still) modern equipment and the equipment of the institute is predominantly very good to excellent. However, most of this equipment, which is in the six- to seven-figure price segment, will need to be replaced in the short and medium term in order to meet the high technical requirements in the future. Due to the very different working directions of the research departments, the equipment stock of the service department must meet the requirements of molecular chemistry synthesis labor-

atories as well as those of solid state and surface characterization. In the market, support and service for instruments ten years old and older are often reduced or discontinued altogether. Replacement purchases can hardly be financed from the normal investment budget. In the near future, this will affect a mass spectrometer and an X-ray diffractometer, and in the medium term also an electron microscope.

The **Information Technology (IT)** team ensures the complete digital infrastructure in the institut. In addition to standard tasks and common network services, this also includes the management of the intranet. This is tailored, among other things, to archiving measurement data from the analytical instruments and making it transparently available to users for further processing and evaluation. Due to continuous investments in recent years, the institute is well positioned in the service-oriented provision of IT services for science and the service areas with regard to hardware and software. Since the last evaluation, the IT department of LIKAT has been increased in staff from three to four FTE IT specialists for about 300 employees and guests. In almost all areas of LIKAT, productive work is only possible with reliably provided IT services. In recent years, steadily growing requirements have been added, which include the provision of new IT services for data protection, digitization of research and administrative data, and support for specific, individual IT projects. At the same time, the significantly tightened threat situation in all areas of IT security has significantly increased the effort required to secure IT services and adapt to constantly changing attack scenarios. Continuous efforts have been and are being made to expand and adapt the required high security level of the IT infrastructure in the environment of scientific and industrial projects. To ensure the highest possible level of security, IT has developed a security concept that is constantly reviewed for necessary updates. Since the beginning of 2020, IT has faced additional challenges in the wake of the Corona pandemic. Where possible and desired, colleagues were enabled to work on the move. The technical requirements for this already existed, but required more intensive support during this period. In addition, IT staff provided advice on virtual and hybrid events. In cooperation with the technology service department, the LIKAT seminar room was equipped with the necessary technology.

With 10 FTEs, the technical service department bundles the building services, the workshops and the glassblowing shop. The building services include, for example, the ventilation systems of the LIKAT buildings, which are indispensable for occupational safety, maintenance of the fume hoods and fire protection. The tasks of the workshops include routine repairs and maintenance as well as precision mechanical or welding work and the construction of special apparatus. The in-house glassblowing workshop produces, in addition to small routine repairs, mainly various highly specialized glass devices and glass parts for laboratory equipment in direct consultation with the scientists.

LIKAT takes the following strategic measures to secure the equipment:

- concrete investment planning with prioritized requests, which are decided by the board of directors,
- Consideration of the required investments with prioritization in favor of the large-scale equipment and infrastructures of the service departments analytics, IT and technics used by the entire institute (e.g. replacement of some equipment of the service area analytics, such as gas chromatographs, X-ray fluorescence analyzer, by models of the latest generation, investment in the acquisition of an SEM located at LIKAT),
- Cooperation with the University of Rostock and acquisition of third-party funds within the framework of suitable funding programs (e.g. joint acquisition by the University of Rostock and LIKAT of a new high-performance electron microscope within the framework of the DFG's large-scale equipment program, with location at the Interdisciplinary Faculty of the University,

acquisition of EU funds by LIKAT for a near ambient pressure photoelectron spectrometer (NAP-XPS - Near Ambient Pressure X-ray Photoelectron Spectroscopy) with location at LIKAT,

» Application for a Small Strategic Institute Extension for the sustainable, largely self-sufficient use of the *Catalysis2Scale Transfer Technical Center* in January 2023: for detailed information see *4.9Strategy Catalysis2Scale-Transfer technical Center*, p. 23).p

7.1.3 PERSONNEL

For a long time, high temporary employment rates in the science sector were regarded by politicians and society as a guarantee of innovative strength. In addition, the reputation of a scientific institution was and is strongly influenced by the amount of third-party funding it receives. The result is a very high proportion of temporary employees. The legal basis for their employment is the Wissenschaftszeitvertragsgesetz (German Act on Temporary Scientific Contracts) and the Teilzeit- und Befristungsgesetz (German Act on Part-Time Employment and Fixed-Term Contracts). In our view, fixed-term employment contracts should be limited primarily to doctoral students, postdocs and guests. We strive for reliable perspectives for scientists without ignoring the idea of competition. Uncertain career prospects, temporary employment contracts and the limited ability to plan the future career path reduce the attractiveness of LIKAT as an employer and thus the chances of retaining the best international researchers at LIKAT in the future. From the institute's point of view, an expansion of the budget-financed staff in highly attractive scientific as well as in service areas is urgently needed. At present, only 105 of the approximately 300 employees at the Institute have a permanent contract. Maintaining the scientific mid-level staff with their know-how continues to be problematic. The current pool of non-third-party funded scientific positions is not sufficient for the strategically planned research activities and the sustainable operation of the pilot plant (see *4.9 Strategy Catalysis2Scale-Transfer technical Center*, p. 23). Expiring activities in research fields that no longer meet the requirements of LIKAT are being redeployed. However, these internal redeployments do not solve the actual problem of the lack of budget-funded scientific positions.

In the context of its IT personnel development, LIKAT aims to train its own personnel, to retain them and ideally to increase them by 2 FTEs, taking into account the very tight IT labor market that has existed for years. With the existing staffing level, the rapidly increasing requirements, especially in the operational day-to-day business, are no longer satisfactorily realizable, also with regard to a qualified stand-in.

LIKAT meets the personnel challenges with the following measures:

» Re-appointments on the leading level, in particular of the scientific directorate, are planned and initiated at an early stage in consultation with the *Members' Assembly*, the *Board of Trustees* and the *Science & Industry Council*; active recruitment is carried out, decisive for filling the position are quality and visibility of the research activities as well as the fit to the strategy of LIKAT.

» Positions are made available internally from expiring research on non-current topics.

» Application for a Small Strategic Institute Expansion for the sustainable, largely self-sufficient use of the *Catalysis2Scale Transfer Technical Center* in January 2023: for detailed information, see *4.9Strategy Catalysis2Scale-Transfer technical Center*, p. 23).

In summary, according to current estimates, an increase of about 10 % in LIKAT's personnel is necessary to maintain the institute's performance or to further strategically expand it. In addition, an increase of the current investment budget from about 1 million € to at least 2 million € is necessary.

LIST OF ANNEXES

Catalysis LIKAT
Leibniz-Institut für Katalyse

Catalysis2Scale
The Pilot Plant

Start of work	Autumn 2019
Opening	July 4, 2022
Total area	> 1000 m²
Laboratory area	approx. 200 m²
Office space	approx. 150 m²
Test hall	approx. 650 m²
Total costs	approx. 12.5 Mio. €

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

The topic *Circular Economy* will set the strategic direction for investigations in the pilot plant: The main focus will be on processes that convert CO_2 into valuable and sustainable substances, such as synthetic fuels and basic chemicals.

Primary research topics

» **CO_2-capture** from the atmosphere and point sources (green carbon)

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

» Establishment of the Hydrogen Research Factory MV

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

The technical center has a functional building and a building hall for the infrastructure area. In the 750 m^2 hall, several pilots can be carried out simultaneously. The respective projects/apparatus can be separated from each other by flexible room separation systems.

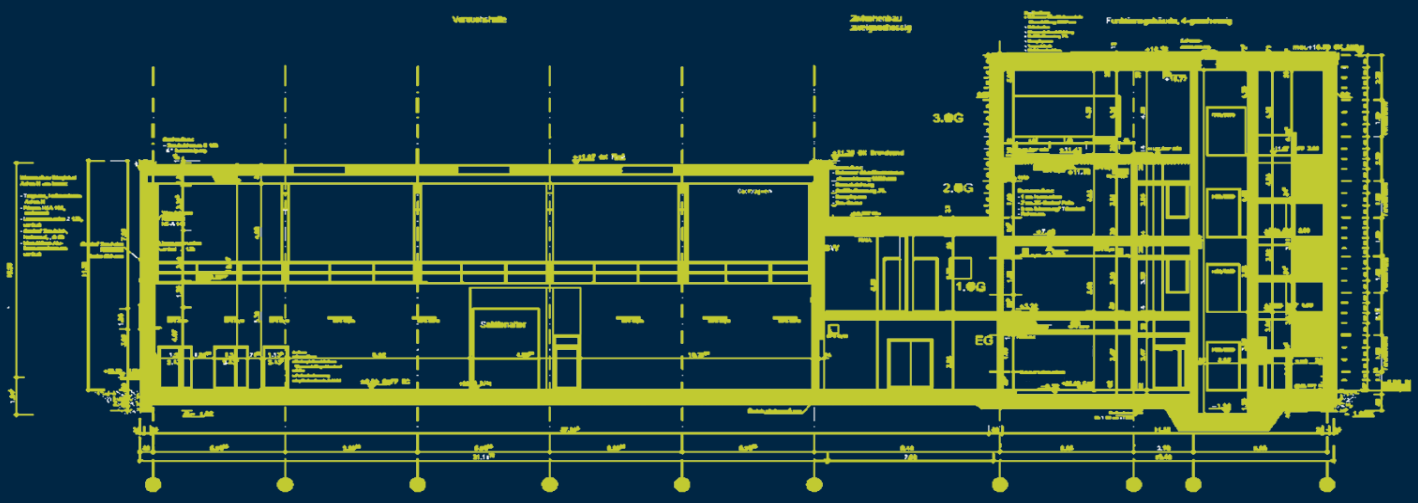
A separate storage area for technical gases or gas bundles (hydrogen; synthesis gas, CO_2, methane; approx. 30 m^2) is provided for applications with these substrates. Generated products are temporarily stored in a fenced outdoor storage area (roofed; 50-75 m^2).

