HELMHOLTZ SPITZENFORSCHUNG FÜR GROSSE HERAUSFORDERUNGEN

MATERIALS RESEARCH STRATEGY OF THE HELMHOLTZ ASSOCIATION

May 2022

Foreword

The Materials Research Strategy of the Helmholtz Association presents the medium- and long-term strategic goals for developing new and improved materials. These materials include nanomaterials as well as structural and functional materials for solving urgent societal issues, such as materials for the energy transition (solar cells, electricity storage, fuel cells and hydrogen technology), lightweight construction and information technology, through to innovative materials for health research. The entire value chain from materials to systems is to be addressed.

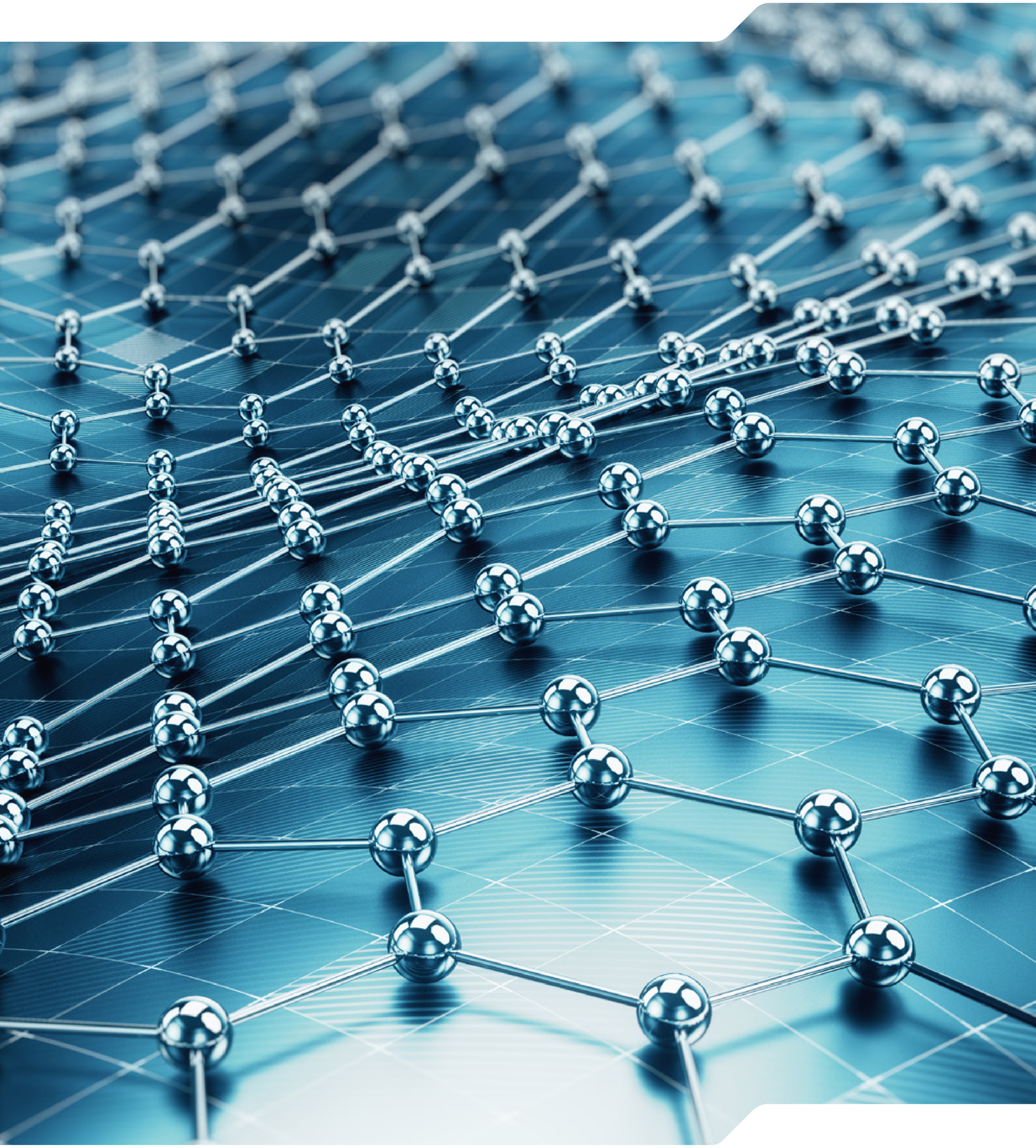
The programmatic research, especially in the Research Fields Information, Matter and Energy, forms the backbone for the strategic positioning of Helmholtz-specific materials research. Other important contributions come from the Research Fields Aeronautics, Space and Transport, Health, and Earth and Environment. Thus, a future-oriented and cross-thematic development and application of new materials and characterization methods is achieved. To this end, thematic bridges between the Research Fields in the Helmholtz Association are being established and expanded, and the competencies are being made usable across the Research Fields in a network.

The Helmholtz Association's materials research has the following unique selling points in the national and international science system: The synergy effects resulting from the combination of expertise available in the individual research units, the long-term, programmatic and cross-programmatic research approach, and the use of outstanding research infrastructures.

First, an overview of the current and future goals of the contributing Research Fields in the field of materials research is presented. Based on this, the activities of Helmholtz Association materials research in the form of *method-oriented "platforms"* and *application-oriented "focus topics"* will be highlighted and will be an essential component for the implementation of the Helmholtz Association materials research strategy.

The Helmholtz Association thus makes an outstanding contribution to the BMBF's Materials Research Impulse Paper and strengthens Germany's international visibility and competitiveness in the field of materials research. The materials research strategy is closely interlinked with the strategies on *digitalization* and *quantum technology* in the Helmholtz Association, and complements them in terms of content.

I. MATERIALS RESEARCH IN THE HELMHOLTZ ASSOCIATION



Materials research combines interdisciplinary scientific approaches from the natural and engineering sciences and thus provides solution options for a variety of socially relevant challenges. Particularly in the major challenges of the energy transition, information and communication technology, health, environmental protection and climate change, essential technological innovations and the associated economic value creation and technical sovereignty that depend directly or indirectly on materials and their research, development and optimization. Materials research thus creates the basis for innovative functionality and sustainable use of components and systems. A prerequisite for this is the precise knowledge of the structure of materials from the atomic, to the mesoscopic, to the macroscopic level, which is investigated with the highest temporal and spatial resolution in the Helmholtz Association. This enables the tuning of mechanical, physical, chemical and biological properties. With the accompanying increase in fundamental understanding of complex structural and property relationships, *digitalization* is opening a new era of knowledge-based materials design with information-based research and virtual design to develop new materials and material concepts along the entire life cycle.

Long-term programmatic research, especially in the Research Fields Information, Matter and Energy, forms the backbone for the strategic positioning of Helmholtz-specific materials research. Other important contributions come from the Research Fields Aeronautics, Space and Transport, and Earth and Environment. For health research, the interface of innovative materials and stem cell research promises groundbreaking advances for medicine and new treatment methods. The Helmholtz Association targets a future-oriented and cross-thematic development and application of new materials and characterization methods. To this end, thematic bridges between the Research Fields in the Helmholtz Association are being established and expanded, and competencies are being bundled in a network with further links to the *digitalization strategy*, the activities in quantum technology ("*Quantum Roadmap*") and hydrogen technology ("*Competence Atlas Hydrogen*") in the Helmholtz Association. The materials research strategy presented here focuses primarily on networking method- and information-based approaches to materials research with the various fields of application. The Helmholtz Association will thus strengthen Germany's international visibility and competitiveness in the field, as called for in the BMBF's impulse paper on materials research.

II. OBJECTIVES OF THE MATERIALS RESEARCH STRATEGY

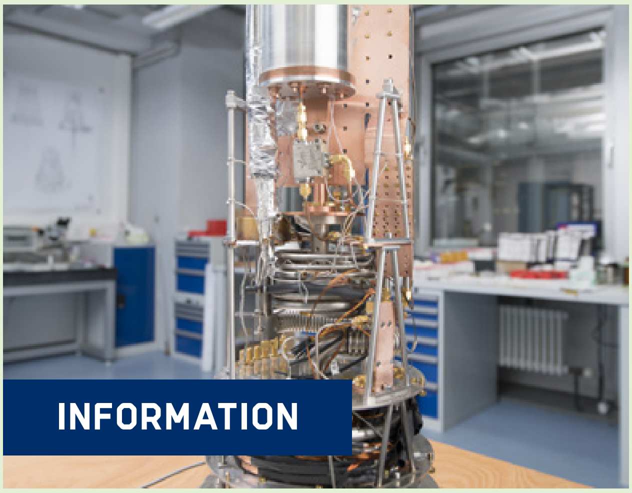
Overarching the Research Fields, the Helmholtz Association Materials Research Strategy presented here pools the competencies and resources of the Research Fields Information, Matter, Energy, Aeronautics, Space and Transport, Health, and Earth and Environment in the Helmholtz Association. The goal is to more closely integrate the materials science activities of the various Helmholtz centers and programs, especially in terms of methods used and concrete applications ("*focus topics*") along major societal issues, and thus increase visibility. Through the partnership of the participating materials research centers (DESY, DLR, FZJ, GSI, HZB, HZDR, Hereon, KIT), completely new opportunities for use in materials modeling, synthesis and characterization at unique research infrastructures will be created for cutting-edge research and expanded in collaboration with research centers from the Research Field Health, also under the area of *digitalization* and *biologization*, i.e., the increasing integration of principles from nature into materials and product development. This is being done on the basis of existing experience and competencies of the individual departments. The research portfolio is being strategically developed accordingly, as well as through the design of cross-functional activities in the PoF IV period. Unique selling points in the national and international scientific system of Helmholtz Association materials research will be achieved through the further development and use of unique large-scale facilities and research infrastructures, through synergy effects between the diverse expertise of the Research Fields, and through long-term, programmatic, and cross-program and cross-domain research.

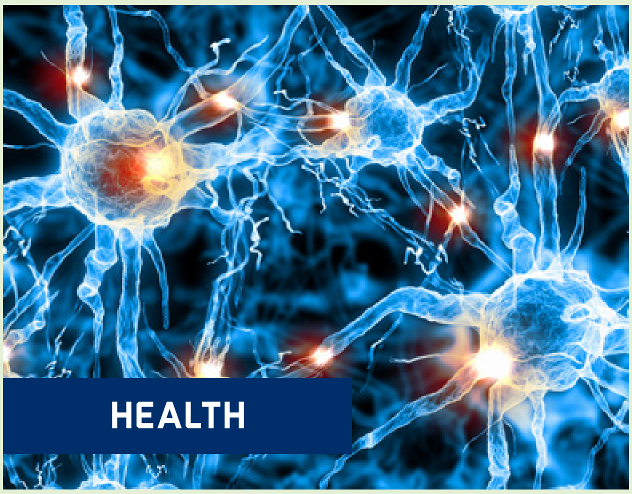
THE MOST IMPORTANT GOALS OF THE HELMHOLTZ MATERIALS RESEARCH STRATEGY ARE:

- The *digitalization* of materials science in data acquisition and research data management, and through further expansion of simulation and approaches to the "*digital twin*" of materials systems
- The *accelerated development* of materials in a wide range of applications for improved material properties and sustainability
- The development and provision of new high-throughput methods for the *synthesis and characterization* of materials
- The comprehensive expansion and use of Helmholtz-wide *large-scale facilities and research infrastructures* for materials research
- *Talent acquisition and promotion* for the maintenance and expansion of competencies in science and industry
- The organization of *technology and knowledge transfer* for the sustainable mastering of societal challenges in cooperation across the Research Fields and with partners in industry and society

It is evident that progress in materials-driven innovations also requires efficient transfer of research and development results along the entire chain from atomic structure to complex material system and component in use. Accordingly, a central task of the materials research strategy is to broaden the basis for comprehensive collaborations between the partners involved and, by generating synergies in materials research, to establish the Helmholtz Association specifically as a research and technology partner in application-related collaborations. Thus, on the one hand, instruments and methods for state-of-the-art material development are created and made available to cooperation partners ("*method platforms*"). On the other hand, the requirements along the entire value chain, including the necessary efforts for *sustainability*, from development, synthesis and characterization to the market-ready product, are dealt with in cooperation with national and international research institutions. The scientific acquisition of knowledge, the development of new technologies and processes, and the Helmholtz Association's unique infrastructures are the basis for the intensive dialogue with industry, through which the results of the Helmholtz Association's materials research are economically implemented (technology transfer). At the same time, the dialogue with society and politics allows a framework to be set for new materials and applications.

III. PARTICIPATING RESEARCH FIELDS AND THEIR COMPETENCES IN MATERIALS RESEARCH





As a scientific organization with 19 scientific-technical and medical-biological research centers, the Helmholtz Association provides expertise in materials science in a wide range of fields. This includes in particular the large infrastructures for materials characterization, modification, and simulation, as well as scientific expertise in materials synthesis, theoretical approaches to the *digitalization* of materials science, and materials engineering as an important basis for technology development in application domains such as energy, mobility, and information. The complementary expertise are strategically positioned in the different Research Fields and programs.

The Research Field Information is designed within the framework of PoF IV as a central link between *materials research, digitalization and biologization* ("information-driven"). In the Research Field Matter, the available large research infrastructures are used to modify materials in a targeted manner and to examine specific aspects of the synthesis and characterization of materials and the elucidation of structure-property relationships and dynamics ("method-driven"). Complementary to this, materials science and engineering in the Research Fields Energy, Aeronautics, Space and Transport, Health, and Earth and Environment make significant contributions to specific technology development ("application-driven") as shown in Figure 1.

In the following, the core competences of the Research Fields Information, Matter and Energy as well as the infrastructures are presented in detail to show the already existing prerequisites for Helmholtz-wide materials research. The points of connection to materials research in the Research Fields Earth and Environment, Health, and Aeronautics, Space and Transport are briefly described.

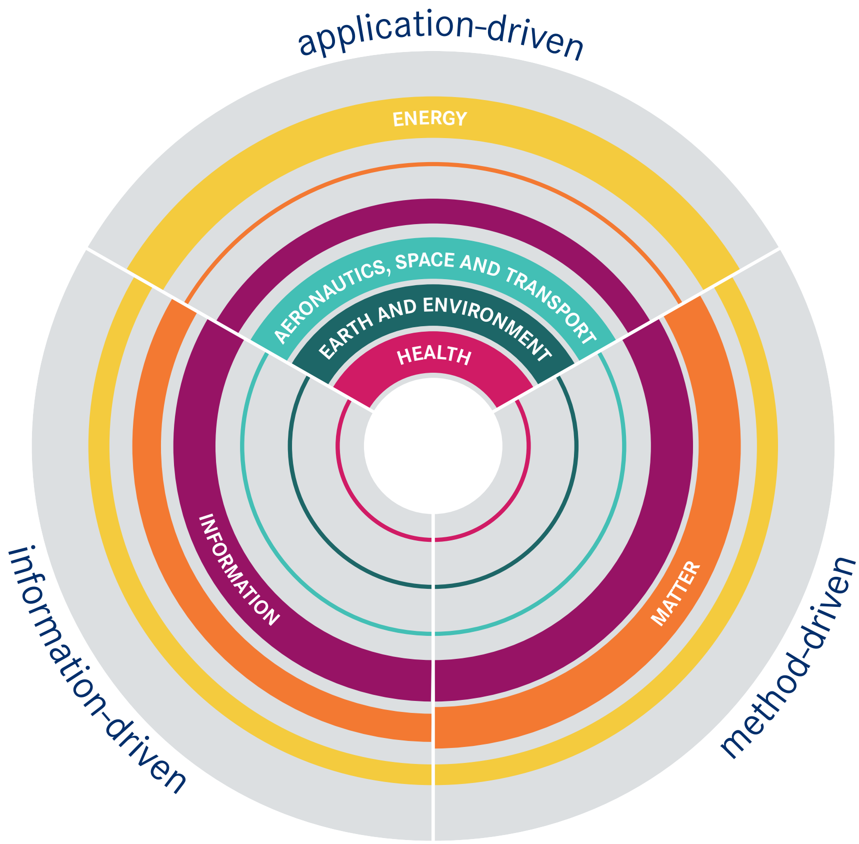
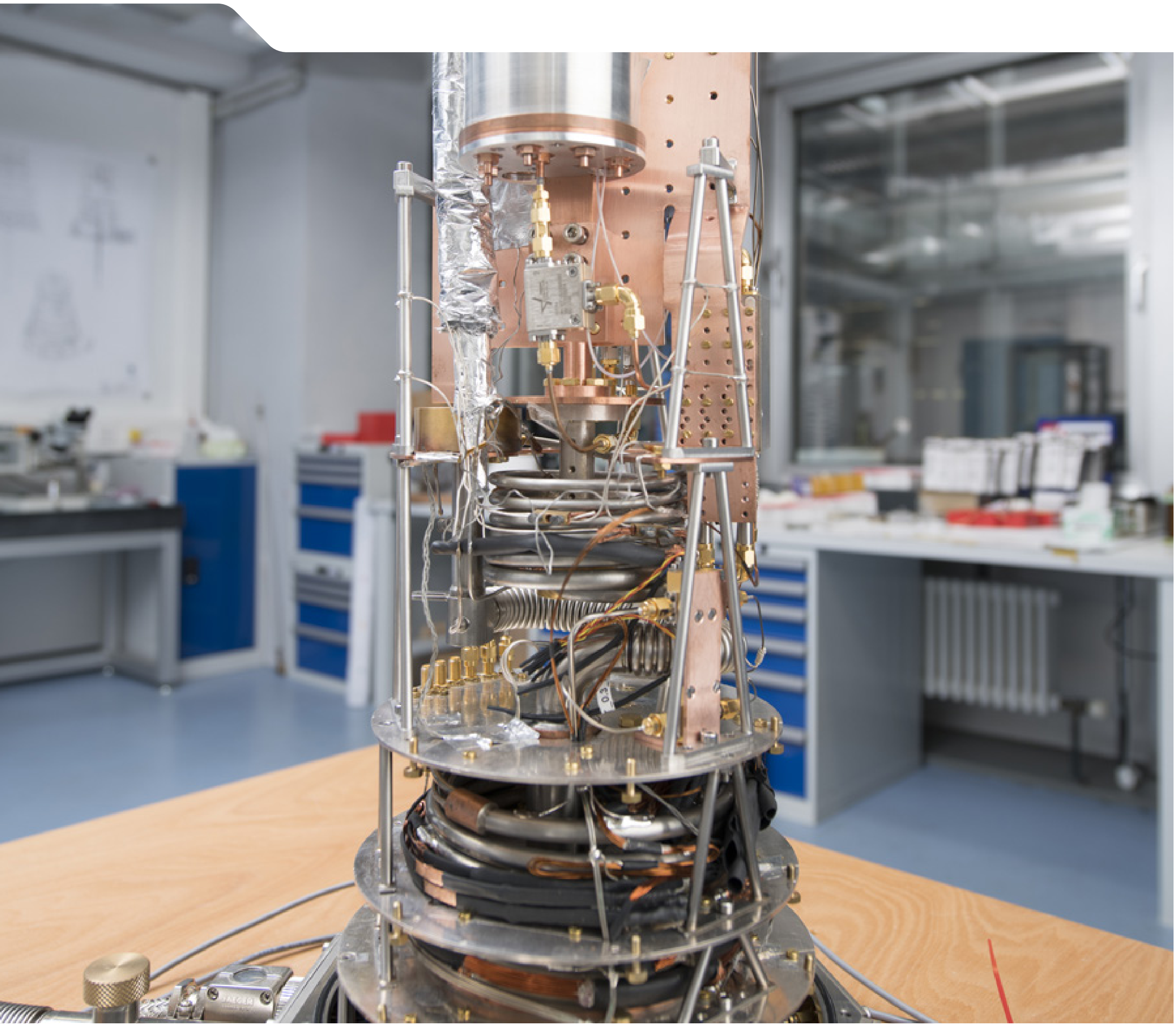


Fig. 1: Materials research in the Helmholtz Association - Complementary core competencies of the Research Fields.

MATERIALS RESEARCH IN THE RESEARCH FIELD INFORMATION

In the Research Field Information, methods for the design of new materials are developed generically and validated on the basis of selected applications, which include material separation and storage technologies, photonics, lightweight construction, information technology, and medicine. By considering the value chain from material to system, a special focus is placed on artificial and biological information systems and technologies. The Research Field develops processes for material synthesis and patterning, including in clean room infrastructures, and provides dedicated characterization methods including *in situ* and *operando* observations in the field of electron microscopy and spectroscopy. In addition, the focus is on digital smart process technology, for example, for semi-finished products made of innovative lightweight materials or materials for medical technology. Taken together, this leads to the development of "*digital twins*" that are intended to encompass the entire life cycle of a material system.



The task of the Research Field Information is to create method- and technology-oriented foundations for the digital transformation of science, industry and society. In PoF IV, the Research Field Information will conduct use-inspired basic research with a specific research portfolio (see following descriptions of the programs). The material sciences and neurosciences, which are located in the Research Field Information, act as a basis, driver and at the same time as application fields of information technology.

PROGRAM "ENGINEERING DIGITAL FUTURES: SUPERCOMPUTING, DATA MANAGEMENT AND INFORMATION SECURITY FOR KNOWLEDGE AND ACTION"

The main objective is to develop solutions to the methodological, technical, instrumental, organizational, and societal challenges facing modern science, engineering, industry, and society in the era of digital transformation. Important are the development of novel methods and tools for simulation and data analysis, as well as the establishment and operation of strategic infrastructures, especially with regard to exascale computing, for the testing of which materials research represents an important field of application, and to a much stronger focus on the field of research on IT security. These efforts, which are based on excellent computer science and information technology, are supplemented by accompanying approaches in order to take a holistic look at societal innovation potentials, value chains, acceptance issues, but also possible risks.

PROGRAM "NATURAL, ARTIFICIAL AND COGNITIVE INFORMATION PROCESSING"

The program has a coordinating role in various initiatives that address the major challenges of advancing *digitalization*. By exploring the connecting elements of inanimate matter and biological systems (including the human brain), the goal is to achieve a comprehensive understanding of the fundamental rules of information processing, and then adapt this to develop new principles for the next generation of computer systems. This includes, in particular, the topics of energy efficiency as a technology driver, self-learning neuromorphic systems as a basis for the realization of Industry 4.0 and of autonomous systems, and quantum materials and quantum computing for the computation of complex systems and with potential applications in many other areas (for example, for improving data security, communication, or metrology). The coordination of these research areas in one program opens up unique opportunities for knowledge transfer and interdisciplinary collaboration. Thus, the program is of central importance for the basic life science research of the Research Field and its bridging towards the integration of biological principles into technical solutions.

PROGRAM "MATERIALS SYSTEMS ENGINEERING"

The objective is to drive the transformation to virtual and data-driven materials research on the basis of experimental and theoretical work in order to (i) enable the *digitalization* of materials science and materials engineering by generating digital images of the materials, the relevant processes and applications, and to accelerate this through predictive approaches, as well as (ii) to realize the research and simulation of multifunctional material systems across the entire process chain up to translation (life cycle analysis). The spectrum of material systems to be investigated includes the atomic and molecular level as well as active and responsive hybrid or composite materials, photonic materials, smart bioactive materials, and hierarchically organized, cross-scale material systems with specific functionalities where applicable.

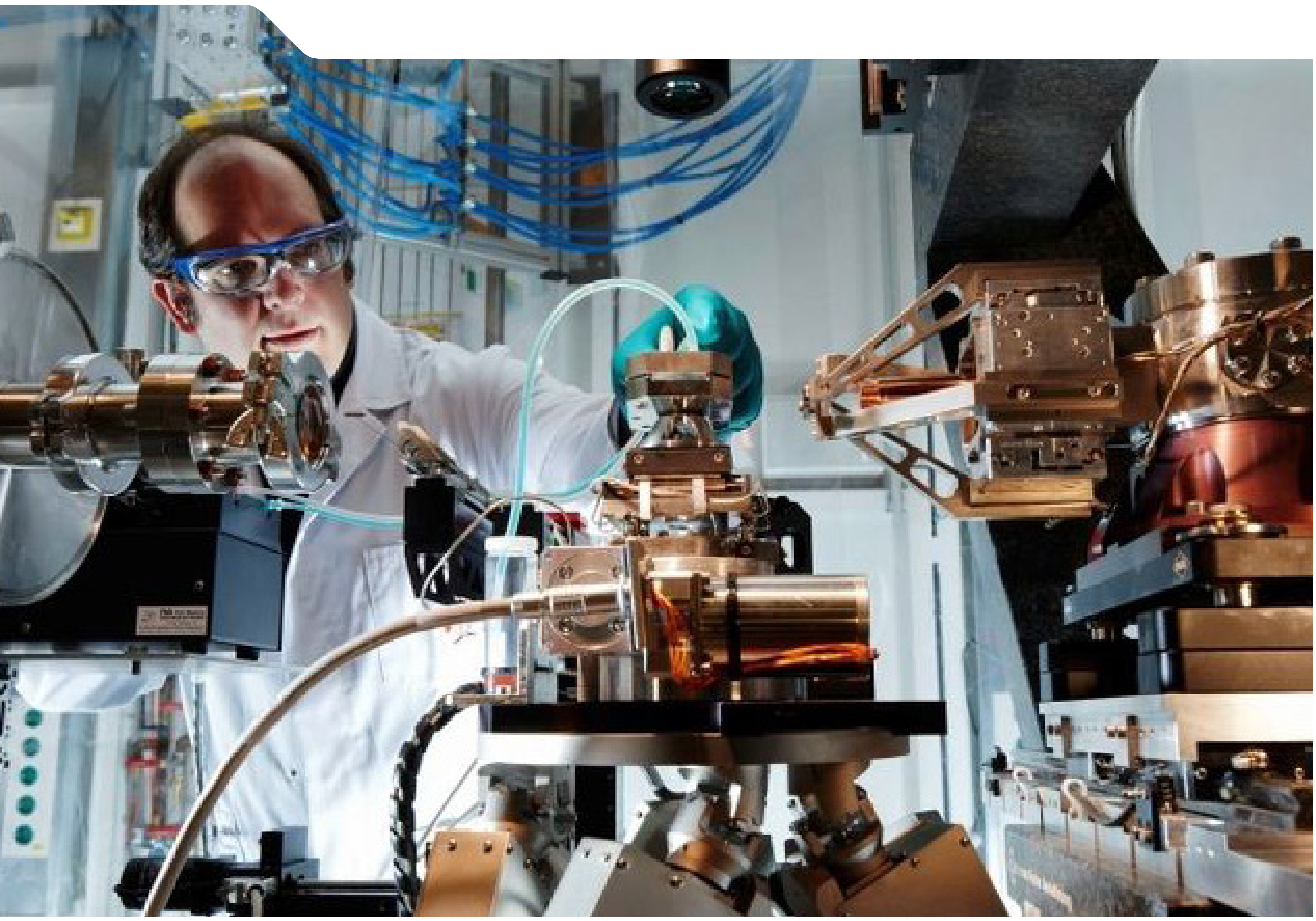
Through virtual and data-driven material development and in conjunction with a uniform data management concept, reverse material development is to be made possible in the medium to long term, i.e., a rational derivation of material properties from the product properties required on the market, with explicit consideration of the *sustainability* of the materials (life cycle analysis). The activities of the BMBF's "*MaterialDigital*" initiative will also be incorporated here. Materials science is becoming the driving force behind rapid further development of information processing technology (fully automated structural analysis, data-driven materials development) as well as modeling and simulation (*ab initio* calculation, molecular dynamic simulation, multiscale simulation).

MATERIALS RESEARCH IN THE RESEARCH FIELD MATTER

The Research Field Matter has special competences in the development, construction, operation and use of large research infrastructures for interdisciplinary questions concerning the characterization, modification and synthesis of materials. The primary goal is to obtain an in-depth, microscopic understanding of matter, materials, and biological systems. The outstanding research infrastructures of the Research Field Matter include large-scale facilities that provide photons, neutrons and ion beams as well as the highest electromagnetic fields.

In particular, the **PROGRAM "FROM MATTER TO MATERIALS AND LIFE" (MML)** focuses on material characterization and investigation of structure-property relationships. The above research infrastructures allow, among other things, investigations on extremely short to atomic length and time scales. In the MML program, the detailed structure and electronic, optical, magnetic, and chemical properties of matter and materials, as well as electronic, catalytic, and (bio)chemical processes are explored. With specific use of the MML large-scale facilities and their diagnostic capabilities, these investigations are carried out on all relevant length and time scales. In-depth knowledge of these processes through *in situ* and *operando* studies and their control serve to develop functional materials and materials for novel devices and applications.

Activities in the **PROGRAM "MATTER AND TECHNOLOGIES" (MT)** consider developments of semiconductor detectors, based on silicon, but also diamond and other materials. These micro- and nano-structured detectors enable high spatial resolutions, for example, facilitating the recording of scattering images of complicated systems at synchrotron radiation sources and FELs or signals at very



high count rates and with picosecond time resolution, as they will occur in future experiments at accelerators at the highest rates.

Thanks to the interdisciplinary nature of the materials research activities of the Research Field Matter, thematic bridges to other Research Fields exist. For example, the ion accelerator facilities of the Research Field Matter are used to study the beam resistance of space electronics and materials developed and applied in the Research Field Aeronautics, Space and Transport. Research on fundamental questions about the behavior of matter and materials under extreme irradiation and pressure conditions are relevant for the application of materials in fusion reactors or for the safe storage of radioactive waste, and open a novel way to synthesize new materials. A bridge to the Research Field Health is provided, among others, with investigations of the dynamics of structural changes in bio-molecules, and with the development of bio and chemical sensors in the field of nanotechnology, or with tumor therapy using ion beams. Materials for the energy transition (for example, in the field of catalysis, hydrogen, thermoelectrics, and batteries) are produced and characterized within the Research Field Matter at various photon, neutron, and ion large-scale facilities, which in turn supports the activities in the Research Field Energy. Similarly, quantum materials for future applications in information technology are also being investigated in the Research Field Information. All of this also requires strategies for the management and analysis of big data. Here, too, the bridge to the Research Field Information, especially within the planned cross-sectional activities for material characterization, plays an important role.

MATERIALS RESEARCH IN THE RESEARCH FIELD ENERGY

The Research Field Energy investigates materials and technologies for the energy transition. It deals with materials research and materials engineering as an essential basis for new technologies for efficient energy conversion, storage and use. This also includes cross-field materials synthesis facilities and characterization platforms, in which the Research Field Energy is actively involved.

Questions of materials research, from new material concepts to their synthesis and the investigation of their reliability, are an integral part of technology development in the Research Field Energy and enable innovative leaps in the corresponding energy technologies. The goals here are, above all, appropriate lifespans and increased energy efficiency, as well as environmentally friendly energy provision and cost efficiency across the entire range of topics within a circular economy approach.

For this purpose, the Research Field Energy operates dedicated synthesis and characterization platforms for energy-relevant applications (for example, Energy Materials Characterization Platform (HEMCP), Helmholtz Energy Materials Foundry (HEMF) or Energy Materials *in situ* Laboratory (EMIL@BESSY II). In addition, methodological developments in the Research Fields Information and Matter are used and contributed in the area of materials development for the various energy technologies, as well as to the targeted further development of characterization and modeling methods.

A successful example is the rapid development of initially basic research in the Research Field Information on the topic of electrochemical energy storage with the subsequent transfer to research related to individual technologies in the Research Field Energy. To strengthen the topics of photovoltaics and catalysis, a similar approach was taken with regard to PoF IV. In general, the interfaces between the Research Fields also ensure that developed methods, for example, for virtual material design discussed above or methods of material characterization, are increasingly used in application-related research.

PROGRAM "MATERIALS AND TECHNOLOGIES FOR THE ENERGY TRANSITION" (MTET)

The goals of the energy transition include not only a massive increase in the share of renewable energies, but also a significant increase in efficiency in the development, provision and use of energy resources, as well as mineral and metal-bearing resources. Therefore, on the one hand, innovative technologies are needed to develop the various renewable energy sources efficiently and cost-effectively and to use them optimally in centralized and decentralized applications. On the other hand, intensive research and development is required for efficient storage in batteries, for the generation and use of hydrogen, and for the entire range of power-to-X technologies, including the use of CO_2, in order to make the future energy system free of fossil fuels and sustainable, i.e., environmentally compatible, reliable, demand-oriented and affordable.

The program incorporates multiple technological options from the scientific basis for disruptive innovations to the timely application of new technologies. Low-cost, high-performance materials are a prerequisite for all technological options.

The MTET program considers technological options in the following five program topics (Topics):

- Photovoltaic and wind energy
- Electrochemical energy storage
- Chemical energy carriers
- High temperature technologies
- Resources and energy efficiency

Materials research and development are an integral part of the respective topics, so that the various technologies are worked on in a process chain from materials research to application in close coordination between the groups involved.

"FUSION" PROGRAM (FUSION)

The Fusion program deals with the physical aspects and the technologies and materials required for the construction and operation of fusion experiments and future fusion reactors.

Topic 3 "Technologies and Materials for Fusion" covers developments of technologies and materials for existing (Wendelstein 7-X), under construction (JT-60SA, ITER), and future fusion facilities (DEMO). In ITER and DEMO, fusion reactions will be realized on a large scale, resulting in new challenges for the materials to be used, especially with respect to neutron reactions. Since the understanding and control of plasma-wall interaction are crucial for the efficient operation of a fusion power plant, key issues in Topic 4 "*Plasma-Wall Interaction*" are also closely related to material aspects, in particular the choice and characterization of wall materials.

Fusion plants impose extreme conditions on structural as well as functional materials (including high temperatures, pressures and magnetic fields, high-energy neutrons, cyclic alternating loads), which, in addition to low activatability, should simultaneously guarantee high operating life and reliability. This exceeds the limits of further development of conventional materials and requires innovative material concepts to ensure technical performance whilst also taking sustainability and environmental aspects into account.

Successful examples of this strategy, which has been pursued for many years, include high-temperature superconducting cables and power feeds, ductile tungsten, diamond windows, graded tungsten protective coatings and additive manufacturing processes, the development of which has not only advanced fusion but can open up application areas far beyond fusion.

NUCLEAR WASTE MANAGEMENT, SAFETY AND RADIATION RESEARCH (NUSAFE) PROGRAM

The NUSAFE program includes basic and applied research on safe nuclear waste management in deep geologic repositories and provides (radio)geochemical and (radio)biogeochemical input to site selection and characterization. It also investigates innovative disposal strategies for the decommissioning of nuclear facilities and for the treatment of radioactive waste streams.

Materials science research in NUSAFE includes the investigation of radioactive materials on research infrastructures and the elucidation of the behavior of structural materials under reactor-typical conditions. For example, ODS steels are studied here in the area of materials and component safety.

MATERIALS RESEARCH IN THE RESEARCH FIELD AERONAUTICS, SPACE AND TRANSPORT

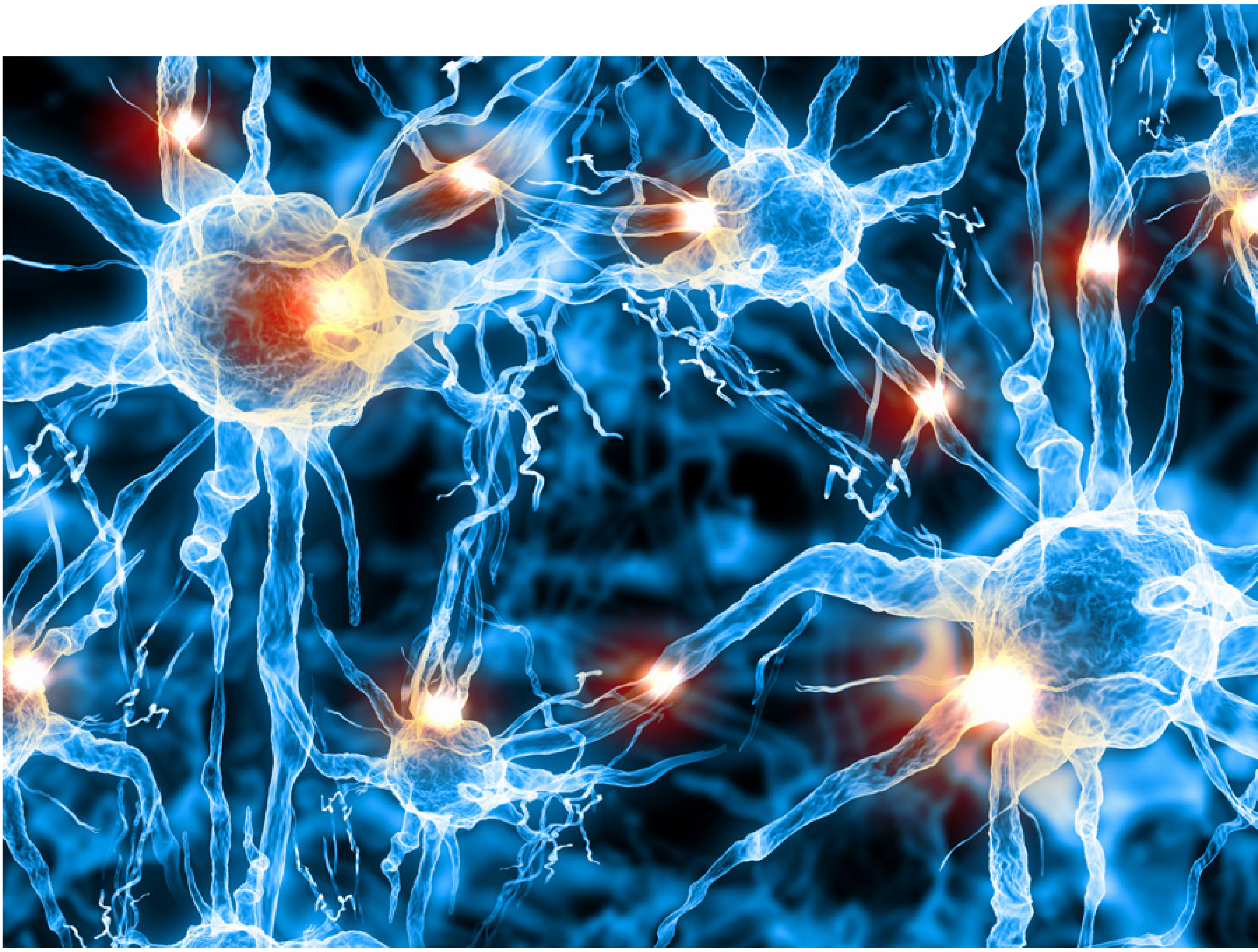
The Research Field Aeronautics, Space and Transport focuses on optimizing existing and developing new materials for high-performance lightweight structures for safe and economical aircraft and spacecraft. The goals are the improvement of economic efficiency and safety in combination with the reduction of the footprint of climate-damaging emissions. In this context, the research addresses new metallic alloys and ceramic composites for high-temperature use in propulsion systems and new light metals and polymer composites for aerospace structures. 3D printing opens up new design options, but also calls for the development of new materials adapted to the process in the aforementioned material classes. The manufacturing processes of composites and 3D printing require the inclusion of all process steps, from the base material to automated production. Only in this way can a complex material provide optimal structural mechanical performance in the target structure. The scientific work for this extends from the simulation of the material and its properties at the atomic and microstructural level, to the design and calculation of structures, the digital integration of the individual process steps along the entire process chain, and the experimental validation of the simulation chain. Physical verification is consistently extended into the full-scale range up to the size of a hull segment. In the future, the goal is the digital evaluability of material solutions in the context of the structure of an entire aircraft, carrier or satellite system. In this context, time and financial expenditures for the development of new materials are playing an increasingly important role. Research in the area of cross-scale digital tools combined with the future use of quantum computing and an integrated digital data management system is expected to reduce development times and costs by more than 50%.