Building

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

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

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



Knowledge & Technology Transfer

Transfer guideline of the Leibniz-Institute for Catalysis

Content

1. Background

The following transfer guideline of the Leibniz Institute for Catalysis explains the transfer understanding of LIKAT, serves as a basis for transfer tasks of the institute and shows current activities.

According to the guiding principle of Gottfried Wilhelm Leibniz *Theoria cum praxi*, LIKAT strives to conduct research for the benefit of the community. This means making scientific knowledge and expertise accessible to society and, ideally, translating research results into practice.

A prerequisite for effective *knowledge and technology transfer (KTT)* at LIKAT is functioning internal communication. On the one hand, this must include specialist information on KTT at LIKAT and, on the other hand, it must aim to raise awareness of the topic and its importance.

The new section on KTT on the catalysis.de website provides information on transfer activities at LIKAT. Furthermore, an offer for support by the transfer officer and an overview of possible activities will be available to all employees on the intranet of the institute.

2. Definition of knowledge & technology transfer (KTT)

Knowledge and technology transfer is now considered the third pillar of science alongside teaching and research. In the sense of the Leibniz Association, transfer means the *exchange between science and the non-academic world*, which always takes place in two directions: On the one hand, the provision of scientific knowledge for societal needs or decision-making processes; on the other hand, the integration of society-generated questions and problems into current research issues. Both require an intensive dialogue on a target group-specific level.

LIKAT understands knowledge and technology transfer as all activities that serve to process scientific findings and technologies in a way that is appropriate for the target group and to transfer them to the non-academic world. In addition, dialogue with society, politics and industry enables research questions to be adapted to social debates and problems.

In particular, technology transfer, as technical utilization and commercial exploitation, has long been one of LIKAT's profile constants. This is expressed in a multitude of transfer examples such as industrial cooperations, transfers and patenting. The close involvement of industrial partners as future users in the research process is an example of successful two-way transfer.

Knowledge transfer at LIKAT is becoming increasingly important: as a *target group-specific and quality-assured translation of scientific findings* and, conversely, as a *translation of problem descriptions and needs from business, politics and society into scientifically workable research questions*. Predestined for such successful knowledge transfer are Leibniz formats such as *Leibniz fragt, Leibniz im Bundestag* or *Book a Scientist*, in which LIKAT regularly participates.

Explicitly excluded from the KTT are all activities at LIKAT that concern research (publications, conference contributions, scientific reports). Even if transfer services can be achieved through them in principle, they belong to the core elements of LIKAT's research mission: the generation of scientific knowledge in the field of catalysis.

3. Goals, transfer partners & resources

As a Leibniz Institute, LIKAT is dedicated to socially, economically and ecologically relevant issues and conducts knowledge and application-oriented research in the field of catalysis, e.g. on the application of catalysis in the socially relevant environmental, energy or health sectors. The target group specific communication of the gained research results of LIKAT, a publicly funded research institution, is understood as an obligation and central task.

The superior goal of KTT at LIKAT is the exchange between science and society, politics and industry in the field of applied catalysis. In particular, it means the transfer of research results and knowledge to strengthen society's ability to reflect. Monetary and human resources, the research focus of LIKAT as well as the identification of societal research needs have to be taken into account. Direct dialogue with various actors in society and industry makes it possible to identify and address research needs.

With regard to technology transfer, a concrete goal for the Institute's scientists is the transfer of at least two catalysts or catalytic processes to industrial pilot scale per year for the utilization and exploitation of scientific results by industry.

With regard to knowledge transfer, the transfer work at LIKAT aims to ensure the transfer of knowledge to the public, as well as to educate and disseminate knowledge on public issues and to provide scientifically sound bases for decision-making.

In order to choose the appropriate language and communication channel, it is essential to analyze and consider the respective target group. The following actors are transfer partners or addressees of KTT at LIKAT:

- Partners from the business community
- Municipal and regional initiatives (e.g. Hy! Rostock hydrogen initiative)
- Regional and supra-regional transfer-relevant networks (e.g. Alumni, NFDI4Cat)
- Politicians of different levels (municipality, state, federal government)
- Level of policy preparation
- Ministeries
- Media
- Interested public
- Students
- Pupils

4. Activities

In the following, various transfer activities at LIKAT are briefly explained. Contact persons at LIKAT for external communication are Dr. Martha Höhne (martha.hoehne@catalysis.de, Staff unit public relations) and Nicole Aulerich (nicole.aulerich@catalysis.de, Assistance to the Scientific Direktor).

4.1 External communication

4.1.1 Publications

Explicitly excluded from KTT at LIKAT are all publications that involve the publication of research results in *peer-reviewed* journals. Even if they basically serve the transfer, they belong to the core elements of LIKAT's research mission.

However, LIKAT staff members regularly report on the latest research findings in articles that are not subject to the *peer-review* process. These include so-called *Perspectives, Commentaries* and

Opinions in renowned scientific journals as well as in non-scientific journals or *preprint* articles. These publications are marked as non-peer-reviewed in the statistics and are used as an instrument of (knowledge) transfer. The publication of specific research results enables potential interested parties to approach scientists of LIKAT.

In addition, there are publications in non-scientific journals or the biennial report of LIKAT, which informs about progress and developments in the institute, as well as the biannual journal *Leibniz-Nordost*. The journal, which is published by the four Leibniz institutes in Mecklenburg-Western Pomerania and the Research Institute for Farm Animal Biology (FBN), deals with current socially relevant research work of the institutes and presents it in a popular science format.

4.1.2 Public relations & Mass media

A suitable way to get in contact with the broader interested public is the classical public relations and the use of mass media like newspapers (print and online), radio and television.

LIKAT regularly publishes press releases about current research results and ongoing projects, which are picked up by various media. The regional and supra-regional press, radio as well as regional and supra-regional television stations report at regular intervals on the research activities at LIKAT. In addition to communicating scientific content, this approach provides the public with knowledge and understanding of the scientific process and demonstrates the sense and benefits of investing in research for society.

4.1.3 Social Media

LIKAT is present on selected social media and maintains profiles on Twitter and LinkedIn.

Social media not only offer the opportunity to increase awareness of content and reach, but also to interact and engage with users. They can be an excellent complement to traditional media and KTT activities.

Another aspect of social media is the opportunity to build transfer-relevant networks. By networking with various stakeholders, it is possible on the one hand to place information in a targeted manner and on the other hand to integrate their interests and needs in turn into research content.

4.1.4 Internet presence

LIKAT has an extensive internet presence (catalysis.de): Here, each research group has the opportunity to present their research work in detail and to introduce scientific contact persons, so that inquiries and needs can be responded to immediately.

An image film, which can be accessed via the homepage, presents the research content and competences at LIKAT in a professional manner. Further video contributions dealing with research contents of LIKAT are linked.

4.1.5 Events for the public

LIKAT regularly organizes scientific colloquia, symposia, workshops and conferences. Likewise, LIKAT staff members actively participate in national and international events of this kind. Even though transfer services can be achieved through these activities, they, as well as publications in peer-reviewed journals, belong to the core elements of LIKAT's research mission and are explicitly excluded from the KTT.

In addition, LIKAT regularly participates in various series of events for the public. Worth mentioning here is the *Long Night of Science*, for which the institute opens its doors every year and provides an insight into scientific work and projects.

Other formats: *Rostocks Eleven*, *Girls Day*, *Wissenskarawane*, *Woche der Umwelt*, *VDI Werkstoffferien*, *Virtual LabDay*, *Leibniz fragt*, *Leibniz im Bundestag*, *Book a Scientist*.

There is the possibility of guided tours of the institutes or to carry out practical training for pupils. In addition, LIKAT sponsors a special prize for the winner of *Jugend forscht* every year, which consists of a three-week internship incl. 1000 € to cover expenses.

4.2 Networks relevant to transfer

4.2.1 Alumni Network

In 2015, an alumni network was actively established at LIKAT and has been maintained since then. This includes the regular information of alumni about current developments, research results and projects, which is done specifically via an alumni group of our LinkedIn profile. Alumni meetings are held at LIKAT every two years to promote networking between alumni and current employees. In addition, an alumni section has been set up on our homepage, which provides information on upcoming alumni meetings, reviews of past meetings, and contact information. Meanwhile, the LIKAT alumni network is maintained via *LinkedIn*.

With their experience and know-how in industry and academia, the alumni support the transfer work of LIKAT. Contacts with alumni result in numerous projects in which research questions and needs are addressed. At the same time, there is the possibility that research results can be transferred into practice in a short way.

4.2.2 Scientific Community

LIKAT is a partner of various networks. These include the *NFDI4Cat* project for the promotion of digitization in central scientific areas, for the networking and provision of important research data of participating partners under the leadership of LIKAT.

Another example is the network for fine chemicals *4chiral*. It comprises 40 partners, 75% of which are small and medium-sized enterprises (SMEs) in central Germany's fine chemicals and biotechnology sectors, as well as universities and research institutes.

4.2.2 Regional non-scientific community

LIKAT is a member of the association *Rostock denkt 365°*. The association *sees itself as a motor of exchange with science in the Rostock region as well as a coordinator of the network necessary for this. Under the umbrella of the association, science, business, politics and culture are jointly committed to a dynamic, creative and cosmopolitan science location*.[1] Numerous events of the association serve to improve the visibility of the science scene in the Regiopole Rostock. The good regional networking of the various transfer actors makes it possible to bundle their activities and thus further increase visibility in Rostock and the surrounding area.

1 Rostock denkt 365 Grad | (rostock365.de)

The network *Leibniz-Nordost* connects all Leibniz institutes[2] located in Mecklenburg-Vorpommern as well as the FBN[3] in various activities.