MATERIALS RESEARCH IN THE RESEARCH FIELD EARTH AND ENVIRONMENT

The Research Field Earth and Environment studies the Earth system and its sustainable use. Materials play an important role in many respects: Raw materials are extracted from compartments of the Earth system and introduced into terrestrial, marine and atmospheric systems as residual and waste materials through and during human use. Persistent substances and pollutants resulting from their degradation are now found in all regions and compartments of the Earth system. In PoF IV, the Research Field has therefore also focused on sustainable use to explore ways of extracting and using raw materials in an environmentally sound manner, in the sense of a circular economy in which environmental protection is an integral part of the systemic approach. Bioeconomic approaches also use biomass and knowledge of biological systems to produce environmentally friendly raw materials and develop biobased materials; biotechnological and bionic research uses knowledge of biological systems to develop and sustainably produce materials with new properties. In addition, new materials can fulfill important contributions to the protection of the Earth system. Furthermore, the Research Field has authoritative expertise in life cycle analysis, which will also be incorporated into materials research.

MATERIALS RESEARCH IN THE RESEARCH FIELD HEALTH

The Research Field Health researches the causes and development of the major widespread diseases. These include cancer, cardiovascular, metabolic, pulmonary and infectious diseases, as well as diseases of the nervous system. Research into complex and often chronic diseases requires interdisciplinary approaches, such as the use of new materials, which the Helmholtz Centers are advancing together with partners from universities, other research organizations, and industry. The Helmholtz Centers in the Research Field Health also contribute their excellent basic research to the German Centers for Health Research initiated by the BMBF in order to transfer research results more quickly into clinical applications. For example, research into nanomaterials plays an important role in establishing intelligent carrier systems that improve the targeted absorption of active substances or even make it possible in the first place. The development of artificial tissues and organs at the interface of materials and stem cell research promises breakthroughs for diagnostics, regenerative therapy and prevention in the sense of personalized medicine.



IV. IMPLEMENTATION OF THE HELMHOLTZ ASSOCIATION MATERIALS RESEARCH STRATEGY

Materials research offers opportunities but also creates challenges, which the Helmholtz Association will address in the coming years with the competencies outlined here to achieve the goals set. Implementation requires a wide variety of measures as well as a continuous dynamic process for the further development of research topics. The Helmholtz Association is already demonstrating its great potential in the Research Fields and beyond, together with national and international partners, which is also built upon its unique infrastructures.

The Helmholtz Association Materials Research Strategy aims to expand this potential and to find innovative contributions to solutions for urgent social and economic issues through interdisciplinary approaches. The visibility of Helmholtz Association materials research in the national and international research landscape is to be further increased by the following key points:

- The complementary competencies of the Research Fields will be expanded as a basis for the Helmholtz Association materials research strategy and oriented towards a high degree of synergy and mutual strengthening of the overarching division of work.
- The exchange of knowledge and methods across Research Fields as well as the dialogue with society and the cooperation with industry will decisively strengthen the innovative power.
- The existing and future planned large-scale facilities and research infrastructures of the Helmholtz Association will be used comprehensively and synergetically by the national and international materials research community.

STRUCTURE AND NETWORKING

The establishment of a Helmholtz Association-wide materials research network will support the cross-Research Field exchange of knowledge as well as contribute to the visibility of materials research in the Helmholtz Association. By means of structure-giving elements, the research landscape at the Helmholtz Association and throughout Germany is to be strengthened in order to better position itself among the international competition. Essential elements are a cross-Research Field data infrastructure, also as part of the National Research Data Infrastructure (NFDI), as well as an overview of available methods and contacts, which will also expand and strengthen contacts and cooperation with industry.

The complementary work of the Research Fields is brought together on selected topics and the added value based on knowledge exchange for processing in the respective globally visible and strategically relevant topic is shown. These selected activities are characterized by a critical size and will have the following functions for cross-Research Field materials research:

- Methodological development for the benefit of multiple topics, programs and Research Fields in the Helmholtz Association.
- Formation of a cross-Research Field scientific community within the Helmholtz Association (for mutual support).
- Efficient use of resources in the Helmholtz Association (coordinated use of infrastructures and planning of large, unique facilities).
- Responding to socially relevant questions.

As a baseline scenario, the activities here are organized into two **method platforms** and **application-oriented priority topics**. The method platforms, "*Accelerated Material Development*" and "*Correlative Material Characterization*", are dedicated to the overarching questions of modeling/simulation, synthesis and processing, and characterization; the answers to which are important for a variety of applications. The Joint Labs "*Virtual Materials Design*" (VMD) and "*Integrated Model and Data driven Material Characterization*" (MDMC), which have already been established in the Research Field Information, represent an essential part of the information-based method-oriented integration of the Helmholtz Association materials research strategy. The priority topics "*Materials for Information Technology*", "*Battery Materials*", "*Materials for Hydrogen Technology*", "*Photovoltaic Materials*", as well as "*Materials for Health*", "*Bio-based and Bio-inspired Materials in the Bioeconomy*" and "*Lightweight Construction*", deal with the development of materials along the complete value chain from the atom to the material system in concrete applications in socially highly relevant subject areas. For this purpose, PoF IV bundles related activities in the respective programs into topics (for example, photovoltaics in the Research Field Energy program "Materials and Technologies for the Energy Transition") and thus also contributes to the further development of cross-departmental materials research. In all activities, sustainability and the circular economy of materials are also considered as a central aspect. The mutual transfer of knowledge and the cooperation of the method platforms with the application-oriented priority topics form the matrix of the Helmholtz Association materials research strategy (see Figure 2), which is described in detail in Chapter V.

Planned cross-Research Field activities within PoF IV are examples of the emergence of a value chain that benefits from the competencies of the participants. These include, above all, the "*Joint Labs*" within the Research Field Information, projects within the IVF (for example, pilot projects within the platforms of the Helmholtz Incubator Information & Data Science, which bridge data science to materials science and are to be closely interlinked with the activities in the NFDI), and the Innovation Pool projects of the participating Research Fields, whose topics enable links to the Re-

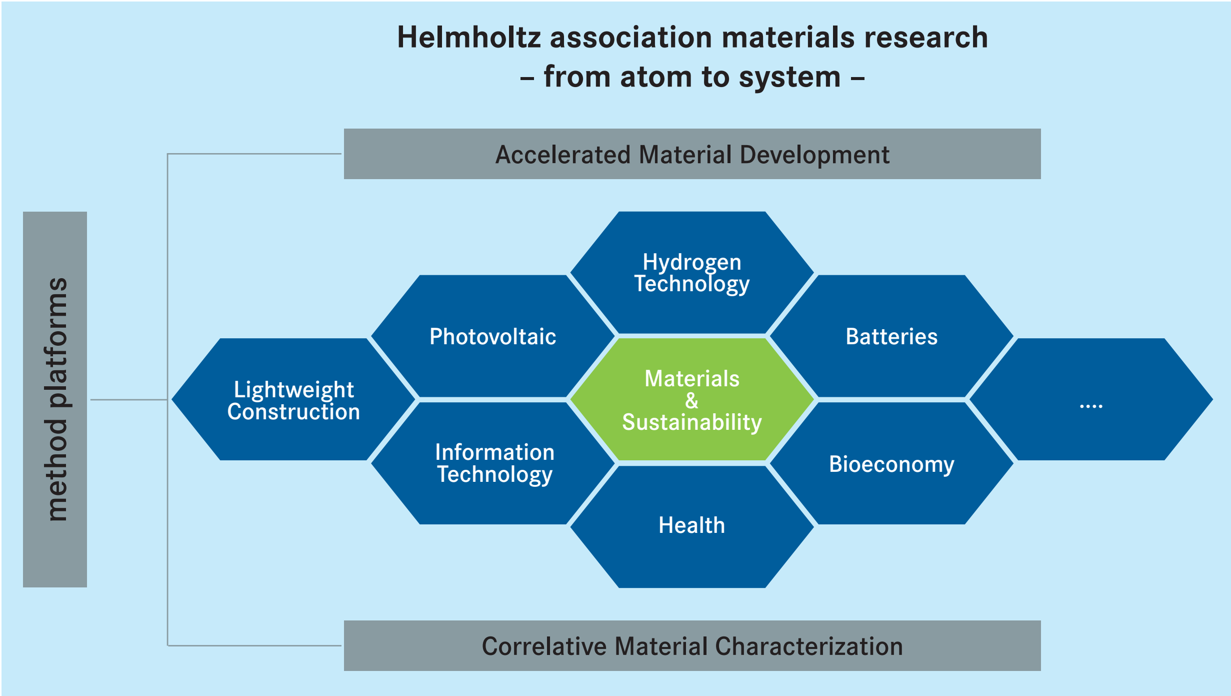


Fig. 2: Activities of materials research in Helmholtz Association; globally visible topics as a common basis for cross-Research Field work. Method-oriented platforms (gray) support application-oriented focus topics (dark blue). Of central importance for all is the topic "Materials and Sustainability" (green).

search Fields Energy, Matter, Aeronautics, Space and Transport, and Health. The aforementioned projects will therefore also play an important role in the implementation of the materials research strategy as focal points of the method platforms and influence the activities of the focal topics in a variety of ways. In order to structure the materials research network, various instruments, such as "*topical meetings*", will be set up, especially in the priority topics, for the transfer of knowledge among one another and also for interested parties from industry and the initiation of coordinated third-party funded projects. The training of young scientists across focal topics is another concern that will be addressed by the activities within the network.

In the long term, these structure-building measures will strengthen the networking of materials research in the Helmholtz Association so that strategic decisions can be made jointly. Successful national and international networking as well as successful technology transfer mean a direct competitive advantage, to which the Helmholtz Materials Research Strategy makes a corresponding contribution. This includes in particular;

- a networked cooperation between programs and Research Fields in the Helmholtz Association on selected topics,
- the expansion of the network towards universities in order to be able to start education and training in a targeted way during studies,
- investments in unique research infrastructures, and
- a transfer strategy that specifically promotes spin-offs and facilitates the path to the product.

INNOVATION AND TRANSFER

The focus of industrial innovation is on sustainable materials that can be used in future-relevant areas such as the energy transition. Thus, materials research retains its great importance for society and for Germany as a business location and contributes to the technological sovereignty of Germany and Europe. Above all, the accelerated and optimized material development that is becoming possible in connection with *digitalization* offers corresponding solutions, especially if the required use of resources and production technology are already taken into account in the development phase. Through the competencies of its centers and the research infrastructures anchored there, the Helmholtz Association contributes to providing industry with appropriate approaches. Through the materials research strategy presented here, the Helmholtz Association is bundling its activities, especially in the priority topics, and thus gaining an invaluable innovation advantage.

[1] The BMBF defines technological sovereignty (TS) as the claim to and ability to cooperatively (co-)shape key technologies and technology-based innovations. This encompasses the formulation of requirements for technologies, products and services in accordance with one's own values and the co-determination of corresponding standards on global markets. International cooperation plays an important role in this. However, TS may require being able to act autonomously in certain key areas (European) if this is necessary to maintain state regulatory sovereignty or to avoid unilateral dependencies. This does not call into question Germany's open global economic and scientific relations. Division of labor, networking and multilateral cooperation continue to be central building blocks for Germany's and Europe's ability not only to endure global developments, but to help shape them according to their own ideas and interests.

An increasingly important driver in business and society is *sustainability* (see also Chapter V). In this context, the deep and diverse anchoring of materials research as a cross-cutting topic in the Research Fields guarantees a rapid translation of materials science innovations into solutions of high societal relevance. At the same time, application issues with a high degree of complexity repeatedly trigger developments in materials science. In this context, the Helmholtz Association faces up in a special way to the increasing demand for *sustainability* in the economy, the environment and society.

In order to remain a leading international location for highly innovative industrial products, it is essential that in the future the demand for increasingly complex materials and their specific processing and recycling technologies can be met reliably and on a national level. In many industrial sectors of particular relevance to Germany, material costs now account for the dominant cost factor due to extensive automation of production (automobiles: 50%, batteries: 80%). In order to remain competitive here, concepts for parallelization, automation and *digitalization* of all elements of the material and process development chains must be advanced. The challenge in industry is characterized by two aspects in particular: First, the innovative strength of a company will in many sectors in the future depend on developing products starting from the nanostructure of the materials and the associated function, from the "*atom to the component*", so to speak. Secondly, in this context it is necessary to close the value chains, which opens up completely new dimensions in the individual design of material systems, in particular through the possibilities of additive manufacturing and the flexibilization of production processes. As a result, companies in Germany that incorporate this cross-sectional technology at an early stage can build up a clear competitive advantage over industries in Asia that are geared towards mass production. However, this poses great challenges to the development and production processes and requires a real technological change, to which the Helmholtz Association can contribute.

It will be the Helmholtz Association's task to establish the focal topics and method platforms (similar to the "*material platforms*" and "*material hubs*" mentioned in the BMBF impulse paper) or to network the already existing activities in order to be able to design a successful transfer from basic research to the product. The analytical instruments of the Helmholtz Association represent an added value that cannot be provided by any company or other organization. All in all, it will be important that developments that are crucial for transfer are taken up across centers and departments and tailored to industrial needs. In this context, the connection to the other three non-university research institutions (Fraunhofer, Leibniz, Max Planck) is an important building block in order to be able to answer industrial questions with the broad competence of the German research system. Furthermore, relevant industrial partners will be invited in order to advance the linking of research and industrial needs in a target-oriented way.

Knowledge and technology transfer is already successfully practiced as part of the Helmholtz Association mission. With the help of consulting and information services, continuing education offerings, Internet portals, citizen dialogues, real laboratories and other formats, knowledge is prepared in a comprehensible manner and made available for an intensive exchange with the respective target groups of politics, administration, business, civil society, education and the media. The Helmholtz Association student laboratories

and so-called citizen science are also used for this purpose. Materials research is also to make use of such formats and thus become accessible to a broad public.

Internal funding programs as well as **innovation and transfer managers** at the Helmholtz Centers enable research results, data and technologies to be brought into application in a targeted manner. The success can be seen in the numerous patents, and spin-offs that have also been able to establish long-term economic prospects.

TALENT DEVELOPMENT

Talent development and promotion is another crucial pillar of the materials research strategy and is applied at all levels of scientists' early but also advanced academic careers. The Helmholtz Association already offers a high quality of subject-specific but also interdisciplinary training in materials science and engineering through its cooperation with universities in more than 15 graduate colleges and schools. The participating centers make a decisive contribution to the promotion of doctoral students. The networking of these schools through joint activities or exchange formats is intended to further increase the impact in the training of young talent. This is already being expanded by the Helmholtz Association within the framework of the "*Information & Data Science*" incubator of the Initiative and Networking Fund in the field of information technology. Overall, therefore, materials research activities between the programs of the Helmholtz Association will be further improved by optimized networking at the level of doctoral students, thereby also promoting opportunities for further qualification, as well as careers in science. To this end, suitable formats are to be developed, such as training networks and summer/winter schools, which in particular bring the overarching topics of the methods platforms closer to all doctoral researchers in the community.

For example, a cross-center "*Training Network Computational Materials Design: Advanced Tools and Techniques*" is currently being planned for PhD students and postdocs in the Research Field Information's "*Materials System Engineering*" program. In addition, individual funding is provided for publications, participation in conferences, invited talks, and training to help young researchers become scientifically independent. Furthermore, master's students, PhD students, and postdocs will be encouraged to participate in specific mentoring programs in materials research and various staff development schemes at the centers.

Furthermore, within the framework of the materials research strategy, the formation of networks at the career level of junior professors and junior research group leaders is to be promoted. This is also financially supported by the participating centers, but networks supported by the members are to organize joint activities such as scientific lecture events with internationally renowned materials scientists, measures to encourage further personal qualifications, idea workshops for new research activities, and more.

FUNDING INSTRUMENTS

It is clear that the topics of materials research of the Helmholtz Association are not only promoted by the programs, but also by a variety of third-party funded projects. Outstanding examples are the participations in the clusters of excellence "*3D Matter Made to Order*" (3DMMO) for the development of novel printing processes for the production of nanomaterials, "*Post Lithium Storage Battery Research*" (POLiS) for the development of materials for sustainable batteries and "*Complexity and Topology in Quantum Matter*" (ct.qmat) as well as "*Matter and Light for Quantum Computing*" (ML4Q) for the research of complex and topological quantum materials and their use in technical applications. Accordingly, strategic funding of materials research in the Helmholtz Association should not focus on individual topics, but rather promote methodological expertise across the board and thus continue to create the basis for achieving outstanding results in the fields of application.

In many application fields, the development of high-throughput methods and the automation of processes is the key to an enormous acceleration of product development and significant cost savings in production. Outstanding examples are the automotive, aircraft and electronics industries, whose products today either cannot be manufactured at all or cannot be manufactured cost-effectively without the use of automation strategies. This trend is increasingly being applied to research infrastructures as well, but is still in its early stages in materials research (for example, EU-Battery2030+-FET Proactive materials acceleration platform). The Helmholtz Association will pursue with great commitment the potential arising from the parallelization, automation and *digitalization* of all elements of materials and process development in its materials research strategy, including the integration of correlative characterization methods through the platforms presented here (Chapter V), and will also promote the transfer of this methodology to industry, for example, in a possible pioneer campaign of the Helmholtz Association. Through the partnership of the Research Fields involved in materials research, the implementation of this research direction will create completely new possibilities for materials modeling, synthesis and characterization at existing research infrastructures and establish innovative mechanisms for their transfer to industrial materials development.

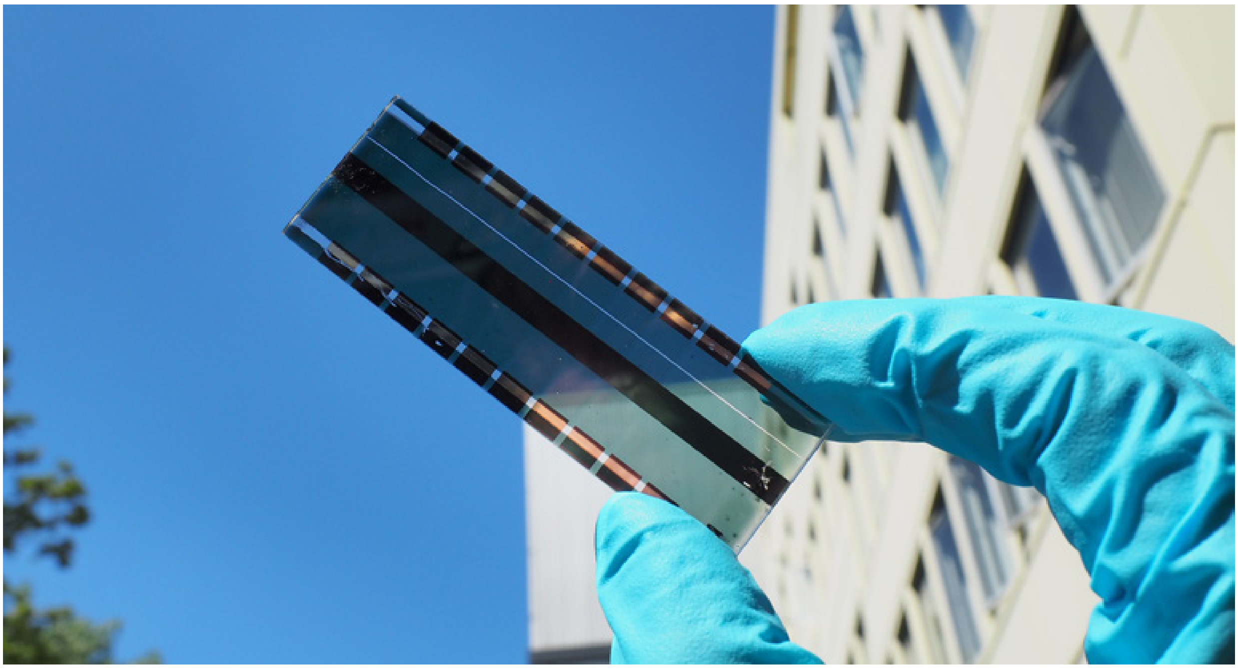
Funding from the Helmholtz Association's Initiative and Networking Fund via a pathfinder campaign would, in addition to achieving the goals in the medium and long term, above all improve the use of the existing potential of young scientists. In this context, already established instruments and methods can be used as examples, such as current funding activities of the BMBF (for example, NanoMatFutur and MaterialDigital). In the future, with regard to the BMBF's impulse paper on materials research, the newly established funding opportunities of the "*Material Hubs*" should be brought into line for the priority topics of the Helmholtz Association materials research strategy. The collaborative projects of such a pathfinder campaign of the Helmholtz Association will especially promote cooperative relationships that support the achievement of the goals of young researchers and technology transfer.

V. PRIORITY TOPICS & PLATFORMS OF HELMHOLTZ ASSOCIATION MATERIALS RESEARCH

In order to make optimal use of the available resources, the network will be built on the strategically relevant and globally visible topics selected here, the so-called priority topics, and this will be continuously adapted (see Figure 2). This will focus on issues that address the challenges facing society and the economy by means of the development and use of new materials and the methods required for this purpose.

The interaction of the centers across the boundaries of the Research Fields, integrating the existing and planned infrastructures, will make an essential contribution to addressing the priority topics. The materials research strategy is intended to strengthen the innovative capacity of the Helmholtz Association without neglecting the fact that this requires a broad competence base in the various Research Fields.

To this end, some of the participating centers contribute their own thematic focal points with their corresponding competencies. For the activities planned in PoF IV, interrelated activities of the different departments, which are already represented in topics in the respective program (such as photovoltaics in the Energy department, MTET program), are bundled and can thus contribute to the further development of cross-departmental materials research. In all activities, *sustainability* and the circular economy of materials are also considered as a central aspect. For this reason, a separate section is devoted to this overarching cross-cutting topic.



CROSS-SECTIONAL TOPIC "MATERIALS AND SUSTAINABILITY"

SUMMARY

Materials are related to *sustainability* in many ways: On the one hand, materials must be produced sustainably and integrated into an efficient circular economy. On the other hand, new materials in application, as will be shown by many examples in the following key topics, contribute to the goal of *sustainability*. In this context, (a) sustainable production and raw material bases are to be aimed for and (b) changes in consumption behavior, the service life of products, and material development are to be supported. A third area of application is (c) materials in applications to protect the environment or clean up environmental compartments.

The amount and variety of use of raw materials is constantly increasing, especially for building renewable energy systems, for energy efficiency, or electromobility, but also for the sustainable production of chemicals, and for digital communication more and new materials are needed. Therefore, the sustainable use of resources is a key element for responsible consumption and production, as called for by the United Nations in the "*Sustainable Development Goals*" (SDGs). This affects a wide range of resources for materials, from mineral and metallic (inorganic) to biological resources and carbon from anthropogenic sources. At the same time, the challenges of providing raw materials in an environmentally and socially sustainable manner are increasing: Many geogenic deposits suitable for mining and other primary sources of raw materials are located in fragile ecosystems, in inhospitable areas, or deep in the Earth's crust or the ocean. The trend toward increasing complexity and variability of building elements and material systems means that their use as secondary raw materials is becoming increasingly difficult. A reversal of the trend is necessary here: In order to secure a sustainable supply in the long term, raw materials in the economic cycle (circular economy) must be used as efficiently as possible in terms of energy and raw materials, waste must be minimized, and they must be recycled in an environmentally friendly manner. These goals must already be taken into account in the design phase of new materials and construction elements. This requires the inter- and transdisciplinary development of innovative technologies and solutions, digital platforms and data-capable models for the material, chemical and energy infrastructure. Modern materials research therefore aims to improve raw material and energy efficiency. Increasing the circular economy will make it possible to reduce the enormous social consequences of the extraction of primary raw materials.

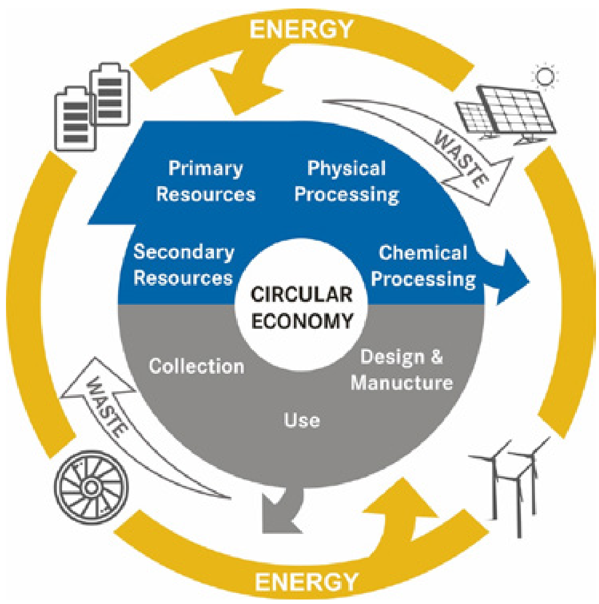


Fig. 3: The desired circular economy is closely linked to the energy system. Both interact with each other and limit each other (Source: HZDR).

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

Improvement of the resource situation

- Development of innovative and sustainable technology concepts for resource- and energy-efficient processing of complex resources.
- Testing of novel technologies for chemical processing of complex resources.
- Development of new strategies and methods for **multidimensional and multiscale raw material characterization** through a diverse method platform.
- Integrating process and feedstock knowledge to quantitatively predict resource and energy efficiency.

Circular economy and sustainable use

- Development of a platform for quantitative assessment of parts of the circular economy.
- Digitally assisted design of **highly specific separation processes** (membrane design).
- **Additive manufacturing:** Expanding the range of materials towards ceramics, metals, and composites for resource efficient manufacturing.
- **Process modeling** to reduce material consumption in additive manufacturing processes.
- Extending the **service life of metallic structures** by developing new concepts for environmentally friendly corrosion protection.

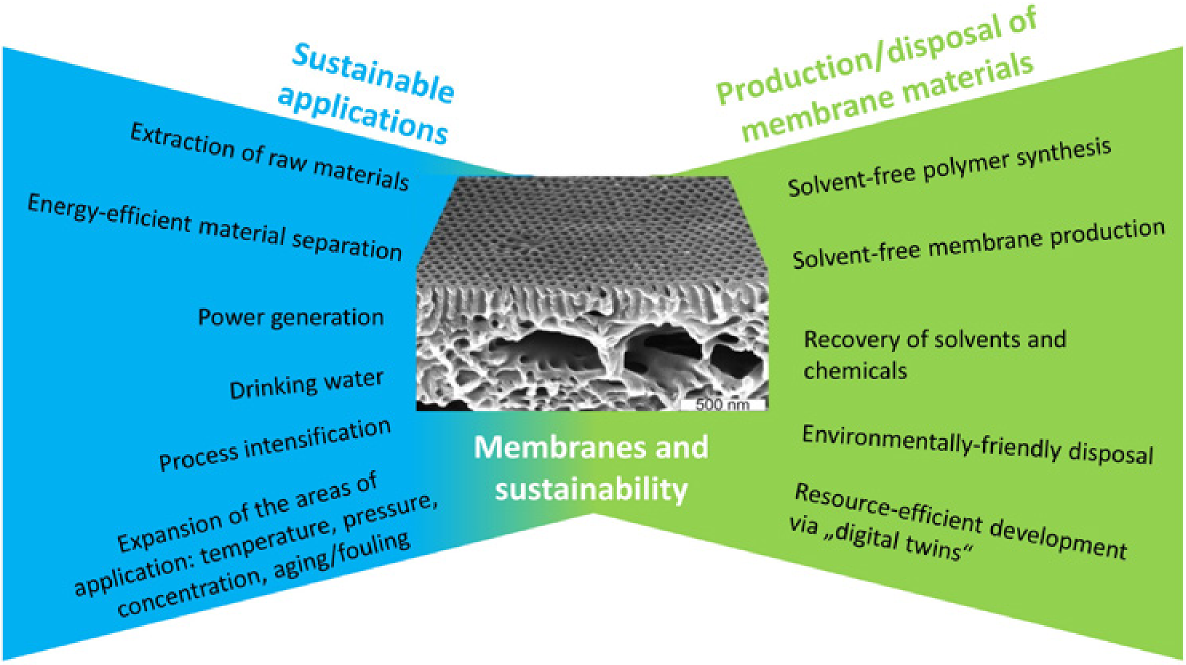


Fig. 4: Exemplary illustration of materials and sustainability using the example of membranes. Membranes are used in a wide range of applications that are necessary for sustainable management, climate protection and environmental protection. At the same time, the goal is sustainable production and use throughout the entire life cycle of membranes, from production to recycling (source: HZG).

Reduction of environmental pollution

- Membranes and membrane processes, as well as the associated simulation tools for closing material cycles, for example, for CO_2 separation or zero-discharge approaches in the use of water resources.

LONG-TERM STRATEGIC GOALS

The goals mentioned here are relevant with regard to material development, but can only be addressed in cooperation with other partners from research and industry.

Improvement of the resource situation

- Develop and deploy digital tools specifically with the goal of **saving resources and enabling environmentally friendly materials** development and manufacturing.
- Expansion and improvement of methods for **energy-efficient material separations** in industrial processes.
- Development of (for example, membrane-based) **separation processes for environmentally friendly extraction** of raw materials.
- Environmentally friendly development of raw material sources, for example, from deep in the sea or from complex geogenic deposits.

Circular economy and sustainable use

- Closing of relevant material cycles through **innovative energy- and resource-saving technologies** (for example, for construction materials and functional materials).
- Establishment of design principles that integrate the circular economy and recycling aspects into material, component, and product design.
- Development of sustainably applicable material combinations, for example, of polymers and inorganic materials, as support structures, transport-active matrix materials or catalysts.
- Expanding the application ranges of efficient materials in terms of temperature, pressure and composition as well as chemical resistance and aging.
- Consistent use of material and environmentally friendly additive manufacturing methods.
- **Life cycle extension of material structures by implementing active protection concepts** and preventive maintenance approaches.

- Development and use of appropriate tools for quantitative assessment of the efficiency and *sustainability* of recycling and circular economy in transdisciplinary alliances with environmental researchers and economists.

Reduction of environmental impact
- Develop sustainable and scalable approaches to close the anthropogenic carbon cycle through biological and chemical recycling.
- Develop material systems and separation processes to separate pollutants from different environmental compartments (water, earth, air).

MAIN FUTURE ACTIVITIES

Improvement of the resource situation
- Integration of data from **multidimensional resource analytics** with machine learning approaches. This improved understanding of materials will be achieved in real time to better characterize and more efficiently process material flows.
- Creation of **novel, so-called geometallurgical models for geogenic raw material bodies** (deposits) by integrating process data with raw material data. Similar models will be developed for secondary resources.
- Closed-loop **modeling of polymer membrane production** and its use for process simulation and optimization (*"digital twin"*).

Circular economy and sustainable use
- Development of a quantitative label for consumer goods for the Society for Resource and Energy Efficiency.
- Development of novel membrane materials and processes based on mathematical model predictions and increased integration in process intensification.
- Manufacturing gas separation membranes using solvent-free processes.
- Reduction of environmental impact.
- Development of AI approaches to **predict the lifetime of materials or components under complex environmental conditions** and establishment of intelligent predictive maintenance concepts with the goal of extended lifetime.
- Development of materials for *"negative CO_2 emissions"* to reduce CO_2 pollution of the atmosphere.

SUSTAINABILITY AS A CROSS-CUTTING TASK FOR FOCAL TOPICS AND METHOD PLATFORMS.

The *sustainability* of the use of raw materials and materials is an important and overarching aspect that must be taken into account in any development of innovative materials or products in all focal topics and in the method platforms. When selecting and developing materials (for example, for information and hydrogen technologies or the manufacture of photovoltaic modules or batteries, etc.), the availability and sustainable usability and recyclability of the raw materials used should be analyzed at an early stage and the associated ecological and social consequences over the entire life cycle assessed. In subsequent product development, not only should material savings (for example, through lightweight construction) be a central target parameter, but other sustainability aspects such as durability, ease of repair and recyclability should also be taken into account. The generation of residual materials should be minimized and recyclable materials should be kept in as closed a loop as possible. To this end, it will be necessary to develop approaches and tools that enable a qualitative and quantitative view of both the opportunities in the form of the potentials to be achieved and the challenges, such as tradeoffs and unavoidable losses. This should be done as early as possible during material/product development in the context of the circular economy in order to fulfill the objectives of the cross-cutting topic *"Materials and Sustainability"*.

FOCUS TOPIC "MATERIALS FOR INFORMATION TECHNOLOGY".

SUMMARY

Materials research has always been a driver for information technology: Materials with new and better properties have brought new and better possibilities in the processing, storage and transmission of data.

While until the late 1990s microelectronics almost exclusively used silicon semiconductors (and compound semiconductors in optoelectronics), the spectrum of materials has steadily expanded since then, for example, with *high k dielectrics* or germanium. This was necessary in order to be able to continue to drive miniaturization and the associated increase in performance in accordance with *Moore's Law*. Research in this direction continues today, with the semiconductor alloy GeSn as an example. However, *Moore's Law* is heading towards saturation and research is therefore being conducted into a variety of alternative ways of processing information, which require other concepts and thus other classes of materials. Quantum materials with novel topological, electronic, and transport properties occupy a central position here. Two important new concepts consist of the extension of computing paradigms by neuromorphic computing and quantum computing.

Base materials for neuromorphic computing are a wide variety of oxides that can be used as memristive devices, but also simply as resistive memories. In addition to redox-based oxides, phase change materials such as GeSbTe and increasingly also magnetic multilayer systems such as Co/Pt play an important role.

There are several different solid-state-based approaches to quantum computing. One is to use certain defect states in semiconductors such as SiC as qubits. Here, a challenge lies in the controlled fabrication of these defects. Second, in even more forward-looking concepts, topologically protected excitations such as Majorana fermions, for example, consisting of skyrmions or nanowires in contact with superconductors, will be used as qubits. The basis for this is research on the above-mentioned quantum materials: These include, for example, topological insulators or Weyl semimetals, but also semiconductor nanowires and quantum dots.
An independent Helmholtz Association strategy paper already exists for the entire area of quantum technology, within which the activities are coordinated.

A materials science revolution has occurred with the discovery of graphene and other so-called 2D materials (including transition metal dichalcogenides such as MoS_2). These materials consist of atomic single layers that can also be stacked to form heterostructures with new, tailored properties (Fig. 5). This "*2D construction kit*" offers a wide range of possibilities for the use and manipulation of electronic and spin states, but also for the control of redox processes. This enormous potential is reminiscent of the revolution in semiconductor physics brought about by the invention of molecular beam epitaxy and subsequently semiconductor heterostructures in the 1970s and 1980s. For 2D materials, however, there is still a major challenge in depositing them over large areas using standard thin film methods and doping them appropriately.

Magnetic materials represent a special focus of the Helmholtz Association centers involved. While these have so far been used mainly as sensors and for data storage, research has also been going on for a long time

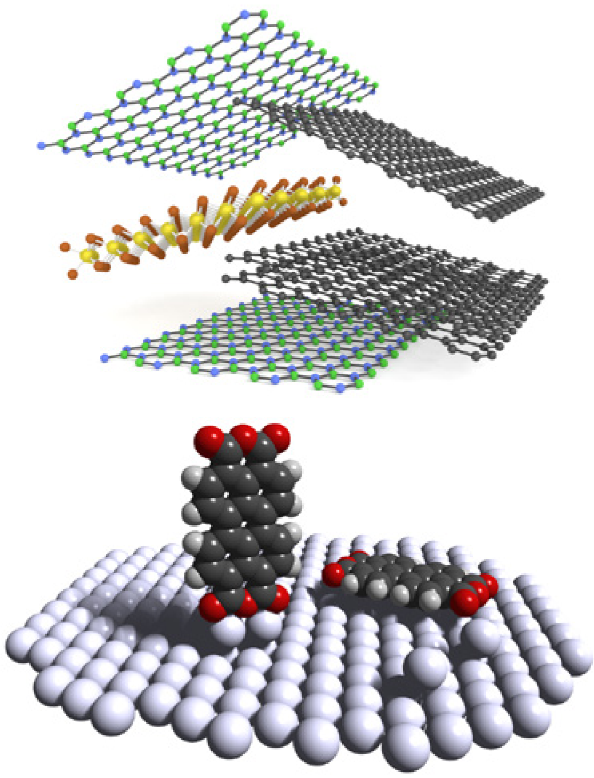


Fig. 5: Two approaches to fabricate nanostructures: Stacking monolayers of 2D materials in any order (top), and 3D nanostructures by molecular manipulation (bottom) (Source: FZJ).

into spintronic devices in which electron spin is used instead of charge for information processing. Collective excitations such as spin waves (magnons) can also play a role in *on-chip* information transfer. Special topological spin configurations, such as the skyrmions mentioned above, could enable higher density data storage and neuromorphic functionalities, or even bridge the gap to quantum computing.

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

According to the relevant research programs in the Research Fields Information and Matter, the detailed structure and electronic, optical, magnetic and chemical properties of materials as well as the electronic and chemical processes will be investigated. The most important classes of materials such as semiconductors, 2D materials, oxides, magnetic materials, phase change materials and topological materials will be synthesized for this purpose. The investigations are to be carried out with the highest time and spatial resolution and with targeted use of large-scale equipment and its diagnostic capabilities (program MML "*From Matter to Materials and Life*" of the Research Field Matter), with the aim of **identifying the most energy-efficient processes possible and also new functionalities for information technology**. In particular, the focus here is on the two computing paradigms neuromorphic computing and quantum computing, which are also represented in the program "*Natural, Artificial and Cognitive Information Processing*" of the Research Field Information in PoF IV. The newly established cross-program Joint Labs "*Virtual Materials Design*" (JL VMD) and "*Integrated Model and Data Driven Material Characterization*" (JL MDMC) complement materials development with simulation- and data-driven methods. Materials science thus acts as a foundation and driver, but at the same time also as an application field for information technology through virtual materials design.