4.3 Education & Training

The support of education and training of young scientists and technicians in cooperation with universities, especially the University of Rostock, is a statutory task at LIKAT.

4.3.1 Training

In close cooperation with the University of Rostock, LIKAT offers a variety of topics for the preparation of doctoral theses as well as bachelor and master theses. In particular, the topics of the doctoral theses are often integrated into tasks of industry-relevant research and introduce the future specialists to related issues at an early stage.

This transfer instrument is extremely well integrated at LIKAT. Numerous doctoral students take up employment in the respective companies after successful completion of their dissertation due to the industrial contacts already established during their dissertation period.

4.3.2 Transfer via individuals

Scientists, students and alumni contribute their knowledge to various institutions and organizations. This happens in the context of dual-supervised theses (with cooperation partners from industry), student internships or through career entries of qualified alumni. The permanent participation or membership of scientists in bodies and committees is also a means of KTT via individuals. Examples are the memberships in the *German Academy of Sciences Leopoldina,* the *German Catalysis Society GECATS*.

4.3.3 Further training

LIKAT recognizes priorities in the training and further education of LIKAT employees on special transfer-relevant topics such as science communication, contract management for research contracts and patenting. There is the possibility of organizing further training measures for this purpose.

Through explanations, in this specific case on issues of contracting and patenting, by the transfer officer, knowledge on these topics is continuously imparted and thus the sensitivity of all employees of LIKAT from science and administration for knowledge and technology transfer is increased. Already in the doctoral phase, doctoral candidates deal with the exploitation potential of their research work.

Scientists interested in a spin-off can be referred to appropriate experts by the transfer officer. The WGL office (Wissensgemeinschaft Gottfried Wilhelm Leibniz) also provides detailed information on its website *Start-ups at Leibniz*.

4.4 Transfer pilot plant Catalysis2Scale

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

2 Leibniz-Institut für Katalyse (LIKAT), Leibniz-Institut für Atmosphärenphysik (IAP), Leibniz-Institut für Ostseeforschung (IOW), Leibniz-Institut für Plasmaforschung und Technologie (INP)

3 Forschungsinstitut für Nutztierbiologie (FBN)

Institute for Catalysis has another significant unique selling point. The pilot plant was opened in 2022 and enables in-house piloting for the transfer of innovative laboratory results from catalysis research into practice. This opens up further avenues for collaboration with SMEs and non-chemical user industries that do not have the corresponding facilities themselves. It also provides the basis for closer networking with researchers at the University of Rostock and other research institutions in Rostock and MV through joint use.

4.5 Joint facilities with industry

Joint research projects with representatives of industry usually have short project durations of a few months to a year. LIKAT has the resources for long-term framework agreements and is thus a reliable partner for industry. These long-term cooperations allow practice-relevant research over a longer period of time and a sustainable transfer: research concerns are directly taken up and results can be directly implemented in practice.

4.6 Industrial property rights (patents & licenses)

The scientists at LIKAT focus on recognizing and exploiting potentials in their research work and publications. The young scientists are taught this from the beginning of their work.

As a rule, results achieved in collaborative projects are initially patented throughout Europe. In order to benefit from the expertise and infrastructure of the partners and to be able to transfer research results quickly, the patents are preferably filed jointly with the industrial partners.

Individual advice on intellectual property issues is provided by the transfer officer Ute von Zweydorff (ute.zweydorf@catalysis.de).

5. Internal communication

Increasingly, the KTT already plays an important role in the application process for projects. In order to sensitize the employees of LIKAT for the importance of the topic, a transparent internal communication is aimed at. LIKAT's transfer guideline is published on the institute's intranet and thus accessible to all employees. The transfer officer Ute von Zweydorff (ute.zweydorf@catalysis.de) has been appointed and can be contacted for support and advice. The focus here is on support in patent and contract matters for collaborations and corresponding non-disclosure agreements. The close networking of all departments in LIKAT promotes a fast flow of information and the bundling of all transfer-relevant expertise. In this way, KTT can be systematically considered throughout the entire research process, from project planning to dissemination of results.

6. Success & indicators

KTT is essential for the exchange of Leibniz institutes with society. In order to evaluate and track the impact of the transfer lines at the Leibniz Institute for Catalysis, the development of various indicators is necessary (taking into account personnel and economic possibilities). In addition to quantitative indicators, these should also take into account qualitative criteria.

In order to verify the success of the transfer work, transparent, traceable and evaluable quantitative indicators are recorded and communicated transparently at LIKAT. The documented indicators include in each case the number of:

- Cooperation projects with the industry
- Transfers
- Patents & property rights
- Target group specific events incl. visitor numbers
- Interviews on radio and television
- International cooperations
- Publications in terms of Perspectives, Opinions and Comments as well as preprint articles (see section 4.1.1, p. 6)
- Press releases
- Tweets and their reach
- Articles in trade & general press (print, online), radio & television, Twitter

In 2022, professional media monitoring was added to the toolkit in order to track and respond to the direct media response to output. In this way, input and output of the KTT at LIKAT can be measured well.

However, the informative value of quantitative metrics alone is limited. Measuring the success of transfer services requires the introduction of so-called qualitative indicators. These are far more difficult to measure and often emerge only with a time lag. Nevertheless, knowledge about the impact of the transfer services provided is important in order to continuously adjust and improve research questions and communication of results.

LIKAT intends to develop a set of quantitative and qualitative indicators to evaluate KTT at the institute. They should be collectable at a reasonable cost, be proportionate to human and monetary resources, and be consistent with the statutory research mission.

The KTT guideline of LIKAT will be evaluated regularly and adapted according to relevant developments. The indicators to be developed will serve as an additional instrument to facilitate the continuous adaptation of LIKAT's transfer work to new challenges.

Publication & Open Access Guideline of the Leibniz Institute for Catalysis - LIKAT Rostock

Content

1. Background

This document serves as a guideline for publishing scientific work of the Leibniz Institute for Catalysis. It is based on LIKAT's mission statement and on current requirements in the field of scientific communication. Within the last decade, about 15.7 million scientific journal articles have been published worldwide. The number of journal articles per year increased by about a quarter in the period 2011 to 2020 (from 1.26 million in 2011 to 1.79 million in 2020).[1] So-called science-to-science communication is increasingly taking place outside traditional publication channels, in the form of blogs, via Twitter or in academic social networks.

The guideline summarizes recommendations & obligations for publications by LIKAT scientists. It also provides information on different possibilities of Open Access publishing, Creative Commons licenses as well as a glossary.

2. Objective - Quality Assurance & Open Access

Against the background of excellent scientific productivity, LIKAT's main future goal is to increase the quality, visibility and impact of its publications. Prerequisites for maximum impact are high relevance and quality of the research results as well as reputation and quality of the publication medium. At LIKAT, transparent, traceable and evaluable quality indicators and criteria (e.g. peer review) are recorded and communicated transparently. Key individual goals of the publication guidelines for increasing the influence as well as the visibility and perception are:

1. Publication of >50% of all journal articles in international journals with high impact factor (>5).
2. LIKAT documents books, book chapters and journal articles in journals in its publication list. Journal articles that have undergone a *peer review* process are identified as such. *Corrigenda* and withdrawn publications are not considered publications. *Preprints* (e.g., on *chemRxiv*) are reported as open access publications without a *peer review* process as long as they have not appeared in a journal with a *peer review* process. Once published, the *preprint* will be linked to the publication and documented as one publication.
3. Increase international collaborations,
4. Increased inter- and transdisciplinary research,
5. Promotion of Open Access, Open Data and Open Science in the context of the science (funding) policy of the EU and national funding agencies (NFDI4Cat),
6. Raising awareness about fake journals and predictive publishing,[2]
7. Archiving and securing research data for at least 10 years,
8. Access to stored research data in consultation with researchers and in accordance with legal requirements,
9. Administration and operation of the official LIKAT Institute account on Twitter and LinkedIn is carried out exclusively by the Public Relations Office.

As a publicly funded, non-profit research institution, LIKAT has set itself the goal of making its research results accessible via the Internet without financial, technical or legal barriers as far as possible. As a

1 https://www.webofscience.com/
2 http://thinkchecksubmit.org/

member of the Leibniz Association, the institute follows the Berlin Declaration on Open Access to Knowledge in the Sciences and Humanities[3] and the Leibniz Association's Open Access Policy.[4] Open Access supports scientists in researching and publishing, accelerates scientific innovation processes, and improves the visibility and utility of research. The institute aims to make at least 40% of all journal articles available in open access and supports its scientists financially as far as possible *4 Implementation & Funding*).

As a Leibniz Institute, LIKAT addresses socially, economically and ecologically relevant issues and conducts knowledge- and application-oriented research in the field of catalysis. Its science communication and public relations activities focus on socially relevant questions, e.g. on the application of catalysis in the environmental, energy or health sectors. Research results are to be made public in appropriate formats and tailored to different target groups (*science-to-professionals or science-to-public*).

3. Recommendations & Obligations

1. All researchers of LIKAT are obliged to publish their scientific results in order to demonstrate research performance and expertise.
2. For quality assurance purposes, LIKAT demands its researchers to follow the *LIKAT rules and regulations on Good Scientific Practice* when publishing.
3. For publications of scientific results in the form of journal articles, only journals with *peer review* procedures are to be chosen. If a publication has already been made on a pre-print server, the researchers are encouraged to submit the finished manuscript to a journal with a *peer review* process.
4. LIKAT urges its scientists to publish their research results in accordance with the Open Access principle. This can be done directly via OA first publications or, within the scope of legal possibilities, via OA second publications in repositories, where a timely publication is to be aimed for (see section 5, p. 4). In the case of direct OA publication, the Institute strongly recommends publication under a free use license (*Creative Commons Attribution*,[5] see section 7, p. 9). This is the only way to ensure free access.
5. LIKAT recommends the free use license for text-based publications: **CC BY-NC-ND**.
6. If, from the authors' point of view, there is no suitable open access publication journal for an article, it can be published in an access-restricted format.
7. LIKAT encourages its scientists to apply for external funding for Open Access publications when applying for projects.
8. The affiliation of authors belonging to LIKAT has to be stated:

   Leibniz-Institut für Katalyse e.V., Albert-Einstein-Str. 29a, 18059 Rostock, Deutschland.