LONG-TERM STRATEGIC GOALS

Central is the targeted identification of the optimal material with the suitable functionality for the respective application, its characterization and optimization, in order to be able to manufacture optimal components from it.

- Establishment of a platform for the fabrication of controlled layer structures of 2D materials, as well as for the fabrication of quantum systems on an **atom-by-atom basis.**
- Overcoming problems with stability under ambient conditions, sufficiently high purity and **reproducibility of new material systems**.
- Establish multidimensional phase and property diagrams for selected families of quantum materials.
- Establish a **database for protocols for synthesis of quantum materials** from nanoscale building blocks based on extensive automated series of experiments.

MAJOR FUTURE ACTIVITIES

It can be expected that in the post-PoF IV era, the new computing paradigms and hence the materials relevant to them will play an even greater role, and at the same time classical semiconductors will become somewhat less important. Moreover, it is not unlikely that by then another new class of materials will be discovered that will also offer new perspectives for information processing; this is particularly the case because by then it is probable that much more systematic and effective methods for **finding new materials with specific, desired properties** will be available.

SELECTED INFRASTRUCTURE USE

Major infrastructures are used in the fabrication, processing, and characterization of materials and their dynamics: The most important are the **Helmholtz Nanoelectronic Facility (HNF), the Ernst Ruska Centrum (ERC), the Ion Beam Center (IBC), the UNILAC ion accelerator and CRYRING (GSI-FAIR), High Field Magnet Laboratory Dresden (HLD), the Jülich Center of Neutron Science (JCNS), the synchrotron radiation sources PETRA III, BESSY II, the FELs FLASH and European XFEL, and the radiation source ELBE**. In the international area, additional light sources (**ELETTRA, SOLEIL, ALS,** etc.) are used.

SYNERGIES

Synergies arise from the cooperation of different Helmholtz Association centers within the PoF, also across departments, but also within **BMBF or EU projects**. In addition to thematic cooperation, joint method development and the mutual use of large-scale equipment also play a role.

KNOWLEDGE TRANSFER WITH METHOD PLATFORMS

The method platform "*accelerated material development*" supports the main topic by designing materials using a cross-scale approach (for example, from DFT to FEM) with parameters that are optimal for application (for example, optimal electrical, magnetic, optical properties), which can be generated using automated workflows.

The method platform "*correlative material characterization*" will enable the development of a comprehensive material database on structural, electrical, magnetic, and optical properties, and will contribute significantly to their experimental investigation.

Goal: Develop and investigate novel materials for the post-Moore era of information processing
Participating Research Fields: Information, Matter
Participating Centers: FZJ, HZDR, HZB, KIT, GSI
Infrastructure: HNF, ER-C, JCNS, IBC, ELBE, HLD, UNILAC, CRYRING@ESR, BESSY II, PETRA III , FLASH, European XFEL

FOCUS TOPIC "BATTERY MATERIALS"

SUMMARY

The aim is to develop particularly cost-effective, safe, durable and sustainable electrochemical energy storage systems for mobile and stationary applications. In the context of targeted materials development, advanced modeling and characterization techniques are necessary to understand both novel synthesis routes and degradation behavior as well as potential shortcomings of current battery materials. Based on this and already advanced in the program, various solutions for Li-ion batteries, as well as new battery concepts, will be developed. Both the atomic and the mesoscopic structure of the materials play an essential role. The special feature of materials research for energy storage is that all components interact with each other through contact with the electrolyte. With regard to material development, this means that the optimization of individual cell components is therefore only a partial step. For a comprehensive and final evaluation of the materials, investigations at cell level (in a full cell where possible) are therefore necessary. For this reason, materials development for batteries is an independent task located in the "*Electrochemical Energy Storage*" topic of the MTET program. While it is already clear today that lithium-ion batteries will hold their own on the market in the long term, other electrochemical energy storage concepts have yet to prove their market potential. In addition, new battery concepts are to be developed for long-term, i.e., seasonal to annual energy storage, which is not currently addressed in the current strategic planning for PoF IV. For an assessment of specific opportunities, all cell components, i.e., both storage-capable active and supporting inactive materials, must first undergo significant further development. The overall assessment will consider *sustainability* aspects over the entire life cycle of a battery.

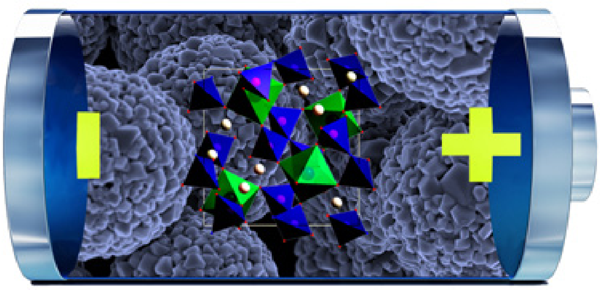


Fig. 6: Active and passive materials within a battery determine the performance characteristics tailored to applications. Side reactions are largely responsible for limiting the service life (source: KIT/Adobestock 56417722_Battery).

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

Currently, different cell concepts are being intensively researched and the following material aspects are being considered in particular:

- The **utilization of metallic lithium anodes**. This requires material solutions through coatings of electrodes or the development of new electrolytes and electrolyte compositions. This is a cross-sectional task for numerous cell concepts of lithium-based batteries, i.e., both with liquid electrolyte formulations including the establishment of suitable additives with polymer electrolytes and in pure solid batteries, as well as for Li-sulfur or Lioxygen cells. Hybrid electrolytes (for example, multi-layer approach) are also conceivable.
- For lithium (ion) batteries, **new cathode materials** with higher redox potentials as well as higher capacities are to be developed to further increase the energy density. In this context, Co and also Ni are to be largely dispensed with. Higher energy densities also require new multifunctional electrolytes (for example, polymers and hybrids) that are more stable and more conductive than the current state of the art. Inactive material components such as binders or separators are being optimized with regard to more environmentally compatible cell production and safety.
- For metal-sulfur cells, **new electrodes** based on nanostructured carbon and graphene-based aerogels are being developed to further increase gravimetric energy density. The main issues to be overcome are capacity losses and low electrode utilization. Polysulfide retention in the conductive mesoscopic structures is the most important material aspect here. This can be further optimized by combining metal-containing substances with a polar surface to increase the adsorption of polysulfides to accelerate redox reactions taking place. Separators produced using ion beam technology, among other techniques, are also being investigated.

- For cell chemistries that do not require lithium and could possibly enable more sustainable energy storage for some applications, **material concepts** are to be developed that overcome current limitations. These include organic active materials and new electrolyte systems including solid electrolytes. Among other things, new environmentally friendly seawater batteries are being developed for use in remote areas. The focus here is on metal anodes, for example, based on magnesium alloys, and novel electrolyte additives to increase efficiency and ensure long-term reliable performance. After demonstrating the principal functionality on a small scale, an upscaling step will be performed and the performance characteristics will be evaluated using larger cells. During PoF IV, an evaluation of the different cell concepts will be performed and the work will be focused on a few particularly promising systems.

For all cell systems, material development will be accompanied by **comprehensive modeling** in order to help interpret complex measurement results on the one hand, but also to identify the most important influencing variables by flexibly adjusting individual material parameters, and thus to steer and accelerate material development in particularly promising directions.

LONG-TERM STRATEGIC GOALS

The overriding goal of materials research for batteries is to provide the best possible electrochemical intermediate storage of energy as the foundation of sustainable energy technology. This will also involve the use of various cell concepts in different applications. Material aspects are of central importance along the entire value chain. This begins with:

- Resource availability and use of materials in a closed-loop economy that is as complete as possible, on
- the development of new materials and morphologies with improved properties and the
- the processability of the materials in cell production, through to the
- material-related performance characteristics over the entire service life and in possible damage scenarios.

Due to high complexity and many degrees of freedom in the material parameters, a purely empirical optimization is not target-oriented; instead, materials research for batteries must be based on comprehensive understanding of underlying effect and failure mechanisms:

- The **elucidation of all property-decisive processes** within a battery is therefore just as much an important strategic goal of materials research for batteries as the development and investigation of new material systems, including the modeling of cell behavior and critical material parameters over all relevant time and length scales.
- the development and investigation of new material systems including
- the modeling of cell behavior and critical material parameters over all relevant time and length scales.
- The development and validation of modern simulation tools that can describe processes within as continuous a simulation chain as possible, from the atomic to the cell scale, represents an important concern of the focus topic "*Battery Materials*". As a cross-sectional topic, the developed modeling techniques could be applied to different battery concepts and relevant materials there, whereby methodological adaptations will be necessary in individual cases.
- In the ongoing work, new electrochemically active electrode materials as well as innovative or improved electrolytes are formulated and synthesized in order to achieve better performance characteristics, increased safety and longer lifetimes.
- Inactive components, such as binder materials and separators, are also being further developed to improve the processability and recyclability of cell components and thus contribute to battery *sustainability*.
- For cells with high energy densities, the interfaces must be designed to withstand the extreme oxidative and reductive operating conditions over the long term.
- To create a validated simulation basis for battery development, a **closer coupling of simulation techniques at different scales** is sought, not only to systematically expand the transfer of atomistic information from density functional theory and molecular dynamics to continuum techniques of microstructure simulation of electrodes and macroscopic cell design simulations, but also to more specifically advance materials development.

In 10 years, it can be assumed that there will be an **application-oriented consolidation of selected cell concepts**. The focus will then be on the upscalability of materials and optimum processability in cell production, which can also be directly taken into account in new developments in materials research. Ideally, battery performance characteristics can then be derived from fundamental material parameters using available modeling tools, leading to **accelerated optimization of both materials and cell designs**. These then need to be validated on the materials side and implemented in practice. **In the area of materials simulation, in the long term, the use of quantum simulation techniques could provide unprecedented opportunities for the development of energy materials** and complement existing density functional techniques. Planning and development of appropriate simulation techniques of high-performance energy materials is currently underway.

MAJOR FUTURE ACTIVITIES

- **Hybridization of electrolytes for solid-state batteries**, for example, the development of polymeric interlayers for ceramic-based electrolyte/electrode combinations.
- Provision of polymeric components for functional layers for variable cell chemistries.
- Developing **efficient concepts for upscaling battery materials.**
- Combining machine learning techniques and physics-based modeling including novel quantum simulation techniques for energy materials. This will make simulations for describing battery components even more realistic, and promising material combinations can be proposed more reliably and then tested via high-throughput experiments.
- **Development of novel battery materials using advanced synchrotron- or neutron-based characterization techniques** in combination with application-oriented design of next-generation batteries (for example, metal-sulfur, post-lithium, and polymer-based batteries).

SELECTED INFRASTRUCTURE USE

- Special *in operando* methods are needed to characterize material behavior in complete cells, providing the maximum information about the underlying processes at the highest possible spatial resolution and under real operating conditions. This ranges, among other things, from electrochemical methods to gas and structural analysis to diffraction and spectroscopy using synchrotron (**BESSY II, PETRA III**) and neutron radiation (**MLZ**).
- For the upscaling of material developments, the advanced powder ceramic synthesis technologies and colloid chemical processes within the nanoparticle synthesis laboratory of the H*elmholtz Energy Materials Foundry (HEMF)* are used, among others. These materials are used in the *Battery Technology Center,* the *NextGenBatt Laboratory*, and the Battery Laboratory for the fabrication and evaluation of medium- and large-sized cells.

SYNERGIES

Materials characterization uses all the major infrastructures of the Helmholtz Association available for this purpose. Materials research for batteries within the Helmholtz Association is linked to all major national funding activities, either through intensive collaboration or coordination by senior Helmholtz Association scientists. Helmholtz Association Materials Research contributes substantially through materials expertise to the BMBF umbrella concept "Battery *Research Factory*" and the associated competence clusters.

As a particularly extensive EU project, the large-scale research initiative Battery 2030+ (**https://battery2030.eu/**) should be mentioned here, in which, for example, accelerated material development is to be advanced using artificial intelligence methods.

Electrochemical storage devices, such as batteries, are an example of a priority topic that is being worked on along the entire value chain from the idea to the marketable product. The planned joint labs of the Research Field Information, VMD and MDMC, are also an important link here and support material development through data-driven simulation, establishment of quantum simulation techniques and characterization.

Goal: Development of sustainable storage systems of the highest efficiency for the global energy transition
Participating Research Fields: Energy, Information, Matter
Participating Centers: KIT, FZJ, DLR, GSI, DESY, HZB, HZDR
Infrastructure: HEMCP, HEMF, KNMF, ER-C, BESSY II, PETRA III, KIT-BaTeC, Energy Lab 2.0, NextGenBatt, Battery Laboratory, UNILAC

FOCUS TOPIC "MATERIALS FOR HYDROGEN TECHNOLOGY"

SUMMARY

The sustainable and efficient production, storage, distribution and use of hydrogen, and chemical energy carriers based on hydrogen from renewable, carbon-neutral sources will make a significant contribution to our future energy system, replacing our current fossil-based production routes and mobility concepts. Hydrogen enables the transport and import of energy as well as a flexible coupling of the electricity, heat, industry and mobility sectors. To realize sector coupling, new process and value chains for hydrogen and derived chemical energy carriers are being developed using renewable energies. This can bridge the gap between fluctuating electricity generation from renewables and demand on different time scales, as well as provide hydrogen for decarbonization of mobility and industrial processes, for example, in steel and cement production or the chemical industry. To be carbon neutral by 2050, intensive research and development efforts are needed for large-scale deployment of hydrogen technologies. A fundamental understanding of materials and materials technologies can tailor the necessary components and maximize the efficiency of the overall system. Moreover, new materials drive innovation and open up additional new possibilities. In this context, materials research for hydrogen technologies includes the following key functional elements:

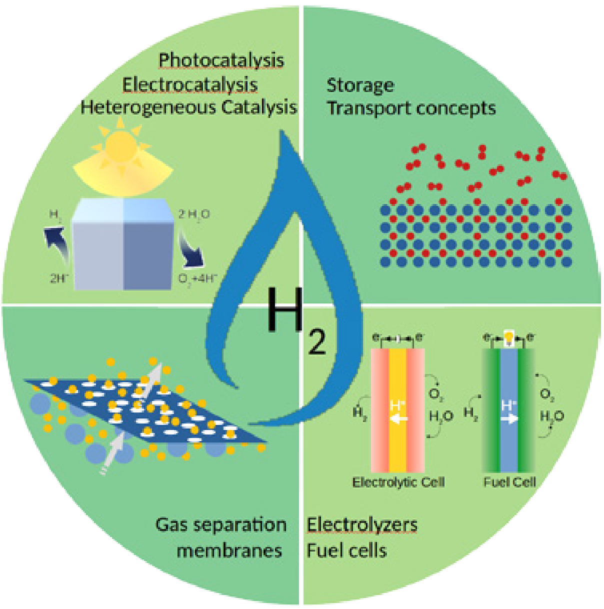


Fig. 7: Thematic focus points of materials research for sustainable and efficient production, storage, distribution and use of hydrogen (source: FZJ).

- Heterogeneous catalysts, electrocatalysts and photocatalysts for extraction and conversion
- Membranes for separation and processing, and hydrides for compression
- Ion conductors and electrodes for electrolyzers and fuel cells
- Materials for storage and transport concepts

Material aspects are of central importance along the entire value chain. This begins with the availability of resources and the use of materials in a closed-loop economy that is as complete as possible, and continues with the processability of the materials for the individual components, through to the material-specific property profiles over the entire service life and the avoidance of possible failure scenarios. *High throughput* methods, unique critical *in situ* and *in operando* experiments, and comprehensive multiscale simulations and modeling are combined to reach solutions and successful implementation faster given the high complexity of the requirements.

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

The application-oriented basic research of the Helmholtz Association addresses the tasks and challenges of the "*7th Energy Research Program of the German Federal Government*", the "*Hydrogen Roadmap Europe*" and contributes to the **implementation of the hydrogen strategy of the German Federal Government**. Hydrogen research is carried out in cooperation with partners from industry and scientific research.

(Photo-)catalytic processes as well as the corresponding interfacial dynamics during the phase formation and reaction processes play a decisive role in the materials studied. For a comprehensive understanding, the processes have to be investigated on the atomic and nanoscale. For this purpose, the processes are investigated *in situ* at the interface with highest time and spatial resolution in close cooperation of the different research areas. Element-specific analyses are performed under *operando* conditions. These experiments provide important input parameters for simulations and can be used for systematic validation of models. Due to the flexible variability of individual material parameters, comprehensive modeling supports the interpretation of complex measurement results and provides important insights into critical influencing variables. **The interaction of experiment and modeling steers and accelerates material development in particularly promising directions**. Focus is on the following activities:

- Development of **Ni-based electrocatalysts for alkaline membrane electrolysis, supported catalysts for PEM electrolysis**, and new concepts such as exsolution for high-temperature technology.
- Modeling of photo-electrochemical devices and identification of performance bottlenecks.
- Development of synchrotron-based *in situ* and *operando* methods for studies at solid-liquid interfaces.
- Development of **thin film catalyst systems based on powder catalysts**.
- Conceptual design and prototype development of scalable and stable photo-electrochemical devices and of integrated photovoltaically driven electrolysis devices for **solar water splitting**.
- In situ characterization of reactive hydride composites with working temperatures between 100 °C and 200 °C. Embedding of storage materials in polymer membrane matrices to **ensure long-term stability**.
- Investigation of activation issues and reaction rate determining steps in interstitial metal hydrides using atomistic and phase field simulations.
- Determination of the application characteristics of CO_2-selective membranes for the **treatment of different process gas streams**: H_2-containing bio and industrial gases, waste gases, natural gas.

LONG-TERM STRATEGIC GOALS

The overarching goal of materials research on the priority topic "*Materials for Hydrogen Technology*" is to provide tailored materials and materials technologies for the comprehensive implementation of a sustainable and **efficient energy and raw materials economy based on hydrogen as a green energy carrier**. A central goal is a comprehensive and in-depth understanding of the complex processes in the various (partly multifunctional) materials over their entire life cycle. With regard to the various areas of application, a correspondingly broad portfolio of materials and process technologies is to be made available that can be combined to form efficient overall systems, whereby, in addition to the optimum property profiles, the aspects of resource availability and recyclability must always be taken into account in the sense of a sustainable circular economy. The specific strategic goals for the key building blocks and components of hydrogen technology are:

- Long-term stable and cost-efficient heterogeneous catalysts, electrocatalysts and photocatalysts for the **production and conversion of hydrogen**,
- Membranes for efficient separation and processing of hydrogen, and l**ow-maintenance compressors based on hydrides**,
- Fast ion conductors and corrosion-resistant electrodes for electrolysers and fuel cells,
- Efficient carrier materials for efficient, compact and safe **storage of hydrogen**,
- Development of multi-physics modeling and simulation tools that enable virtual material development of complex components (for example, electrode, transport layer, up to the fuel cell).