   The English name is also permissible:

   Leibniz Institute for Catalysis, Albert-Einstein-Str. 29a, 18059 Rostock, Germany.
9. For coordinated public relations, press releases are prepared in cooperation with the Public Relations Office and published exclusively by them.

3 Berlin Declaration on Open Access to Knowledge in the Sciences and Humanities.
4 Open-Access-Policy der Leibniz-Gemeinschaft.
5 https://creativecommons.org/about/cclicenses/

4. Implementation & Promotion

1. The publication performance of LIKAT is documented under consideration of relevant quality criteria, updated monthly and communicated regularly in the extended board meeting as well as on the intranet for all employees.
2. LIKAT endeavors to list freely available publications of its scientists in *LeibnizOpen*. Publications published via the Leibniz subject repository *ReNaTe* (Repository for Natural Sciences and Technology) are automatically entered into the central open access portal of the Leibniz Association *LeibnizOpen*.
3. LIKAT informs and advises its scientists on Open Access as well as on legal issues related to Open Access publications of their research results.

   The OA contact person at LIKAT is Dr. Sandra Hinze (sandra.hinze@catalysis.de).
4. LIKAT participates in transformation contracts, e.g. *Wiley DEAL* or *Springer Nature* (outside of DEAL), and thus provides its scientists with financing options for publication fees of Open Access publication media:

   For example, the institute covers the costs incurred by LIKAT authors in the Wiley-DEAL contract. Payment has to be made for each publication regardless of whether it is published Open Access or not.
5. The APC for other journals have to be financed by external funds of the respective research departments.
6. It is possible to apply for financial support via the *Leibniz Open Access Publication Fund*. Further information can be found on the intranet under *Management/Licensed Journals & Databases/Leibniz Open Access Publikation Fund*.

5. Open Access secondary publications

The European Commission (EC) and the European Research Council (ERC) require the widest possible dissemination and worldwide access for publications funded by them.

LIKAT generally recommends publication in genuine *open access* journals (*gold OA*). If the publication takes place in conventional (*closed access*) journals, the secondary publication (*green OA)* is recommended.

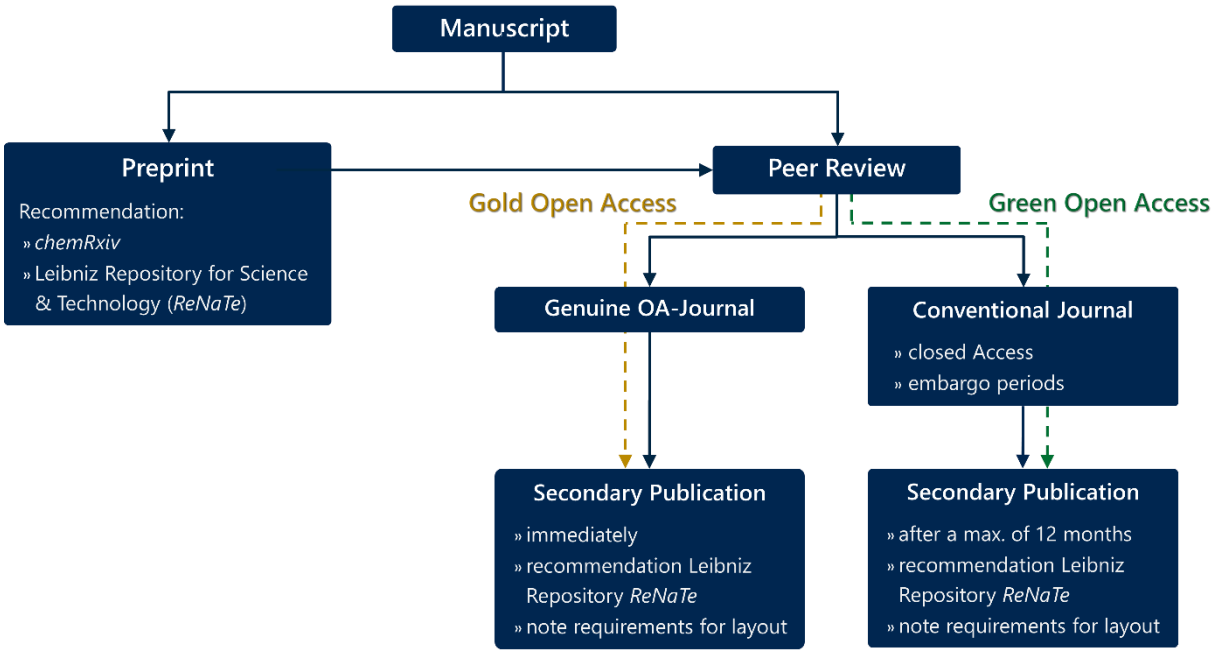


Figure 1. Options for secondary publication of a manuscript.

Recommended repositories

LIKAT recommends depositing *Open Access* first and second publications in the *Leibniz Repository for Science and Technology ReNaTe* in order to maintain a uniform standard. It is a subject-specific, institutional repository that bundles publications from all Leibniz institutions of the subject sections D and E and is linked to the Leibniz Association's central Open Access portal *LeibnizOpen*.

Das Leibniz Repository *ReNaTe* is operated by the TIB (Leibniz Information Centre for Technology and Natural Sciences University Library) and is indexed by search engines, subject search services and library catalogs.

Both first and second publications can be submitted to the repository free of charge. A second publication can be published in the repository as a *preprint, postprint*, and as a final publisher's version, depending, among other things, on what a possible publishing agreement allows.

Procedure

In principle, it is possible to have the TIB staff take care of the posting of publications: Contact: re-anate@tib.eu.

Alternatively, you can create your own account under User Registration | Repository for Science and Technology (tib.eu).

1. posting of publications that have already been published under **CC-License** (Open Access Publications):
   - » Submit a publication list (without full text, without publication agreement) via the online form
2. posting of (first and) second publications without **CC-License**:
   - » Enter the metadata in the corresponding online form and upload the full text
   - » Submit the signed publication agreement (for first publications „Publication Agreement ReNaTe v2.0.pdf" or for second publications „Publication Agreement ReNaTe v2.0 ZV.pdf")
   - » Secondary publications without CC license may usually only be published as accepted manuscript (last version after scientific review with all changes) without publisher's own layout
   - » Review (and, if necessary, amendment) of the entries by TIB administrators

6. Glossary

APC

The *Article Processing Charge APC* is a publication fee that is charged for the first publication of a scientific article in a pure Open Access journal or a hybrid journal. A research institute can provide support for the payment of *APCs*, either within the framework of trans-formation agreements or funding instruments (e.g. *Leibniz Open Access Publication Fund*).

Alternative terms are Article Charges, Processing Charges, Page Charges, Publication Charges.

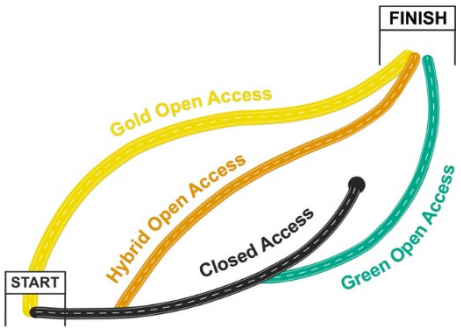


Figure 2. Pathways to open access. (Image: open access network)

Bronze Open Access

Bronze Open Access describes articles that are freely accessible via the publisher's website but have not been published under an Open Access license. These can be downloaded and read free of charge, but not redistributed or reused.[6]

Closed Access

Closed Access refers to restricted, non-free access to scientific literature that is only possible after payment (*paywall*). When publishing in *closed access*, authors cede the exclusive rights of use and exploitation to the publisher and can no longer decide on the further use of their own content.[7]

6 Gold, Green, Bronze, Blue...: The Open-Access-Color Theory - TIB-Blog

7 Universitaetsbibliothek der HU Berlin - Glossar (hu-berlin.de)

Creative-Commons-Licenses

Creative-Commons-Licenses (*CC*) licenses provide everyone from individual creators to large institutions with a standardized way to grant the public permission to use their creative work under copyright law. From the perspective of the reuser, the existence of a Creative Commons license for a copyrighted work answers the question: *what can I do with this work?* The various *CC licenses* are described in detail in Section 7. *Creative Commons Licenses* (p. 9).

DEAL

DEAL is a project initiated by the Alliance of German Science Organizations and the German Rectors' Conference. It aims to negotiate nationwide transformative *publish and read* agreements with the largest scientific publishers (Elsevier, Springer Nature and Wiley). This is intended to reduce and restructure the overall German costs for access to scientific literature. The aim is to give all scientists the opportunity to publish Open Access themselves on the one hand and to have access to the entire portfolio of electronic journals on the other.[8]

First publication

This is the first publication of a scientific work.

This refers to the publication of a scientific publication (usually an article or book) by a publisher at the end of a publication process. Scientific publications published by another institution (research reports, etc.) are also included. An initial publication can be non-open access (see *Closed Access*) or open access (see *Open Access*). The latter corresponds to *Gold Open Access*.

Free Access

Free Access articles are articles from subscription journals that are freely accessible to non-subscribers. In contrast to *Open Access*, this access is usually limited in time and the articles are not provided with a *CC license*, so that their subsequent use is not possible.