Over the next five years, activities will focus on further development of the best materials to date, as well as scaling up synthesis and process methods to present working technology demonstrators that enable the necessary rapid implementation. In parallel, analysis and modeling will be performed to expand the fundamental understanding of the processes and mechanisms to provide improved and novel materials in the medium to long term. This will further increase the energy efficiency of the building blocks for hydrogen technology and further reduce costs. Specifically, this involves:

- Demonstration of durable and efficient fuel cells and electrolyzers with very low precious metal loading, including alkaline technology completely free of precious metals.
- Knowledge-based **development of novel thin-film catalysts for sustainable production and transport of hydrogen**, chemicals, and alternative fuels by synergistically combining expertise in thin-film technology and catalysis for industrial-scale application.
- **Prototype development of promising high-throughput photo-, electro-**, and chemo-thin film catalyst systems and develop cost-effective processes for metal oxide-based tandem material systems for photoelectrochemical water splitting.
- **Efficient polymer and ceramic membranes** for hydrogen purification and integration into membrane reactors for power-to-X technologies. Polymer membranes for the separation of CO_2 from H_2 and for the separation of H_2 from the natural gas grid are used for separation tasks in application-oriented research activities and their integrability with other process technologies is investigated.
- Fundamental **analysis of new material systems for hydrogen storage** using critical *in operando* experiments and computer simulations: Reactive hydride composites and in H_2-selective membrane scaffolds for temperatures < 100 °C.
- Development of a fundamental understanding of reaction mechanisms at solid-liquid interfaces in scal-

able thin film catalyst systems at the molecular level, in view of the design of novel chemo-, electro-, and photo-catalysts via *in operando* analysis and modeling.

- Identification of **novel, chemically stable metal oxide-based semiconductors** with band gaps between 1.5 - 2.1 eV for application as "top" absorbers in photo-electrochemical stacked cells and analysis of the essential mechanisms for solar H_2 generation and CO_2 reduction.

The long-term goal is to provide optimal solutions for the various applications:

- **Long-term stable and cost-effective heterogeneous catalysts with minimal precious metal content.**
- Cost-effective photocatalysts with high efficiency and suitable concepts for corrosion protection to ensure long-term stability.
- Demonstration of long-life, cost-effective, large-area prototype cells for stand-alone solar water splitting.
- A **new generation of temperature-stable polymer and ceramic membranes** allows selective addition of reactants and separation of products from membrane reactors at temperatures up to 300°C and 900°C, respectively, becoming an "*enabling technology*" for process intensification in the hydrogen economy.
- **Low-maintenance compressors based on hydrides** with suitable thermodynamics and temperature/pressure characteristics.
- **New durable polymer membranes** with high ionic conductivity for electrolyzers and fuel cells in the temperature range around 120°C for simplified heat and water or moisture management.
- **New ionic conductors** (anions or cations) for fuel cells and electrolyzers in the 300 to 500°C temperature range for industrial applications.
- Material solutions enable reversibility of cell technology for the production or conversion of hydrogen (flexible switching between fuel cell and electrolysis modes).
- Comprehensive portfolio of material and storage tank systems enables cost-effective, copact and safe storage of hydrogen in stationary and mobile applications (sector coupling, seasonal storage, ships, trains, buses).

KEY FUTURE ACTIVITIES

- Development of novel tailored thin-shell catalysts for large-scale production and conversion of hydrogen, as well as chemical energy carriers and processes using an integrative knowledge-based approach: Digital catalysis, *in situ* and *in operando* analysis, thin-shell processes, scaling and prototype development (CatLab project, jointly with MPG).
- **Core-shell catalysts** with long-term stability in polymer fuel cells.
- **Establish digital libraries** to support the implementation of tandem photoelectrochemical material systems via kinetic spraying and other scalable fabrication techniques.
- Develop critical nanofabricated experimental model electrodes for validation of computer simulations of electrode properties.
- Development of **Reactive Hydride Composites** with reduced working temperatures and combination with polymer scaffolds by combining *operando* experiments with parallel computer simulations.
- New polymer membrane materials for H_2 separation at high temperatures and optimized and application-specific CO_2 separation by thermally rearranged polymers or facilitated transport membranes.
- **Exploring process intensification approaches** through the use of membranes in membrane reactors and integrated processes.
- Exploration of novel metal oxide-based semiconductors and optimization of their efficiencies and stability.
- Application of synchrotron-based *in situ* and *in operando* methods for solid-liquid interface studies.
- Conceptual design and prototyping of scalable and stable photo-electrochemical devices.

SELECTED INFRASTRUCTURE USE:

- The **HEMF and HEMCP platforms** provide extensive, and in some cases, unique infrastructures for the synthesis and analysis of innovative materials for hydrogen technology. Specially designed and unique *in situ* and *in operando* environments at synchrotron **(BESSY II, EMIL, PETRA III)** and neutron facilities **(MLZ - FRM II)** are used to analyze the material, providing time- and spatially-resolved direct insight into the underlying processes and mechanisms under real operating conditions. For example, solid-solid and solid-liquid interfaces of electrochemical and photoelectrochemical material systems are investigated to identify new photoactive materials and contribute to the provision of cost-effective and efficient photoelectrochemical cells. Other infrastructures such as the **Polymer and Hydrogen Technology Centre (PHTC)** allow the synthesis of nanoscale materials and new polymers up to pilot scale for the fabrication of larger storage tanks and membranes, as well as their testing at technical scale over wide temperature and pressure ranges. At the **Membrane Center,** membrane systems for new energy-efficient technologies are developed and investigated, for example, for catalytic membrane reactors and novel fuel cells. Various manufacturing processes, such as film casting, PVD and dip coating processes are used and the new materials and components are extensively characterized with regard to structure and performance.

SYNERGIES

In the field of materials research for hydrogen production, processing and storage, the activities in the Research Field Energy, the Research Field Information as well as the Research Field Matter complement each other and jointly use the special infrastructures (HEMF, HEMCP, PHTC, ...).

The Joint Labs VMD and MDMC (Research Field Information) support material development by multiscale comprehensive modeling and simulation as well as by intelligent data-driven characterization and evaluation methods. In a cross-scale approach, the link between fundamental material developments via new process technologies to the optimization of the performance profile of complete modules and systems is elaborated and linked in parallel with different modeling and simulation approaches.

All activities are closely integrated into European research projects within the framework of Hydrogen Europe and the activities of the "*Hydrogen Technology Collaboration Program*" (TCP) of the International Energy Agency (IEA), for example in Task 40 "*Energy Storage and Conversion Based on Hydrogen*".

Goal: Materials research for sustainable production, storage, distribution and use of hydrogen for the energy transition
Participating Research Fields: Energy, Information, Matter
Participating Centers: FZJ, DLR, KIT, Hereon, HZB, UFZ, DESY, GFZ, HZDR, GSI
Infrastructure: HEMCP, HEMF, KNMF, ER-C, BESSY II, PETRA III, KIT-BaTeC, Energy Lab 2.0, PHTC, Membrane Center, UNILAC

FOCUS TOPIC "PHOTOVOLTAIC MATERIALS"

SUMMARY

Photovoltaics (PV); the direct conversion of sunlight into electrical energy, is one of the technological pillars for the future supply of renewable electricity in Germany and worldwide.

In order to achieve the strategic goal of offering the lowest cost of electricity (LCOE) of all energy technologies, the development of photovoltaic materials, processes and device concepts to realize an area-related increase in efficiency with new semiconductor systems is an indispensable prerequisite. Innovations from materials research in the participating Helmholtz Centers are key in solving this future task.

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

Thin film solar cells based on hybrid halide perovskites achieve record levels of efficiency. However, these absorber materials contain the element lead and are not stable over time. Therefore, current research focuses on replacing lead while significantly improving the long-term stability of the material, and on new halide perovskite-based materials and processes for high-efficiency tandem solar cells.

- Develop a fundamental understanding of the **design and structure-property relationships** of defect-free and defect-tolerant compound semiconductors, particularly the interplay of static and dynamic structure, for a better understanding of long-term material stability and therefore device stability.
- Develop new strategies to **stabilize halide-perovskite interfaces**, in particular using hybrid heterostructures and 2D/3D perovskite heterostructures, and **develop stable and compatible carrier extraction layers** that effectively passivate both grain boundaries and surface states, with optimal band matching. These activities will be supported by characterization of the chemical, electronic, and structural surface, interface, and bulk properties at the dedicated infrastructures (see below).
- Develop a microscopic and macroscopic description of the **crystallization behavior** of halide perovskites from solution using an experimental and multiscale simulation approach. Based on this, reliable and sustainable fully **solution-processed halide perovskite solar cells** with high efficiency and long lifetime, including the interlayers and electrodes, are developed and optimized. In particular, high-throughput processes are used here.
- Development of new processes for cost-reduced large-area production of **halide perovskite (tandem) solar cells** (inkjet printing, slot die process and co-evaporation).

In order to meet the future challenges for photovoltaics as one of the technological pillars for the supply of renewable electricity, the development of new, innovative absorber and contact materials for highly efficient solar cells is in the foreground. One basis for this is experiment-based and computer-aided material screening.

- Investigation of the structure-property relationships of new absorber materials, especially for use in tandem solar cells (for example, widegap chalcogenides).
- Develop combinatorial materials research methodologies (for example, combinatorial inkjet printing, aerosol printing, slot die coating, pulsed laser deposition, accelerated materials analysis) to create and analyze material libraries of new photovoltaic materials or combinations of materials relevant to high-efficiency solar cells.
- Develop a methodology for reporting efficiency and stability data for "*emerging*" PV materials.

Newly developed materials and concepts must be subjected to systematic testing in solar cells and opto-electronic devices.

- Development of **new device concepts and architectures** for improved energy yield under real conditions. Optical simulations coupled with energy input simulations are used to evaluate and optimize new device concepts (for example, 3-terminal) and light management concepts.
- Development/optimization of new **analytical methods** for the investigation of material properties and long-term stability **under operating conditions**. For the progressive development of an "*autonomous laboratory*" and "*autonomous manufacturing processes*", the **targeted implementation of intelligent diagnostic methods and acquisition as well as AI-based analysis** of material and process data is necessary.

The impact of degradation processes on the performance of photovoltaic systems will be an important area of research, as the presence of critical contaminants in certain environments can drastically shorten their lifetime leading to premature failure.

- **Investigate the corrosion** of various key components in relevant environments and develop predictive models.
- **Demonstration of photovoltaic-powered water treatment systems** (without batteries) in Africa is planned within the Research Field Earth and Environment ("*Bioeconomy*").

LONG-TERM STRATEGIC GOALS

- Helmholtz Association materials research focuses on the **development and realization of new, highly efficient photovoltaic technologies and device concepts** with efficiencies above 30%. This will overcome the current efficiency and electricity production cost limits. Important aspects for new PV technologies are not only the production costs of the modules, but also their long-term stability.
- **Development of new material functionalities** that meet the key criteria of sustainability, resource conservation and cost-effective production, and enable system integration, especially with a view to global deployment on a tera-watt scale. This concerns not only photovoltaic absorber materials, but the entire range of materials needed to manufacture solar modules (for example, for contacts, electrical connections, encapsulation).
- Development of **high-throughput experimental methods** for the acquisition of physical characteristics of new photovoltaic materials, both in the laboratory and on large-scale equipment. Methods for accelerated material development (for example, computational and experimental high-throughput material screening with stage-gate process) will be established for the search of new photovoltaic materials. As well as this, cost-effective, scalable, and resource-efficient layer fabrication processes and dedicated characterization environments that specifically combine different analytical approaches with *in-system* or *in-situ* measurement facilities are being developed. To complete this, AI-based algorithms are required for quantitative acquisition and interpretation of predicted and measured characteristics of the variety of materials and material combinations.
- Develop **material libraries** of new photovoltaic materials or material combinations, and establish database-based data management relevant to high-efficiency solar cells. They will also serve to collect and exchange photovoltaic-relevant research data between the individual Helmholtz Centers. This will make it possible to identify the "*next generation*" of absorber materials of different bandgap regions for multi-layer solar cells (for example, triple-junction solar cells).
- Predict real **efficiency and lifespan potential** of new photovoltaic materials focused on chemical/crystallographic structure and based on key material parameters of absorption, mobility and carrier lifespan. Analogous parameters (for example, selectivity and passivity) will be determined for the functionality of interfaces (for example, between absorber and contact materials).
- Establishment of **cradle-to-cradle life cycle analyses** of photovoltaic materials, devices and technologies. Photovoltaic materials and processes must be in compliance with all national and international requirements necessary to establish photovoltaics as a dominant renewable energy source with system relevance. Furthermore, the long-term stability and environmental friendliness of processes and materials must be included in the overall evaluation.

KEY FUTURE ACTIVITIES

Information-driven materials and device research will be central to the development of future photovoltaic technologies beyond PoF IV. A strategic goal must therefore be to expand core competencies and methods in this area:

- **Expansion of Helmholtz Association platforms** (for example, AMANDA) and databases as well as

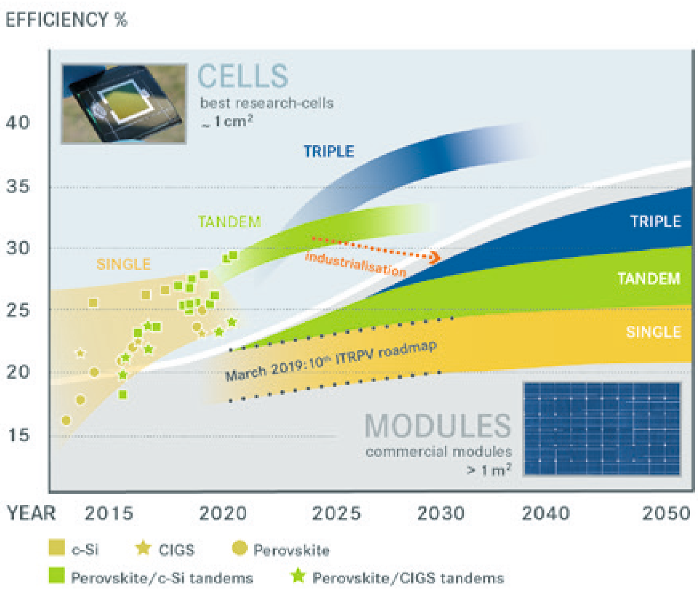


Fig. 8: Roadmap for PV efficiencies of solar cells (1 cm2) and commercial modules (> 1 m²) (Source: HZB, based on Nat. Energy (2017) 16196; Adv. Energy Mater. (2020) 1904102).

pilot projects (for example, "*in situ characterization platform for liquid-processed perovskite solar modules*" (IN-SIPERO)). The unique combination of materials synthesis and synchrotron X-ray based analytics at the EMIL@BESSY II infrastructure is of crucial importance in achieving the strategic goals.

- The **integration of fundamental machine learning principles** that significantly improve throughput in terms of data acquisition and analysis is mandatory when investigating the properties of combinatorial material libraries. In addition, modeled and measured material properties (**digital twin**) must be linked to external databases and standard characterization data to provide a holistic understanding of the relationships between fundamental physical properties and the performance of solar cells or their components.

Progress in optimizing the heterostructure of photovoltaic devices is also expected through the targeted investigation of new materials for contact and transport layers in conjunction with newly developed absorber materials:

- Application and targeted tailoring of, for example, 2D materials in conjunction with their 3D analogs.
- Application of non-destructive depth-resolved X-ray spectroscopic characterization techniques in combination with *in-system/in situ* sample preparation or treatments.
- Investigation of the influence of real operating conditions on the chemical and electronic structure in the solar cell and at its interfaces (*in operando* investigation methods), crucial, among others, for the understanding of aging processes in solar cells and the development of mitigation strategies.

New generations of photovoltaic materials will be even more versatile and variable, driving the global integration of PV into everyday life. New technologies for solar energy conversion, such as solar lasers pumped by luminescent solar concentrators or photocatalytic microreactors for air or water treatment, will develop. Energy autonomy in industry, transportation, and construction will require additional technologies with high variability and integration potential without sacrificing efficiency, durability, or cost.

SELECTED INFRASTRUCTURE USE

The large energy range of X-ray light provided by **BESSY II** allows the investigation of material surfaces as well as deeply buried layers and interfaces. In addition, the chemical, atomic and electronic structure of photovoltaic materials can be fundamentally investigated using the versatile instrumentation at the beamlines.

In **EMIL@BESSY II**, various energy materials can be fabricated and characterized using a combination of different X-ray and electron-based analytical techniques. This enables *in-system, in situ,* and *in operando* measurements on layer systems fabricated in industry-relevant deposition systems, among others.

In particular, experiments at **FLASH** and **European XFEL** can provide important contributions to the understanding of charge separation during photoexcited processes, whose lifetimes are extremely short, in order to specifically optimize materials according to rational methods. For the analysis of atomic and electronic structure as well as complete devices, a wide range of analytical techniques in the harder X-ray range is available at **PETRA III**.

The **Helmholtz Energy Materials Foundry (HEMF)** is a large, collaborative research and development platform dedicated to the synthesis of new and improved materials for energy conversion and storage applications. HEMF serves the scientific community and is operated as an international user facility for academic and industrial partners. Six Helmholtz Centers are involved in HEMF **(HZB, FZJ, DLR, KIT, Hereon, HZDR)**.

The Karlsruhe Nano Micro Facility (KNMF) provides access to laboratories for micro- and nanostructuring as well as in the laboratory for microscopy and spectroscopy to unique fabrication and characterization technologies.

The Autonomous Materials and Device Application platform **(AMANDA)** is a universal platform for automated and autonomous investigation of materials science problems. It combines a generic research automation system with an automated MAP (Material Acceleration Platform) facility for the fabrication and characterization of laboratory-scale solar cells. With its toolset, the AMANDA platform can significantly accelerate materials and process development for solution-processed thin-film solar cells.

SYNERGIES

Synergies with other topics in the Helmholtz MTET program are important for photovoltaic materials research (Topic 3: Subtopic "*Solar Fuels*" and Topic 5 regarding life cycle analysis). Further synergies exist in particular with the Research Fields Matter and Information concerning the use of large-scale research facilities (especially *in situ* and *in operando* methods) and digital material development.

Regarding the *in-situ* monitoring of the growth process of absorber thin films by multiparameter X-ray based methods, there are also synergies with MAXIV, the synchrotron radiation source in Sweden.

In the graduate schools **MatSEC, HyPerCells** as well as the **Helmholtz International Research School HI-SCORE** (collaboration with Israel) there are multiple synergies to research on photovoltaic materials.

Combinatorial materials research is carried out worldwide with great success. Synergies regarding photovoltaic materials exist with HI-ERN, NREL and MIT in the USA, but also with the University of Toronto, Canada.

Researchers worldwide are working on (hybrid) halide perovskites, the basis of highly efficient thin-film solar cells. Synergies exist in this area with groups in the SFB "*Perovskite Semiconductors: From Fundamental Properties to Devices*" and the IPVF/CNRS, France. These materials are also suitable for tandem solar cells. Synergies exist here with the Institute for Solar Energy Research in Hameln (ISFH), the Center for Solar Energy and Hydrogen Research Baden-Würtemberg (ZSW), Oxford University, UK, and the Australian National University.

KNOWLEDGE TRANSFER WITH METHOD PLATFORMS

With the method platform MAP, a collaboration is being developed to create a common database on perovskite semiconductor materials. This can then be expanded with new current solar materials.