Gold Open Access

The golden path of open access publishing refers to the initial publication of scholarly works as articles in *open access* journals, as an *open access* monograph, or as a contribution to an open access edited volume or conference proceedings. The articles usually undergo the same quality assurance process as *closed-access* works, usually in the form of *peer review* or *editorial review*, and are accompanied by appropriate licensing information. They can be secondaryly published immediately after the article appears.

Green Open Access

The green route refers to the publication of a version of an article that has already been published but was not previously open access. Usually, manuscript versions of the publication (*preprints* or *postprints*) or the already published version (*publication version*) are made freely accessible on institutional or disciplinary *open access document servers (repositories)*. For the latter, any embargo periods by the publishers must be observed.

An overview of what publishers allow authors to publish is provided by the Sherpa Romeo directory.

8 Über Projekt DEAL – Projekt DEAL (projekt-deal.de)

Right to secondary publication: As a result of a copyright reform, a right to secondary publication (Section 38 (4) UrhG) has been in force in Germany since January 1, 2014, irrespective of agreements with publishers. According to this, journal articles *[...] that have been produced in the context of a research activity that is at least half publicly funded and that have appeared in a collection that is published periodically at least twice a year may be republished,*[9] twelve months after the first publication. However, only the so-called *accepted manuscript* (last version after scientific review with all changes) without the publisher's own layout may be used for this purpose.[10]

Hybrid Open Access

In contrast to *Golden Open Access*, here the first publication of a scientific article takes place in a journal that is fundamentally subscription-based. Individual articles are made freely accessible (i.e., *open access*) in return for additional payment of *article processing charges* (APC) and are provided with appropriate license information. This model is offered by numerous publishers, especially the large ones, and is attractive for researchers: on the one hand, publication in established and renowned journals is possible, and on the other hand, publication is nevertheless freely accessible.

However, there are justified criticisms of this model: in most cases, it cannot be denied that double payment is required for OA publication - both for subscription and for publication as an OA article. In addition, the *Article Processing Charges (APC)* are on average significantly higher than for pure OA journals. Also, the release of paid articles does not work in every case. As a result, such journals are excluded from funding by many publication funds and in the EU framework program, *Horizon Europe*.**Fehler! Textmarke nicht definiert.**

Metadata

Metadata are independent data that contain structured information about other data or resources and their characteristics. They are stored independently of or together with the data they describe. Usually one differentiates between technical and technical and/or administrative metadatas. While the latter have a clear metadata status, technical metadata can sometimes also be understood as research data.[11]

Postprint

In contrast to a *preprint*, a *postprint* has already gone through the review process and has been accepted for publication. This can be the publisher's version or the accepted manuscript version which, although not identical in layout, is identical in content to the publisher's version. The latter is relevant for the Green way of Open Access.

Preprint

A *preprint* is a form of manuscript that has not yet undergone an official *peer review* process. The publication takes place on so-called *preprint servers* (e.g. *chemRxiv*). The article differs from the publisher's version in terms of both layout and content, as changes resulting from the *peer review* process have not yet been incorporated.

9 § 38 UrhG - Einzelnorm (gesetze-im-internet.de)

10 https://open-access.network/informieren/open-access-grundlagen/open-access-gruen-und-gold#c7776

11 Glossar | Praxis kompakt | Forschungsdaten und Forschungsdatenmanagement

Publish & Read fees

Publish & Read (PAR) fees are fees negotiated as part of the *DEAL contracts* that combine the costs of *open access* publications and comprehensive reading access into one amount.

In this context, the usually uniform fee per article is intended to replace the non-transparent type of subscription-based funding. The amount of the fee is determined by the total subscription expenditure in Germany and the total number of articles published annually (by German research institutions).[12]

Pure open access journal

The *pure/genuine OA journal* refers to a journal (or publisher) that publishes exclusively *OA publications* from the beginning. The publication is provided with an appropriate *CC license*.

Repository

Repositories are either subject-specific or institutional document servers on which various publications or scientific data are made available to the public without access restrictions.

Institutional document servers are usually operated by university libraries, other infrastructural institutions or research organizations. *Disciplinary repositories* are inter-institutional. Essentially, a repository consists of repository software and a database. Data are entered into the *repository* via the web-based user interface. In addition to the actual data, its metadata is required. Metadata describes the content of the research data and provides information about its origin, the software and methods used, and legal aspects.

12 Reduce and redistribute costs - DEAL Operations (deal-operations.de)

7. Creative-Commons-Licenses[13]

Creative-Commons-Licenses offer everyone a standardized way to grant permission to the public to use their creative work under copyright law. LIKAT strongly recommends publishing under a **CC BY-NC-ND** license for text-based publications.

CC-License types

CC BY 	Users may distribute, remix, adapt and build upon the material in any medium or format as long as credit is given to the author. The license permits commercial use.	BY The author must be named.
CC BY-SA 	Users may distribute, remix, adapt and build upon the material in any medium or format as long as credit is given to the author. The license permits commercial use. If changes are made by the user, the modified material must be licensed under the same terms.	BY The author must be named. SA Modified material must be passed on under the same conditions.
CC BY-NC 	Users may distribute, remix, adapt and build upon the material in any medium or format for non-commercial purposes as long as credit is given to the author.	BY The author must be named. NC Only non-commercial use is allowed.
CC BY-NC-SA 	Users may distribute, remix, adapt and build upon the material in any medium or format for non-commercial purposes as long as credit is given to the author. If changes are made by the user, the modified material must be licensed under the same terms.	BY The author must be named. NC Only non-commercial use is allowed. SA Modified material must be passed on under the same conditions.
CC BY-ND 	Users may copy and distribute the material in any medium or format in unedited form as long as credit is given to the author. The license permits commercial use.	BY The author must be named. ND Modifications are not allowed.
CC BY-NC-ND  **Empfehlung**	Users may copy and distribute the material in any medium or format in unedited form for non-commercial purposes as long as credit is given to the originator.	BY The author must be named. NC Only non-commercial use is allowed. ND Modifications are not allowed.
CC0 	Creator relinquishes copyright. Users may unconditionally distribute, modify, adapt and build upon the material in any medium or format.	

13 About CC Licenses - Creative Commons

Guidelines of the Leibniz Institute for Catalysis (LIKAT Rostock) to ensure good scientific practice & to deal with allegations of scientific misconduct[1]

PREAMBLE

The basis of scientific work is the honesty of scientists towards themselves and others. It is the ethical norm and the basis of the rules of good scientific practice. Ensuring the validity and application of these rules in practice is a core task of science.

The Leibniz Institute for Catalysis (LIKAT Rostock) is aware of its responsibility to teach the norms and rules of good scientific practice to all scientists, especially in qualification phases.

LIKAT considers it an important and necessary task to maintain scientific integrity and to sensitize the employees working at the institute accordingly. The present guidelines of LIKAT serve as a self-commitment and define principles of good scientific practice and describe the procedure for dealing with allegations of scientific misconduct at the institute.

[1] Note: This paper is based on both the "Guidelines for Ensuring Good Scientific Practice and for Dealing with Allegations of Scientific Misconduct in the Leibniz Association" and the DFG's "Procedural Guide to Good Scientific Practice". Formulations and sentence constructions are taken from these general documents and are merely adapted and tailored to the situation at the Leibniz Institute for Catalysis (LIKAT Rostock).

1. SCOPE OF APPLICATION

The "Guidelines for Ensuring Good Scientific Practice and for Dealing with Allegations of Scientific Misconduct" define principles of good scientific practice and describe the procedure for dealing with allegations of scientific misconduct at the Leibniz Institute for Catalysis (LIKAT Rostock).

The present guidelines also define possible sanctions for scientific misconduct by employees of the Leibniz Institute for Catalysis.

2. RULES OF GOOD SCIENTIFIC PRACTICE

1. The rules of good scientific practice include in particular:

   a.

   - to work in a *lege artis* manner,
   - fully document all steps and results of an experiment or study, and keep protocols and primary data secure and protected from subsequent manipulation,
   - critically and consistently review the validity and reproducibility of all experimental results and other research designs,
   - to maintain strict honesty with regard to the contributions of contributors as well as with regard to third-party funding sources,
   - to respect the intellectual authorship of others in all publications and to properly identify all citations and takeovers,

   b. to provide appropriate guidance to scholars in the preparation and academic evaluation of qualifying papers,

   c. the responsible cooperation and the responsible performance of the editorial tasks in working groups, including the appropriate supervision of their members,

   d. the responsibility of the authors of scientific publications for their content, including the presentation of results and their discussion,

   e. to always give priority to originality and quality over quantity as performance and evaluation criteria for promotions, appointments, appointments and allocation of funds.

2. Scientific publications should describe scientific results and how they came about in a complete and comprehensible manner. Previously published results and texts can only be part of later publications in a clearly identified form (duplicate publication) if they are necessary for understanding the context of the publication.

3. Only those who have contributed substantially to the conception of the studies or experiments, to the preparation, analysis and interpretation of the data and to the formulation of the manuscript and who have agreed to its publication, i.e. who are responsible for its publication, may be considered authors of an original scientific publication. A so-called honorary authorship is excluded. These regulations should be the subject of a cooperation agreement, for example in the case of large collaborative research projects.

4. Primary data and experimental documentation must be kept accessible for at least ten years. Data for which there are central, public repositories should be made available to them.