Goal: Development of new concepts and materials for highly efficient and long-term stable solar cells
Participating Research Fields: Energy, Information, Matter
Participating Centers: HZB, FZJ, KIT, Hereon
Infrastructure: BESSY II, EMIL@BESSY II, PETRA III, HEMF, HEMCP, KNMF, AMANDA, FLASH, European XFEL

FOCUS TOPIC "MATERIALS FOR HEALTH"

SUMMARY

The development of new materials and material systems for life and health research is a driver for innovations in diagnostics, treatment, prevention, and research into disease mechanisms. These include: (1) Understanding **bio-material interactions** (*bio-instructive materials*). (2) **Intelligent delivery systems** (*advanced delivery systems*) for drugs and diagnostics. (3) **Regenerative therapies** and *in vitro* test systems *(artificial tissues and organs*). (4) **Multifunctional implants** (Fig. 9).

There are numerous challenges for basic research in this area, since interaction with living systems is associated with a considerable increase in complexity. The interdisciplinary research approach encompasses the design of materials with tailored multifunctionality, interaction with biological materials, and material behavior, including degradation processes over the whole lifetime in the organism. Integrative structural analysis allows the characterization of the interaction and interfaces between biological tissue and inorganic materials with high spatial and temporal resolution.

In translational biomaterials research, smart biohybrid delivery systems are being pursued for targeted and controlled release of drugs and diagnostics ("*smart*" drugs) and for overcoming biological barriers. Transformative opportunities for modern medicine arise from materials that can modulate *in vivo* regenerative processes. These also serve to create artificial functional tissues and organs for transplantation into patients and, in the form of biological barriers, organoids and organ-on-a-chip for pharmacological screens, and thus as an alternative or complement to animal testing. Multifunctional materials enable degradable as well as actuator and sensory functional implants, especially for minimally invasive treatments.

The development of new methods for the determination of *in vivo* data (sensor technology, imaging) provides completely new possibilities for improved prevention, diagnostics and treatment. Ideally, this should result in technologies that enable patients to self-monitor the impact of their lifestyle on their health, the success of a medical treatment, or the condition of their implant, and if necessary, to communicate with their treating physician via eHealth apps, for example.

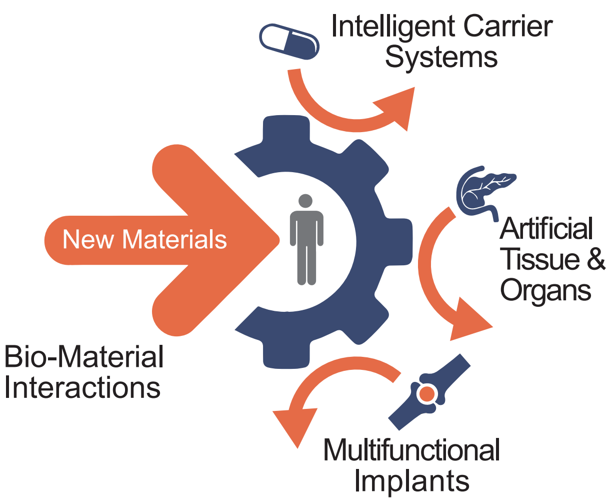


Fig. 9: New materials and their application for health research and medicine (source: HMGU).

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV.

Bio-material interactions

Biomaterials research requires **an integrative, cross-scale analysis of the structure and interaction of organic and inorganic matter**, as well as a fundamental understanding of biological processes underlying specific disease patterns. For this purpose, modern methods of structural analysis and imaging are developed and applied.

In addition to X-ray and scanning probe-based methods, imaging and computer-aided techniques, cryo-EM and NMR spectroscopy are combined with X-ray and neutron scattering. Biological material structures (for example, amyloid fibrils in Alzheimer's disease and diabetes), and self-assembly of macroscopic structures are studied *in vitro* and *ex vivo* (in cellular environments). Highly sensitive optical methods can be used to analyze weak and transient bio-material interactions that (for example, as a "*soft protein corona*") influence the behavior of nanoparticles in vivo. Supercomputers enable the analysis of experimental information through AI-based methods and multiscale tissue simulations (for example, tumor tissue or tissue regeneration).

Using high-throughput synthesis and characterization methods, and supported by AI algorithms, databases on polymeric biomaterials are being built. The development of sensor technology that allows working with minimal sample volumes or *in vivo* is a major challenge but of essential importance, as usually little biological material is available for analysis. Surface modifications of materials should optimize interactions with proteins and other biomolecules or track the *in vivo* behavior of new materials or physiological changes in the body using implantable sensor technology.

Intelligent carrier and delivery systems

A central problem in the development of new drugs is their **transport to the site of action across various biological barriers** in the body. Nanotechnology in particular is providing important impetus for this ("*nanomedicine*"). Bacteriomimetic and bacteriogenic nanocarriers are being researched in order to combat infectious diseases more effectively. The penetration of nanoparticles into hair follicles enables non-invasive immunization. Aerosolizable nanocarriers, novel deposition systems, and pharmacokinetic models for pulmonary drug delivery are being investigated. Inorganic nanocarriers and encapsulation of cytostatic drugs are important approaches for the treatment of infectious and tumor diseases. DNA origamis, nanocarriers, and bioresponsive polymers, which can also be integrated into an implant, provide access to effective and safe therapies. Self-assembling nanoparticles are being developed for theranostic monitoring using optoacoustic and multiscale imaging.

Regenerative therapies and in vitro testing systems

Human pluripotent stem cells are the starting material for the development and production of cells for **3D tissue repair**, **organoids** for disease modeling, or whole **organs for cell replacement therapy**. Of particular note are the organoid systems already developed for the brain, heart, lung, pancreas, and intestine. The integration of advanced material design is key to improving *tissue engineering* for diabetes and respiratory diseases, cardiovascular and neuromuscular diseases, and infectious diseases in the core area of the Helmholtz Health Centers. Through miniaturization and parallelization, 2D and 3D cell cultures can be characterized cost-effectively with new omics tools. Here, approaches such as Langerhans islet, or lung epithelial tissue are grown and analyzed on chips ("*organ-on-a-chip*") on a micrometer scale. Defined tissue structures are built on hydrogel scaffolds of synthetic and natural polymers by additive manufacturing processes such as 3D printing. Printing methods based on single/multi-photon or digital light projection stereolithography are used to process synthetic polymers, metals and living cells.In particular, coatings of high-precision, nm-scale polymer structures (*nanoscribe*) with biocompatible materials are explored to achieve optimal light yield and structural resolution.

Furthermore, research is conducted on human cell culture models of biological barriers (intestine, lung, skin), especially in the pathophysiologically altered state, for example, chronic infection by biofilm-forming bacteria. Clinical studies on initial applications of investigational products based on materials that can modulate regeneration processes are performed. Translation into clinical application is performed via a method platform at BCRT. This includes the design, fabrication and biological testing of investigational products and the conducting of clinical trials for first use in humans.

Multifunctional Implants

Implants made of bio-responsive polymers react to physiological (pH, ROS concentration, etc.) as well as exogenous stimuli (ultrasound, magnetic field). This allows "*on-demand degradation*" of only temporarily needed implants. The controlled mobility of implants opens up visions such as "*soft robots*" and continuum robots, which, driven by artificial muscles ("*shape memory polymer*" actuators) or flexible materials, can move autonomously in the environment and, with appropriate miniaturization, also in the human body.

Degradable metallic biomaterials, for example, magnesium, offer great potential if they dissolve in an application- and patient-specific manner. Ideally, the released ions trigger tissue regeneration, which in turn influences the rate of degradation. This type of physiological feedback is unique and opens up new possibilities, for example, for the local treatment of cancer. If optimized coatings or adaptive bioinstructive properties are incorporated, further functionalities can be implemented: Control of antimicrobial properties of implant surfaces or biofilm diagnostics on explants. Combinatorial (bioorganic) chemistry is used to identify new material systems (for example, MOF-based). Digital production technologies for the fabrication of multifunctional implants are developed at Hereon. Essential insights into the *in vivo* behavior of new materials or physiological changes in the body are provided by implantable sensor technology.

LONG-TERM STRATEGIC GOALS

The information-guided development of innovative materials and systems for health and quality of life holds unique perspectives for **innovations in the research of disease mechanisms, diagnostics, treatment and prevention**. In this context, scientific and engineering methods are combined with medical-pharmaceutical research. **Accelerated digitalization**, especially using **artificial intelligence** (AI), is a necessary prerequisite for world-class competitiveness. The complexity of the biological environment requires a fundamental understanding of material-tissue interactions to develop **customized materials for biologization**.

Bio-material interactions
Detailed understanding of mechanisms at biotic/abiotic interfaces is required to develop and optimize bioinstructive material systems:

- Molecular understanding of bio-material interface interactions.
- Integrative structural analysis *in vitro* and *in situ* (for example, cryo-EM, NMR, fluidAFM, optical, acoustic, and X-ray-based methods) and multichannel imaging for molecular actuation (for example, optogenetic, electromagnetic stimulation).
- Design and synthesis of multifunctional biomaterials.

Intelligent carrier and delivery systems
In order to deliver drugs (therapeutic proteins, gene therapeutics, small molecules) and contrast agents for diagnostics specifically to their site of action and release them in a controlled manner, optimized materials are being developed as transport systems ("*advanced delivery systems*").

- Biomimetic and biogenic nano-carriers for enhanced and directed transport as well as exo- or endogenously controlled release of drugs or genetic information, for disease- and patient-specific approaches.
- Self-assembling nanostructures for diagnostic & theranostic applications.

Regenerative therapies and *in vitro* test systems
Bio-functional materials and corresponding processing technologies are required for the modulation of regenerative processes, the assembly of artificial tissues for *in vitro* test systems, and artificial organs for transplantation medicine.

- Bio-functional materials for building complex tissue structures with heterogeneous cell types (i) to study human physiology and complex disease mechanisms, (ii) to modulate regeneration processes and immune homeostasis, and (iii) for organ replacement.
- Additive manufacturing technologies to build complex tissue structures, and platforms to culture physiological tissues at micro to macro scales ("*organ-on-a-chip*", organoids, organs) for drug testing.
- Reduction of animal testing.

Multifunctional implants
Implants should stimulate tissue regeneration, be minimally invasive in application, and guarantee the patient unrestricted mobility and activity as much as possible.

- Consideration of the entire life cycle of implants and drug delivery systems with adaptive, sensory, and actuator functions, especially using "*dynamic digital twins*".
- Automated, robotic and AI-assisted design and manufacturing workflows.

KEY FUTURE ACTIVITIES

Bio-material interactions

- Development and application of **integrative analytics** (cryo-EM, NMR spectroscopy, AI/ML-assisted optical imaging, and molecular manipulation) to study the molecular properties of nanoparticles (lipid vesicles, nanofibrils, self-assembling protein nanocompartments, bio-material interfaces).
- **Computational methods and AI** for understanding and optimizing materials and bio-material interfaces.
- **Multiparametric analysis** of thin films and 2D / 3D materials for mechanistic understanding of assembly, remodeling and degradation behavior.

Intelligent delivery systems

- Novel technologies and models for transport of antimicrobial agents (including nucleotides) across the gram-negative bacterial cell wall (HIPS).
- Self-assembling nanocarriers and nanocompartments generated in living human cells for directed transport of drugs and diagnostics into cells and organs (Hereon, HIPS, HMGU).

Regenerative therapies and in vitro test systems

- New materials, including those with programmable cell and tissue instructivity, for future patient applications that allow functional nanocompartments to be generated from human cells, tissues, organoids, and organs (pancreas, liver, retina, heart tissue) at scales relevant for transplantation (HMGU, MDC, Hereon).
- Upscale production of specific cell types and develop 3D/bio-printing methods for **the production of complex, controllable, functional tissue scaffolds and biological structures.**
- Development of barrier models and biochips with biophysical interfaces and inks from synthetic and natural biopolymers (HMGU, KIT, HIPS, MDC).

Multifunctional implants

- Controllable implants and drug delivery systems by implementing sensing and actuation. Intrinsic signals are sensed by implants and cause the adaptation of the material to its environment, for example, structure, degradation behavior, and release kinetics (Hereon, KIT).
- Implement computer/robotic automated manufacturing and 3D printing to integrate material functions into implants and other medical devices.
- Accelerating translation by addressing bottlenecks in the development chain: Integrated processes, manufacturing and characterization of test products.
- Predicting optimal implant materials through multi-physics and cross-scale simulation and AI approaches ("*digital twin*").

INFRASTRUCTURE USE

The specific challenges of materials research in health care research require a multi-method approach. For this purpose, the highly developed infrastructures of the Helmholtz Association are essential and should be further developed. In particular, **X-ray** and **neutron-based methods,** *in situ* **microscopy, multiscale imaging, cryo-electron microscopy, ultra-high field NMR spectroscopy, high-throughput synthesis and characterization, and supercomputing** are central.

SYNERGIES

Scientists from different Helmholtz Centers are already collaborating in multidisciplinary consortia to develop new materials in health research at national (BMBF) or European level (**IMI, Marie Curie, ITNs**). The synergy between materials and health research will be strengthened in the future through (i) interdisciplinary workshops or hackathons and (ii) the establishment of a cross-center and cross-research area graduate school "*Materials Research for Health*".

KNOWLEDGE TRANSFER WITH METHOD PLATFORMS

The work presented here can benefit greatly from the two cross-focus method platforms. In addition to using the excellent characterization capabilities bundled in the "*Correlative Multimethod Materials Systems*" platform, the exchange with the "*Accelerated Materials Development*" method platform allows the digitalization of biomaterial development. The degradable metallic implants made of magnesium are one of the flagship projects being worked on in the method platform "*Accelerated Material Development*" within the framework of the JL VMD (Research Field Information) and the JL MDMC (part of the platform "*Correlative Multimethod Material Systems*"). The program ("*Materials Systems Engineering"*) also contributes to these activities with several topics (including work on the characterization of degradation products of polymeric implant materials).

Goal: Biofunctional materials for health research and medicine
Participating Research Fields: Helath, Information
Participating Centers: HMGU, HZI-HIPS, MDC, DKFZ, Hereon, KIT, FZJ
Infrastructure: MLZ, JSC, ER-C, KNMF, GEMS, BNMRZ, BMT, BCRT, PETRA III

FOCUS TOPIC "BIO-BASED AND -INSPIRED MATERIALS IN THE BIOECONOMY"

SUMMARY

Bio-based and bio-inspired materials hold great opportunities as sustainable alternatives for materials made from fossil raw materials. However, derivation from biological raw materials alone is not sufficient; rather, for these materials, too, (1) sustainable use must be achieved through adequate design and targeted introduction into cycles with the least possible negative effects on natural systems, (2) practical use must be made possible through competitive prices, and (3) the functionality of the materials must be at least as good as that of competing materials from fossil raw materials. At the same time, (4) nature also offers structural and functional models that enable new applications as bio-based design. (5) In addition, the bioeconomy has a high demand for specific material development. This includes, for example, catalysts for the conversion of biomass in biorefineries or membrane materials for the separation of complex mixtures of bio-organic liquids or gases. Bioeconomy thus has components in which biological materials are implemented, these are used as inspiration for structures or functions of materials, but also a need for new materials for the implementation of bioeconomic processes. All approaches must adhere to the principles of *sustainability* and environmental relevance.

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

Bioeconomy research in the Helmholtz Association has a long tradition in topics related to the efficiency of biomass production in plants and its conversion by microorganisms (Topic 7). So far, the main focus has been on the use of biomass as a raw material in the chemical industry, in addition to its production for food. **The integrated consideration of biomass production, its conversion in biorefineries or in biotechnological processes** (parallel to the use of organic residue streams) to modified raw materials or chemicals and the **development of material cycles** is an essential concept of sustainable bioeconomy. Bio-based materials are thereby either rebuilt from the (platform) chemicals or built up from partially modified biomass, as in the use of fibers, chitin or lignin, for example. Cascade utilization in this sense uses, for example, in building materials first the grown biological structure of the wood, then breaks down the structure into chips or fibers, then uses chemical monomers, and only in the last step in energy utilization does the conversion into CO_2 take place. Target systems are also biopolymers that either replace fossil raw materials as drop-in products, but also new polymer systems that allow recycling of materials in a special way. Research activities in the Research Field Earth and Environment that contribute to this research topic are summarized in Topic 7 Bioeconomy.

In addition to the classic use of biomass and the application of the grown structures, value-adding material properties are increasingly being researched as bio-based coating or functionalization materials. For example, polymer nanochannels are being fabricated using ion beam technology and then biochemically modified to mimic the functionality of protein biochannels (GSI). Systems are also being developed in which reactive surfaces or surfaces that release substances in response to certain stimuli are constructed. Structures and functions of plants (FZJ) and marine organisms (AWI) are analyzed to develop **new bio-inspired approaches** for the development of structurally optimized engineering structures and materials. Here, biophysical principles of biological composite systems are analyzed and derived principles are applied by generative design software to (a) develop resource-efficient multifunctional lightweight structures optimized for robustness, permeability and vibrational properties, (b) to build nanocomposites in complex lightweight geometries and material substitution (for example, biodegradable plastics), and (c) to derive the development of morphogenetic algorithms for sustainable product development.

LONG-TERM STRATEGIC GOALS

- Expand the portfolio of Helmholtz Association bioeconomy research on bio-based materials to include relevant application examples.
- Intensify collaboration of bioeconomy research with materials research and infrastructures in the Helmholtz Association.
- Demonstration of **cascade use of biomass** with a significant share of raw material use.
- Establishment and implementation of structural and functional design approaches based on bio-inspired materials.
- Application of life cycle analysis and *sustainability* assessment of (bio-based) material systems in interaction with the environment.
- Demonstration of bio-based materials for sustainable use.
- Integration of research on bio-based materials into the materials research activities of the Helmholtz Association.
- Establish **analysis of environmental impacts of raw material extraction**, production and use of new materials in parallel with material developments in other areas of the materials research strategy.

MAIN FUTURE ACTIVITIES

- **Cascade use of bio-based materials and raw materials.**
  In a circular economy, innovative biorefinery concepts must integrate biomass use for food and feed production with value chains for material and material use using renewable energy. This includes the production and refinement of chemical building blocks for material and energy use (cascaded biomass use and polygeneration). In such advanced biorefineries, biomass by-products and organic residues or waste streams from agriculture, forestry, aquaculture, food industry, municipal biowaste, etc. are recycled into intermediate or final products for the provision of bulk chemicals, platform chemicals, and energy carriers, thereby closing nutrient cycles and substituting fossil resources.
- **Bionic solutions for material design**
  The analysis of structures and functions of plants and marine organisms can also be used to establish new bio-inspired approaches for the development of structurally optimized engineering structures. Natural structures and functions are analyzed and applied to sustainable materials, including bio-based materials such as bagasse, cellulose, and degradable plastics. This includes (a) application pathways for resource-efficient multifunctional lightweight struc-

Fig. 10: ELISE stands for the AWI concept of "Evolutionary Light Structure Engineering". The aim was to systematically transfer the construction principles of the extremely light but mechanically stable shells of radiolarians and diatoms to technical components. Through the integrative software approach, a powerful, universally applicable development software was developed for all industries; from shipbuilding to aerospace engineering. Synergies with the main topic "lightweight construction" are available here (source: AWI).

tures optimized for robustness, permeability, and vibration properties, (b) nanocomposites in complex lightweight structures and material substitution (for example, biodegradable plastics), and (c) the application of dynamic evolution of structures (for example, morphogenesis of complex biogenic lightweight structures) to understand biophysical principles and transfer them to algorithms for generative design software. The goal is also to further implement the technologies for application in the broader bioeconomy.