3. SCIENTIFIC MISCONDUCT

Scientific misconduct occurs when false statements are made intentionally or through gross negligence in a context relevant to science, intellectual property rights are violated, or the research activities of others are impaired. In addition to violations of scientific ethics, especially through inhumane or deceptive procedures, scientific misconduct includes, among other things:

1. Incorrect data, in particular:
    a. making up data,
    b. falsifying data (e.g., by selecting desirable or rejecting undesirable results or evaluation procedures without disclosing this, or by manipulating a figure),
    c. providing incorrect information in publication lists or grant applications (including incorrect information about the publication organ and about publications in print),
    d. multiple publication of data or text without disclosure.
2. Infringement of intellectual property rights, in particular:
    a. regarding a legally protected work created by others or essential scientific findings, hypotheses, doctrines or research approaches originating from others:
        » the unauthorized adoption or other use of passages without adequate proof of authorship (plagiarism),
        » the exploitation of research approaches and ideas without consent, especially as a reviewer,
        » the presumption or unfounded assumption of scientific authorship or co-authorship, as well as the denial of justified co-authorship,
        » falsification of the content or
        » unauthorized publication and unauthorized making available to third parties as long as the work, finding, hypothesis, teaching or research approach has not yet been lawfully published;
    b. claiming the (co-)authorship of another person without the latter's consent.
3. Interfering with the research activities of others (including damaging, destroying, or tampering with experimental setups, equipment, records, hardware, software, chemicals, or other items needed by others to conduct an experiment).
4. The disposal of primary data, if this violates legal regulations or recognized principles of scientific work. This also applies to the illegal non-disposal of (especially personal) data.

Co-responsibility for misconduct may result, among other things, from participation in the misconduct of others, gross neglect of supervisory duties, or co-authorship of publications containing falsifications.

4. ORGANIZATIONAL STRUCTURES THAT PROMOTE "GOOD SCIENTIFIC PRACTICE" AT LIKAT

1. According to the statutes, the board of LIKAT is responsible for the scientific orientation of the institute. The direct responsibility for the scientific work is assigned to the research department heads, who shape the working style in their departments, ensure a high scientific standard and can delegate the responsibility for sub-areas to the research group leaders assigned to them. The explanation of rights and duties of each employee is to be given when the employee is hired or changes his or her area of responsibility.
2. The research department heads shall hold regular meetings with the scientists in their departments for the purpose of internal coordination, setting goals, and identifying and solving problems.

3. The overall responsibility of the department heads extends to the individual studies and publications of the subordinate working groups only to the extent that responsibility is involved in the context of co-authorship.
4. Supervisors of Bachelor, Master, and doctoral students are obliged to ensure that the scientific as well as the organizational and technical supervision is secured at all times.
5. The duties of the research group leaders also include upholding the principles of "good scientific practice" in their field of work. Scientific personnel, doctoral candidates and diploma students are to be instructed accordingly. Young scientists must be comprehensively informed about the nature of "good scientific practice" and the consequences of scientific misconduct.
6. Scientific and technical staff as well as Bachelor, Master, and doctoral students may pass on materials and results of their research work only with the explicit approval of their research group leaders.

5. OMBUDSPERSONS

5.1 Ombudsperson of LIKAT

1. The scientists of LIKAT elect an ombudsperson and a deputy as a contact persons in case of disagreements, suspicions and disputes (so called decentralized ombudsperson within the Leibniz Association). Re-election is permitted.
2. Scientists who already enjoy a scientific reputation and have exercised leadership responsibility should be appointed as ombudspersons. Personal and professional independence are important and promising criteria for the selection of an ombudsperson. In order to avoid conflicts of interest, the task may therefore not be performed by members of the Board of the Leibniz Institute for Catalysis.
3. The term of office of the ombudsperson and the deputy ombudsperson at LIKAT is fixed for a period of four years. The Board of LIKAT is responsible for the execution of the election.
4. A deselection of the ombudsperson (or the deputy ombudsperson) can take place if a permanent reliable fulfillment of tasks seems to be no longer possible or the confidence in the appropriate fulfillment of tasks no longer exists. Such a deselection must be approved by at least two thirds of the scientists at LIKAT. The (deputy) ombudsperson has to be heard before the decision on the dismissal.
5. The procedure for the examination of allegations of scientific misconduct by the ombudsperson at LIKAT is regulated below under points 6, 7 and 8 of these guidelines.

5.2 Central Ombudsperson of the Leibniz Association

1. Within the Leibniz Association, *a central ombudsperson* and a deputy are elected by the Senate of the Leibniz Association on the recommendation of the Presidium. Both of them ensure good scientific practice and deal with allegations of scientific misconduct for all institutions of the Leibniz Association.
2. The *central ombudsperson* investigates allegations of scientific misconduct against employees and former employees of member institutions of the Leibniz Association.
3. The *central ombudsperson* becomes active when the (decentralized) ombudsperson elected at LIKAT appeals to her. In justified cases, the *central ombudsperson* can also become active if he/she is in-

formed directly from LIKAT by a whistleblower about a suspicion of scientific misconduct with the request for a review.

6. INVESTIGATION OF ALLEGATIONS OF SCIENTIFIC MISCONDUCT AT LIKAT

1. Allegations of scientific misconduct are usually to be addressed in writing to the ombudsperson of LIKAT.
2. The review of anonymous reports has to be weighed by the ombudsperson. In principle, an appropriate investigation requires that the name of the whistleblower be mentioned.
3. The name of a whistleblower shall be treated confidentially. Disclosure of the name to the accused person may be required in individual cases if he or she cannot otherwise defend himself or herself properly. However, the name of a whistleblower shall only be disclosed if the whistleblower does not suffer any disadvantages for his or her own scientific and professional advancement.
4. The ombudsperson shall confirm receipt of the report to the whistleblower within one week.
5. The ombudsperson reports to the LIKAT Board and, if applicable, to the concerned department within LIKAT about his or her actions.
6. The ombudsperson shall conduct a preliminary examination. In order to carry out this examination, the ombudsperson shall at least hear the accused and, if necessary, also the whistleblower.
7. The ombudsperson may hear further persons and commission external expert opinions.
8. As a result of the preliminary examination, the ombudsperson decides whether to discontinue the proceedings (either because the accusations have proven to be unfounded or because a simple and uncomplicated reconciliation of interests has been achieved) or whether it is necessary to set up an investigating committee (see no. 7). The latter is the case if, in the opinion of the ombudsperson, the suspicion of scientific misconduct is substantiated. In justified cases, the LIKAT ombudsperson has the possibility to call the *central ombudsperson* of the Leibniz Association (see section 5.2) and to hand over the proceedings to that person.
9. As a rule, the ombudsperson informs the whistleblower in writing about the result of the preliminary examination.
10. The ombudsperson shall inform the LIKAT Board in writing of the result of the preliminary examination and the reasons for it.
11. If the ombudsperson discontinues the proceedings, the Board shall deal with the decision and its reasons at its next meeting at the latest (after receipt of the information). If the Board does not agree with the decision to discontinue the procedure, it may decide to set up an investigative committee or to forward the matter to the *central ombudsperson* of the Leibniz Association.

7. INVESTIGATING COMMITTEE TO REVIEW ALLEGATIONS OF SCIENTIFIC MISCONDUCT

1. The ombudsperson shall, at his or her discretion or upon resolution of the Board, establish an *Investigating Committee* to review allegations of scientific misconduct. It shall select its members and invite them to serve on it.
2. The *Investigating Committee* shall consist of at least three members who have the professional qualifications required for a comprehensive understanding of the scientific facts of the matter. If the allegations are particularly serious, members who are not employees of LIKAT may also be

appointed. In special cases, a fully qualified lawyer can also be appointed to the *Investigating Committee*. The *Investigating Committee* shall appoint a chairperson from among its members.

3. The LIKAT ombudsperson shall, as a rule, be a member of an *Investigating Committee*.
4. All members of the *Investigating Committee* shall have equal voting rights. The bias rules of the *Leibniz Competition* apply.
5. The *Investigating Committee* shall deliberate in non-public and oral proceedings. It shall agree on rules of procedure at its first meeting. In any case, there is a duty of documentation and a duty to record all steps taken.
6. The Board of LIKAT fully supports the work of the *Investigating Committee*.
7. All data and documents requested by the *Investigating Committee* shall be made available to it.
8. The members of the *Investigating Committee* and the involved employees of LIKAT as well as all persons involved in the proceedings or informed about the proceedings are bound to confidentiality.
9. The *Investigating Committee* shall examine at its own discretion whether scientific misconduct has occurred. It shall hear the accused person and the whistleblower and determine the context of the conduct complained of. The *Investigating Committee* may question further persons and commission experts as well as consult them in an advisory capacity.
10. As a rule, the review by the *Investigating Committee* shall be completed within a maximum period of six months from the constituent meeting of the *Investigating Committee*.
11. The *Investigating Committee* may decide to discontinue the proceedings.
12. The *Investigating Committee* shall draw up a report which either justifies the discontinuation of the proceedings or establishes the existence of scientific misconduct.
13. If the *Investigating Committee* concludes that scientific misconduct has occurred, i.e., if the majority of the *Investigating Committee* considers scientific misconduct to be sufficiently proven, the report shall, in particular:
    a. determine whether such conduct was grossly negligent or intentional; and,
    b. assess the seriousness of such scientific misconduct.
14. The report shall also state what further action the *Investigating Committee* recommends (referral to further institutions and bodies, initiation of appropriate measures, etc.).
15. The report will be submitted to the Board of LIKAT, which shall deal with the report at its next meeting (after receipt) and, if necessary, decide on further measures (see section 8).

8. CONCLUSION OF THE PROCEEDINGS

1. The Board of LIKAT decides on the basis of the report of the *Investigating Committee* on the existence of scientific misconduct on the necessary measures or the termination of the proceedings. In cases of scientific misconduct by employees of LIKAT, consequences under labor law shall always be examined first:

   a. warning,
   b. extraordinary termination,
   c. ordinary termination,
   d. termination of contract,
   e. particularities of employment contracts similar to civil service contracts.

2. If, on the basis of the *Investigating Committee* report, the board determines that the academic misconduct may result in the revocation of academic degrees, it shall forward the matter to the awarding university.

3. If, on the basis of the *Investigating Committee* report, the board determines that the academic misconduct could result in civil consequences, it shall consider the following civil consequences:

   a. issuance of a ban from the premises,
   b. claims for restitution against the person concerned, for example for the return of stolen scientific material or the like,
   c. claims for removal and injunctive relief under copyright law, personal rights law, patent law and competition law,
   d. claims for repayment, for example of grants, third-party funds or the like,
   e. claims for damages by LIKAT or by third parties in case of personal injury, property damage or the like.

4. Criminal consequences are always considered if there is suspicion that scientific misconduct simultaneously fulfills an element of the Criminal Code (StGB) or other criminal norms or administrative offenses. Criminal consequences would have to be drawn, for example, because of:

   a. copyright infringement,
   b. forgery of documents (including falsification of technical records),
   c. damage to property (including data alteration),
   d. property crime (including fraud and embezzlement),
   e. violation of personal life and secrecy,
   f. crimes against life and bodily injury.

   Involvement of investigative authorities should normally be coordinated with or initiated by the directors of LIKAT.

5. Scientific publications that are erroneous due to scientific misconduct must be withdrawn if they are still unpublished and corrected if they have been published (revocation); cooperation partners must be informed in an appropriate form if necessary. In principle, author(s) and publisher(s) involved are obliged to do so; if they do not take action, the Board of LIKAT will initiate possible appropriate measures.

6. The main reasons which led to the discontinuation of the proceedings or to the decision of the Board on measures to be implemented shall be communicated by the ombudsperson to the person concerned and to any whistleblowers.

7. In cases of serious scientific misconduct, the Board shall inform the Leibniz Association and, if necessary, other research institutions or scientific organizations concerned. In justified cases, it may also be appropriate to inform professional organizations.
8. The Leibniz Institute for Catalysis may be obliged to inform affected third parties and the public in order to protect third parties, to maintain confidence in scientific honesty, to restore its scientific reputation, to prevent consequential damage and in the general public interest.

9. ENTRY INTO FORCE

The *Guidelines of the Leibniz Institute for Catalysis (LIKAT Rostock) for safeguarding good scientific practice and for dealing with allegations of scientific misconduct* shall enter into force after adoption of the resolution by the Board with the internal announcement of the Institute as of 01 September 2019 and and replace all previously adopted guidelines for ensuring good scientific practice.

Rostock, August 12, 2019 Prof. Dr. Matthias Beller

LIKAT CAREER GUIDELINES FOR YOUNG SCIENTISTS

Leibniz-Institut für Katalyse

CONTENT

PREAMBLE

The LIKAT guideline for supporting young scientists is based on the *Leibniz Guidelines on Career Development*.[1] In addition, further measures of LIKAT are described in this guideline, which are relevant to the research at LIKAT or take into account organizational particularities.

LIKAT is aware of its regional and international importance and therefore tries to train qualified personnel and to support them in their personal and professional development. This is the only way to maintain or enhance the institute's long-term performance. In the course of the new strategic orientation of research at LIKAT, the support of young scientists aims at a thematic and personnel diversification. Young scientists will be encouraged to engage in international and interdisciplinary exchange and will be supported in building networks. The conditions at the institute are ideal for implementing basic research as well as application-oriented projects. Thus, future alumni can optimally prepare for a career in business or science.

1. GROUP OF PERSONS

1.1 Doctoral students

At the Leibniz Institute for Catalysis, about 100 doctoral students conduct research each year with the aim of obtaining a doctoral degree. It is an important concern of the institute to offer a guideline on the organizational procedure and the general conditions of a doctorate at LIKAT for the orientation of doctoral candidates and supervisors alike.

As an affiliated institute of the University of Rostock, LIKAT does not have its own right to award doctorates. The doctoral studies are carried out in cooperation with the University of Rostock.[2] Dissertations can be published either monographically or cumulatively. The latter requires the publication of at least three scientific articles in peer-reviewed journals and the acknowledgement of own contributions contained therein. Doctoral candidates must act as first author in at least two publications. PhD students at LIKAT can enroll as students at the University of Rostock and thus enjoy the same advantages as direct PhD students of the university. For communication with the university and for advising the students, LIKAT appoints a doctoral representative. The current doctoral representative is Dr. Christian Hering-Junghans. Furthermore, there is a cross-institutional representation for all PhD students and PostDocs (see *4.5 PhD & PostDoc Representatives*, p. 5).

For doctoral students, the aim is a three-year employment contract subject to social insurance contributions. Students with very good previous Master's degrees can apply for various scholarships (e.g. *Kekulé* scholarship of the *Fonds der Chemischen Industrie*). LIKAT explicitly supports such applications. In addition, LIKAT awards a small number of doctoral scholarships, especially for particularly well-qualified foreign doctoral students. The scholarships are awarded in accordance with LIKAT's scholarship regulations, in which guidelines as well as rights and obligations are formulated. The institute concludes a scholarship agreement with its doctoral scholarship holders.

PhD students at LIKAT are, regardless of the type of funding, equally placed with regard to the possibility to do a PhD and the scientific supervision of their PhD.

1 Leibniz Guidelines on Career Development

2 https://www.mathnat.uni-rostock.de/studium/promotion-habilitation/promotion

1.2 Researchers after the doctoral phase

LIKAT supports researchers who wish to obtain an advanced scientific qualification. The habilitation is the main degree sought here, which in most cases is required to take over a chair or professorship. As in the case of doctorates, the University of Rostock provides with its habilitation regulations[3] the framework for habilitation candidates of LIKAT and carries out the habilitations in cooperation with the institute. The habilitation theses can be submitted in the form of a (publication-oriented) monograph or cumulatively.

Habilitation candidates usually provide scientific services in the context of externally funded research projects either in the form of employment subject to social security contributions or via a scholarship. At LIKAT, young scientists with a doctorate who aspire to a habilitation are given the opportunity to set up a young research group, which is generally established for a limited period of time. Within this framework, the young scientists have both budget and personnel responsibility, which is advantageous as an additional qualification for a professorship or a leading position in science.

2. AIM OF THE GUIDELINE

The aim of the present guideline of the Leibniz Institute for Catalysis is to ensure good framework conditions for young scientists in all qualification phases. The guideline serves as a guide on how to provide good quality training and supervision. This includes not only the availability of material and equipment, but also personal exchange, motivating discussions and the identification of opportunities for further development. In this way, LIKAT aims to open up attractive perspectives and facilitate the transition to industry or the step into the next stage of an academic career.

The framework conditions in the scientific education should be designed in such a way that a professional focus on the successful completion of the planned career stage is created, taking into account the individual life paths.

3. CAREER PHASES & CAREER DEVELOPMENT AT LIKAT

In order to create optimal conditions for scientists in the qualification phases, they should be offered structured career paths at LIKAT, which include clear marking of important milestones. This includes transparent requirement profiles, which are guaranteed by a doctoral agreement and contribute to the quality of the work through ongoing feedback. Career paths in the Leibniz Association, including the Leibniz Institute for Catalysis, can be divided into four phases: 1. doctorate, 2. orientation after the doctorate, 3. consolidation after the doctorate, and 4. tenure & professorship, which are explained in more detail in the following sections.

3.1 First phase: PhD - Learning to research independently

First, a topic is determined between the doctoral candidate and one or more supervisors, which the doctoral candidate works on largely independently. Supervision by more than one person is necessary if the work is carried out in different *research departments* or *topics*. With the new research strategy at LIKAT, this form of supervision is becoming more common and there are clear rules for communication and responsibilities:

3 https://www.mathnat.uni-rostock.de/studium/promotion-habilitation/habilitation

- signing of a supervision agreement between the doctoral candidate and the relevant supervisors at the beginning of the doctorate,
- documentation of the qualification project (clear definition of the qualification goal, predicted duration, reasons for or measures against possible delays, determination of staff meetings),
- intensive exchange between all participants (for example, in the regular departmental and group seminars or topic meetings),
- regular discussions between doctoral researchers and supervisors with clear definition of research goals,
- various opportunities for doctoral candidates to present their own results (e.g. research group seminars, institute workshops, external events) in order to receive professional feedback and to acquire skills in confident presentation.

As a rule, contracts and project durations for doctoral candidates are set for at least three years from the start of research activities. Employment is to be on a 2/3 full-time basis for all doctoral candidates. During this time, the doctoral candidates should learn to organize and advance their research themselves and to further develop soft skills and languages. For this purpose, they can take advantage of *in house* courses offered by LIKAT or further training opportunities in cooperation with the Graduate Academy of the University of Rostock (e.g. on the topics of personnel management, conflict management, project management, lecture and presence training, etc.). A special annual soft skills workshop is *Rostock's Eleven*, which is organized by the association *Rostock denkt 365°* and in whose organization and implementation LIKAT has been involved as a member for many years. The workshop deals with science & communication. Science journalists from all over Germany support and evaluate the participating PhD students with regard to the target group-oriented communication of their scientific results to a broad public.

All young scientists are encouraged to publish their own research results in international, preferably renowned, *peer-reviewed* journals. The direct supervisor in the doctoral phase provides support in terms of both methodology and content. Participation in conferences is another tool for broadening the doctoral students' horizons and gaining experience in scientific exchange. In addition, PhD students are encouraged to undertake research stays of several months with cooperation partners in Germany and abroad. Travel expenses are reimbursed within the framework of the legal requirements.

3.2 Second Phase: PostDoc - Orientation after the Doctorate

After obtaining the doctorate, the so-called PostDoc phase takes place, the beginning of which is usually accompanied by a change of location and generally covers the first two years after the doctorate. During this time, the young scientists who have obtained their doctorate should sharpen their professional profile, develop personally and gain initial experience in acquiring third-party funding. Getting to know the scientific community should be deepened and expanded. This phase is characterized by new ideas that need space. During the goal-setting process, close exchange with colleagues and mentors is often needed. This exchange is made possible and encouraged at LIKAT. With the supervision of doctoral students and Bachelor or Master students, the PostDocs take on their first leadership tasks, as well as independent publication activities and coordination tasks. After or during this orientation phase, it should become clear to the young scientist where his or her future should lie, for example in academia, industry, public authorities, etc. The next step is to take targeted measures to ensure that the postdocs are able to continue their work in the future. Specific measures are then taken to focus on this goal. For example, if there is a particular affinity for industry-related research, increased work on joint research projects with companies can be offered. In this phase, LIKAT supports not only the professional development but also specific measures for qualification as a leader and in

management. Employment during this period is on a full-time basis, which can also be part-time if desired.

The *Leibniz PostDoc Network* offers itself for networking and orienting exchange.[4] It is an open way to exchange ideas with other postdoctoral researchers, to look beyond one's own horizon and to learn from the experiences of others.

3.3 Third phase: consolidation after the doctorate – determination on a topic

The third phase is mainly entered by outstanding young scientists who have decided to pursue an academic career. In most cases, and as is common in the field of chemistry, the habilitation is pursued. In order to be able to provide the necessary research performance, habilitation candidates at LIKAT are given the opportunity to establish a young research group at LIKAT, provided that the research topic fits the profile of LIKAT. With independently raised funds, post-doctoral researchers can supervise students and doctoral candidates and independently publish the results of their scientific work.

Habilitation candidates are increasingly involved in the institute community and in the institute's committees (*General meeting*, *Board of curators* and *Scientific & industrial advisory board*). The most important goal in this phase is to find and consolidate their own research profile. In this process, they are supported by a mentor who is himself or herself active at LIKAT, through continuous exchange and strategic advice. At least once or twice a year, a qualification meeting is held with the mentors to discuss the progress of the qualification work. In addition to research, the candidates are increasingly employed in teaching at the University of Rostock.

3.4 Fourth Phase: Tenure & Professorship

LIKAT supports the appointment of young research group leaders to a joint professorship with the University of Rostock. In these cases, they are active in research at LIKAT and teach at the University of Rostock. In principle, at least one previous change of location in the course of a scientific career is advantageous, as this contributes significantly to the development of young scientists. The goal of LIKAT is to open up tenure positions for outstanding scientists, provided that funding is available.

For LIKAT's own young scientists who have accepted a call to other universities, there is the possibility of association with the institute within the framework of *Uni in Leibniz*.

4. TARGETED SUPPORTING MEASURES AT LIKAT

4.1 LIKAT Community funds

PhD students and PostDocs are usually employed on a fixed-term basis and funded by acquired third-party funds or receive a stipend. In certain cases, funding may also be provided through the LIKAT Community Fund. The LIKAT Community Fund is an established instrument for providing security for employees in temporary employment during pregnancy, parental or nursing leave, or in cases of particular social hardship. It is a fixed component of the institute's budget and offers employees, including all salaried probationers, postdocs and scholarship holders, planning security and an easier return to work after family interruptions. The special funding is intended to help ensure that the desired degree is attained. Female scientists in the qualification phase mainly work in the laboratory. In the case of pregnancy, this is not possible for safety reasons. The fund can then be used, for example, to provide pregnant employees, regardless of their qualification level, with a laboratory assistant to carry out necessary laboratory work and to ensure the continuity of the laboratory experiments. Planning and

4 https://leibniz-postdoc.de/

evaluation of the experiments as well as the presentation of the research results remain the responsibility of the young scientist.

4.2 Scholarships

With very good previous degrees, young scientists can apply for various scholarships (e.g. *Kekulé* scholarship of the *Fonds der Chemischen Industrie*). LIKAT explicitly supports such applications. In addition, LIKAT itself awards doctoral scholarships. The scholarships are awarded in accordance with LIKAT's scholarship regulations, in which guidelines as well as rights and obligations are formulated. The institute concludes a scholarship agreement with its doctoral scholarship holders.

4.3 Mentoring

In addition to the institute's own mentoring for young scientists with a doctorate, doctoral candidates or postdocs of LIKAT can participate in the *KarriereWegeMentoring* program of the University of Rostock. They are supported in their career planning through seminars, peer-to-peer mentoring and dialogue with selected mentors.

Leibniz Mentoring offers attractive opportunities for female scientists who already hold a doctorate and who aspire to a leadership position in science. Female scientists at LIKAT have already been active as mentors in this framework themselves.

Open to all genders is the *CheMento* program of the *German Chemical Society (GDCh)*. In a kind of tandem relationship, experienced female and male chemists support young colleagues with their questions on career planning, career entry and orientation. With *CheMento*, the *GDCh* offers students, doctoral candidates and post-docs in chemistry the opportunity to make optimal use of the *GDCh* network.

4.4 Further training

The Leibniz Institute for Catalysis supports the further training of young scientists of all qualification phases, e.g. with internal and external offers, which can be used individually or as a group. LIKAT supports initiatives of scientists to attend and/or organize relevant workshops on content-related, methodological or technical issues. The institute offers (also in cooperation with the *Graduate Academy of the University of Rostock*) regular qualification courses in important aspects of scientific work, such as scientific writing, didactics, presentation techniques, time management and project management. Staff members who are to take on or have taken on management functions are enabled and encouraged to participate in seminars for managers and unprejudiced evaluation of people and performance.

Further training on an international level is also recommended and encouraged, for example participation in *summer schools*, e.g. the annual *Ostsee Lehrverbund Katalyse*, a summer school organized by LIKAT and supported by the *German Catalysis Society* (*GeCatS*).

LIKAT is continuously exploring new training opportunities and responding to existing needs.

4.5 PhD & PostDoc Representatives

The interests of the PhD students and PostDocs are protected and represented at LIKAT by the annually elected PhD & PostDoc representatives. As a rule, three persons are elected as representatives. Among other things, they are available as contact persons for organizational matters, supervision and problem solving, they mediate between PhD students and PostDocs and the institute management or the heads of the research departments, they inform about the *Graduate Academy of the University of Rostock*, and they promote cooperation, community and communication between PhD students and PostDocs, e.g. through special seminars and social events. The young scientists also meet regularly in plenary

meetings to discuss common issues and, if necessary, to pass on urgent matters to the elected representatives.

The PhD & PostDoc representatives are firmly integrated, both at LIKAT and at the University of Rostock. One representative participates in the monthly *extended board meeting* of LIKAT and is also actively involved in cooperations with the University of Rostock, especially with regard to questions concerning the realization of doctoral studies.

5. NETWORKING

In addition to the aforementioned support measures, LIKAT promotes the career opportunities and perspectives of its employees through networking: with academia and industry through a very intensive exchange often on the basis of institutional agreements. In particular, international exchange is supported here. For example, doctoral students can spend time as guests at project partners or foreign research institutions, provided that this serves the research objective.

5.1 Graduate Academy University of Rostock

The *Graduate Academy of the University of Rostock* is open to the PhD students of LIKAT. For admission to the academy, a supervision contract between the doctoral student and the responsible supervisor at LIKAT is concluded and presented. The Academy itself organizes courses (e.g. Good Scientific Practice, Fast Reading, Scientific Writing, Leadership Training) on the premises of the University. Furthermore, it provides financial support in case a specific training offer is not available locally.

In addition to this qualification program, the focus is also on networking within the Rostock science landscape. For this purpose, events such as science slams, research camps or regulars' tables are held.

5.2 LIKAT Alumni-Network

All current and former LIKAT staff members have the opportunity to stay in contact with young scientists via the *LIKAT Alumni Network*. This platform is coordinated by the *LIKAT staff unit*. A group in the career network *LinkedIn* has been set up especially for this purpose, in which current developments and research results are also reported.

Every two years, an *Alumni Day* is organized at LIKAT, to which graduates are invited. In lectures, alumni report on their life and career paths. The alumni lectures are accompanied by a poster exhibition of current research topics of PhD students and PostDocs of LIKAT. Thereby, the young scientists can easily exchange ideas with representatives from industry, academia and the public sector.

5.3 Leibniz Networks

LIKAT welcomes the exchange of PhD students and postdoctoral researchers in PhD and PostDoc networks. Especially the cooperation with the Leibniz-internal networks *Leibniz PhD Network*[5] and *Leibniz PostDoc Network*[4] is in the foreground and is actively promoted. The PhD & PostDoc representatives at LIKAT regularly exchange information with the elected representatives of the other Leibniz institutes.

5.4 Society of German Chemists and YoungChemistsForum

Together with the students of the University of Rostock and the Leibniz Institute for Baltic Sea Research in Warnemünde (IOW), the PhD students have the opportunity to get involved in the Rostock *Young Chemists Forum* (JCF) of the *German Chemical Society* (GDCh). Regular get-togethers are held, events

5 https://leibniz-phd.net/

(some of which are highly publicized) are organized, and excursions are organized to open up prospects for later entry into industry or other research institutions. LIKAT offers very committed young scientists the freedom to take up leading positions within these organizations, e.g. to become national spokespersons of the JCF.

In addition, the traditional GDCh lectures take place, to which international guests are invited. Usually once a year such a lecture is organized by the JCF. These lectures are open to all and offer interested LIKAT staff members the chance to look beyond their own professional horizons.

5.5 Leibniz ScienceCampus

LIKAT is leading the *Leibniz Science Campus ComBioCat*, which is dedicated to current challenges facing society: the transition from fossil resources to renewable raw materials for the production of chemicals and the development of alternative energy sources. In this context, catalysis is the key technology. In addition to LIKAT, the *universities of Greifswald* and Rostock, as well as the *Leibniz Institute for Plasma Research* and *Technology Greifswald* (INP) are involved.