- **Chemo- and bio-catalysts and coatings with and of biomaterials.**
  In addition to intensive work on biocatalysts, innovative extensions of classical biotechnological transformation processes are also being pursued, implementing hybrid bio/chemo-catalytic processes based on combinations of whole-cell biocatalysts, enzymes, and chemo-catalysts integrated with novel (bio)reactor technology, including, for example, flow chemical systems and bioelectrochemical reactor systems. Such hybrid processes offer new possibilities for fabrication and promote the linkage of biological and chemical catalysis. To stabilize and optimize multistage processes of this complexity, computational design and integrated process engineering will be critical. Currently, this major challenge can only be met in well-equipped institutes with multidisciplinary research teams, and it offers excellent opportunities for synergies with other areas of materials research.
- **Separation membranes for bioeconomic and biomedical applications in environmental protection**
  Material separations are not only essential for biological organisms, but an important building block in many process chains and therefore for a sustainable economy. Membrane technology allows the interconnection with other separation processes like distillation, absorption or adsorption to hybrid processes, which in their combination are able to achieve energetic optima. Applications such as reverse osmosis for water desalination or organophilic nanofiltration are superior to their competing technologies in terms of energy input. The barrier effect against viruses and bacteria and the high functionalizability of ultrafiltration and microfiltration membranes also demonstrate application potentials of membranes that do not exist for other processes. Examples of the use of membranes have already been listed in the main topics "*Materials for hydrogen technology*" and "*Battery materials*". Further application examples are hemodialysis for renal insufficiency, water desalination for the provision of drinking water, separator membranes for batteries, and fuel cells. Other applications of membranes include the purification of chemicals and pharmaceuticals, the enrichment of desired ions in water, and the use of membrane reactors for material conversion. The development of new membranes with specific functionality requires a wide range of interdisciplinary research, ranging from the synthesis of membrane materials (these can be inorganic in nature or consist of polymers or composite materials) to membrane production and, if necessary, functionalization and their incorporation into modules, right through to the complete technical process. The goal of the research is to enable demand-driven membrane development, where experimentation and model-based computer simulations will go hand in hand to better optimize experimental research and provide society with tailored membrane technologies for various applications.

SELECTED INFRASTRUCTURE USE

The share of material-related research in the Research Field Earth and Environment is manageable so far. Infrastructures belonging to the Research Field Earth and Environment, which are used for its own research work, but also applicable for cooperation with other material scientists, include:

- **Observation platforms** in many relevant environmental compartments, where the environmental impact of materials can also be recorded,
- various **tomographic systems** (CT, MRI, PET) that enable structural analysis of plants and biomaterials from a macroscopic level, and microscopy facilities and technologies for biological materials, and
- **IT-based reconstruction** and **image analysis techniques** and software for bionic lightweight engineering (ELISE).

Of interest to Research Field Earth and Environment researchers could be the use of high-end infrastructures. These include:

- **X-ray and neutron-based methods** (diffraction, tomography, small-angle scattering, spectroscopy **(PETRA III, DESY, BESSY II, Hereon, FZJ)** for the characterization of biomaterials,
- **High energy ion irradiation** for the fabrication of ion track membranes with tailored parameters (GSI),
- *In situ* **microscopy, imaging and cryo-electron microscopy (FZJ, HMGU)**, and the
- Jülich **Supercomputing** Center (FZJ)

SYNERGIES

Contributions from the Research Field Earth and Environment to materials research can provide important elements for the overall materials research strategy of the Helmholtz Association in PoF IV. This is currently still a rather small field in the program, however, it offers very interesting approaches, especially in cooperation with materials research experts in the Helmholtz Association.

- Observation platforms of the Research Field Earth and Environment can provide important information on the persistence and distribution of materials in relevant environmental compartments of the Earth system.
- Bio-based materials and cascade use with successive decomposition of biomass can be interesting starting points for conceptual (for example, circular economy) investigations as well as for alternative materials (C-based).
- Biological principles, which are analyzed in the Research Field Earth and Environment, can provide interesting impulses regarding structures, functions and alternative raw materials in material research.

KNOWLEDGE TRANSFER WITH METHOD PLATFORMS

The method platform "*Accelerated Material Development*" offers opportunities for improved characterization of bio-based materials via robotics, non-invasive methods and predictive simulation approaches.

Goal: Development of bio-based materials and material systems that contribute to the reduction of environmental and climate pollution
Participating Research Fields: Earth and Environment, Matter, Energy and Health
Participating Centers: AWI, HZB, Hereon, FZJ, KIT, HMGU, GSI
Infrastructure: Pflanzen-MRI, Pflanzen-PET, Umweltmonitoring-Plattformen, UNILAC, CRYRING, PETRA III

FOCUS TOPIC "MATERIALS FOR LIGHTWEIGHT CONSTRUCTION"

SUMMARY

Lightweight materials and structures of the future will need to exhibit not only high specific strengths and stiffnesses, but also significantly improved thermal properties, robust processability, sustainable usability over the life cycle, and functions such as electrical energy storage and conduction or self-healing potential. To this end, in addition to the material design for adjusting these mechanical and functional properties, a reproducible process design is being developed in combination with economical and ecological manufacturing technology. The focus here is on new fiber materials, matrix materials, light metal alloys, their manufacturing and joining processes including 3D/4D printing and multifunctional coatings.

Such material systems must be developed across all scales to achieve the desired properties. They also need to be processed, integrated and tested in complex system environments. The physical changes of the material systems during use must be determined for reliable lifespan prediction. For this purpose, it is necessary to cover larger parameter fields than is possible today by classical experimental approaches. The complexity of cross-scale material and process development is to be mastered by characterization and simulation techniques and "*digital twins*".

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

The development fields for lightweight materials are broad. For electric drive units, materials with good electrical conductivity are needed that can serve loss-minimizing energy transport, storage, and structural load transfer simultaneously. At the same time, the additional battery weight requires a further significant improvement in **lightweight vehicle construction**. New development is also required in the field of functional materials which, as energy converters, combine mechanical effects with electrical and magnetic field changes, for example. Also, today's lead-containing piezoceramics will have to be replaced by lead-free functional materials in the medium term. In addition to lead-free piezoceramics, as developed at DLR, there are approaches for nanoporous metal-polymer hybrid materials at Hereon.

The holistic view of the development chain also takes into account **recycling and low CO_2 manufacturing processes**. The process chain of metallic materials from material formation, through their processing (for example, innovative casting, rolling, extrusion and forging, additive processes) to their functionalization must also be developed holistically. The combination of metallurgical material design and knowledge-based technological process design during thermomechanical treatment leads to an increase in the performance of new lightweight alloys.

Sustainable weight reduction can be widely achieved via true 3D or 4D printing. Today's 3D structures created in layers will be replaced in the future by structures printed free-standing in space, for which fast-solidifying materials and associated thermal management are particularly crucial. The use of robots addresses the 4th dimension (time) of 3D printing and promises significantly higher output rates of interest to industry. 3D printing of metals via different processes (SLS, SLM, EBM, FFF, ...) depends on the consideration of the entire process chain (KIT, DLR, Hereon). This starts with the material development specific to 3D printing, considers the process development and extends to the specific design as well as the modeling of complex structures and their function-based optimization (DLR, KIT). To this end, Hereon, KIT and DLR are working on the development

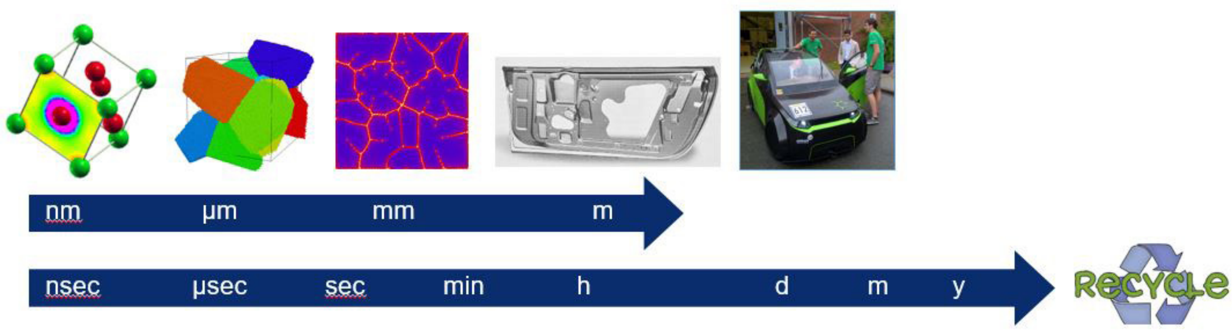


Fig. 11: Cross-scale description of material systems in lightweight construction (source: HZG).

of powders, feedstocks and continuous processes for the production of high-quality base material. Process development is supported by suitable simulation and modeling tools to significantly shorten development times.

For industrial use of new materials, the associated manufacturing processes for component production must also be developed in parallel. So far, lightweight construction potentials cannot be fully exploited, especially in generative processes, due to the strong dependence of structural parameters on the selected manufacturing and joining processes. Here, ontologies need to be developed that link the mechanical and, in the future, also thermal and electrical parameters of manufactured components with the manufacturing conditions (DLR). Friction-based joining processes are also being developed to replace conventional riveting technologies for hybrid material combinations (Hereon). Metallic lightweight structures show great potential for increasing fatigue resistance via residual stress design. Laser shock peening, in combination with a "*digital twin*" in the form of a multi-step process simulation chain up to crack propagation simulation, offers the possibility of tailor-made imprinting of a compressive residual stress field into the respective component and loading scenario (Hereon).

New fiber ceramics (DLR) or TiAl-based materials (Hereon) open up lightweight structures for high-temperature applications, especially in the field of aerospace propulsion. In the case of fiber ceramics, the focus is on new SiC-SiC and oxide composites. The core challenge here is **thermally stable fibers and oxidation-resistant fiber matrix composites** that exhibit higher thermal performance and durability. The integration of numerical models of material behavior with digital models of the components in "*digital twins*" of the test facilities provides insights into the 4D behavior of the material at all scale levels. It also allows optimization of validation experiments by feedback with the calculated material responses.

Lightweight materials and structures can benefit greatly from surface treatment processes. This is particularly important for structural light metals such as magnesium and aluminum, which often suffer from corrosion problems, especially when combined with other structural materials. Therefore, the development of multifunctional surfaces and new strategies to actively control degradation processes in light metals and multi-material structures is a key activity to broaden the field of application and use. Novel functional coatings and surface treatments based on an active nanocontainer such as LDH incorporated into the pores of PEO coatings and combined with functional components encapsulated within LDH structures can provide on-demand triggered delivery. These responsive, active and functional nanocontainers deposited on light metal substrates and hybrid multi-material structures can be used as a toolbox to enable flexible, on-demand design of multifunctional coatings. Designing such surfaces requires a new coupled modeling approach that incorporates aspects of metallurgy, coating and process technology, physics, and electrochemistry using multiscale simulation tools and machine learning approaches.

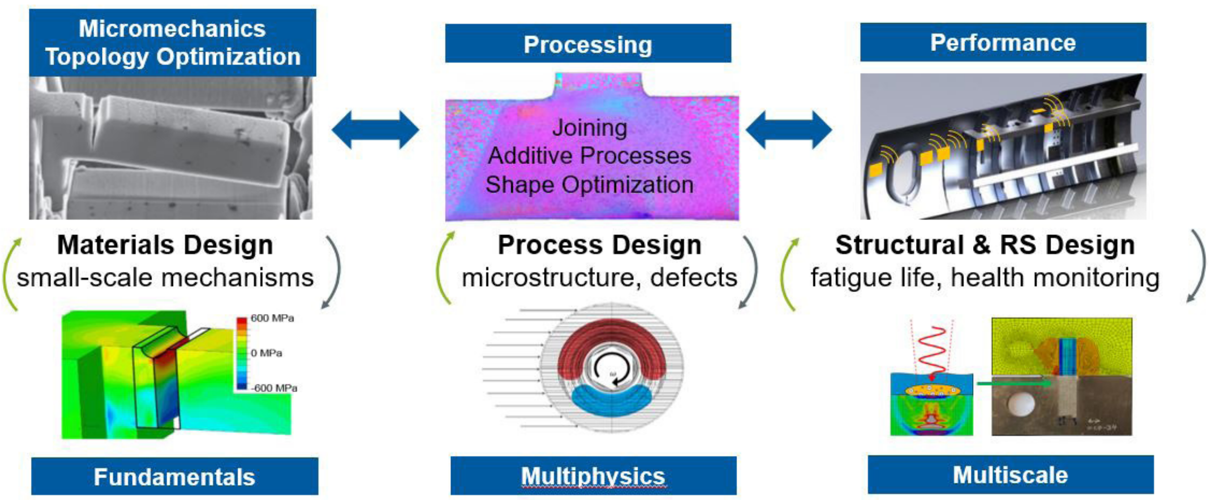


Fig. 12: Coupling of material, process and performance through "digital twins" (source: HZG).

LONG-TERM STRATEGIC GOALS

- **Polymeric fiber composites (PMCs):** Fibers with high thermal and electrical conductivity (for example, pitch-based) are available, expanding the range of applications for PMCs. New **high-performance fibers** (for example, CNT-based) and **new hybrids** with increased mechanical, thermal, and electrical performance are also expanding the range of applications for PMCs.
- **Ceramic fiber composites (CMCs):** New oxidation-protected and lifetime-optimized **SiC fiber reinforced SiC ceramics** are available for applications at temperatures above 1200°C. New oxide ceramic fibers open up application temperatures above 1000°C for oxide CMC. Multiphysical, multiscale methods for calculating properties, failure mechanisms and lifetime allow more precise design of CMC components.
- **Light metal alloys:** Predictive virtual material and process design based on "*digital twins*" allows significantly improved virtual material design. Targeted microstructure design can thus be used to develop alloys that have tailored application-specific property profiles and can be manufactured in a controlled and robust manner in a continuous process chain including recycling.
- **New functional materials:** Lead-free piezoceramics, nanoporous metal/polymer hybrid materials, energy-storing lightweight structures, Mg-based lightweight materials with extended functionality including a reuse or further use concept for the material or the structures made from it, are available.
- **Additive processes:** Ontologies for essential mechanical parameters of components made from additive manufactured materials in interaction with manufacturing processes of lightweight structures are available in a generally usable way. Polymer 3D printers for fiber-reinforced plastic composites, which no longer print layer by layer but directly in the third spatial direction, expand the possible applications. Alloys developed for 3D printing without texture and microstructure drawbacks expand the range of uses of 3D printing for high-performance structures. A physically and digitally integrated process chain is available. Predictive modeling of the fatigue of materials in defined environments including residual stress design based on a "*digital twin*" is available.
- The application of *ab initio* methods allows the precise development of multilayer protective and functional coatings for light metals, hybrid materials and fiber ceramics. The focus is on oxidation protection, corrosion protection and functional surfaces.

KEY FUTURE ACTIVITIES

The process chains considered here include the production of semi-finished products but also structurally and functionally optimized components and their further processing into lightweight components. The system and methodology are being developed using wrought magnesium alloys as an example and will be transferred to other lightweight materials, which will also be evaluated in terms of *sustainability* and climate neutrality. The unique infrastructure for semi-finished product production at the Hereon represents a semi-industrial scale that ensures transfer to industrial applications. First principles methods will allow the prediction of the occurring phases in multicomponent light metal systems in order to identify promising material compositions by a virtual screening of large composition spaces. Procedures that are already in use, for example, in the virtual screening of molecules in chemistry, would thus be transferred to the methodologically more demanding (elevated temperatures) and computationally more complex field of multi-component light metal alloys. In further work, design- and function-optimized lightweight components should thus be realized with the aid of novel material combinations of metal and ceramic (for example, using metal or ceramic fibers) in combination with, among other things, generative manufacturing. Suitable modeling and simulation tools are to be used to significantly reduce the experimental effort in both material and process development. **The combination of bionic and functional surfaces, considering the interaction with the environment, will lead to a significant increase in performance, longer lifespan, and thus improved sustainability.**

SELECTED INFRASTRUCTURE USE

- **3D printer systems** for metallic, ceramic, and polymer materials allow rapid fabrication of new materials and conversion to testable components.
- Robotic **mechanical testing facilities and high-resolution chemical-physical analysis systems with interfaces to digital data management systems and AI-based analysis tools allow rapid materials evaluation**
- A **robotic platform** at Hereon generates Big Data for corrosion of light metals in complex environments.
- A new **MTC testing facility** at DLR will allow superposition of mechanical, thermal and chemical loading of material samples for the first time in 5 years.
- *In situ and operando* **synchrotron and neutron scattering** to study material and component behavior will be provided by DESY, FZJ, HZB and Hereon and, in combination with AI methods, will allow rapid

high-fidelity analysis of materials.

- The **HPC and QC infrastructure** available at the Helmholtz Association (integrated in perspective) up to the highest performance class at the Jülich Supercomputing Center is the basis for accelerating material simulation, especially at the atomic level.

SYNERGIES

By linking experimental expertise with *digitalization* methods, such as material and process simulation, machine learning and linked algorithms, the material-specific process-structure-property correlation is captured and modeled. The development and integration of intelligent sensor technology along the process chain as well as the direct insight into the material behavior under the often extreme application or process conditions by using the characterization platforms from the Research Field Matter is essential for a comprehensive data genesis. The link with the Helmholtz Association platform "*Quantum Technologies*" would open up the possibility of QC/HPC-based material simulation. This could form the basis for efficient process development for lightweight materials and at the same time bridge the gap between the Research Fields Aeronautics, Space and Transport, Information and Matter.

KNOWLEDGE TRANSFER WITH METHOD PLATFORMS

First-class experimental and cross-scale data as well as the description of materials and processes via simulation and modeling is a basic requirement to successfully develop new material concepts. Therefore, cooperation with the two method platforms is essential and is already concretely pursued via joint projects within the JL VMD and MDMC. For example, corrosion and lifetime prediction using a coupled modeling approach that incorporates aspects of metallurgy, coating technologies, and electrochemistry using multiscale simulation tools, machine learning and state of the art characterization techniques for data generation requires close knowledge exchange with both platforms. An integrated Research Field-wide data management system offers further potential.

Goal: Complete digital description of the entire value chain from material development manufacturing, to the numerical description of the resulting properties on all scales, and the long-term levels and behavior in real operation.
Participating Research Fields: Aeronautics, Space and Transport, Information
Participating Centers: DLR, Hereon, KIT
Infrastructure: GEMS, MagIC, PETRA III

"ACCELERATED MATERIAL DEVELOPMENT" METHOD PLATFORM

SUMMARY

The Methods Platform "*Accelerated Materials Development*" (MAP) bundles generic approaches in materials research that aim to shorten the screening of materials by several orders of magnitude through the increased use of automated experiments, increasingly self-controlled by AI, and thereby significantly accelerate the development of new materials. To achieve this, existing potential must be pooled to develop new approaches to materials development. Building on the strategy of "*virtual material development*", demonstrators for MAP are to be developed in particular. Numerous research activities of the partners involved in this platform already aim at the development of individual components required for this purpose, but their complete implementation can only be achieved jointly. Groups in the European Union as well as American and Asian competitors are currently working on the implementation of MAP, but these activities are also still in their infancy. Additional coordinated support for such initiatives therefore gives Germany a competitive edge.

Building on the approaches currently being pursued, fundamentally new approaches to materials research are to be developed and taken into application. An important current challenge in this context is the development of accelerator platforms for materials development. Conceptually, an acceleration platform for materials development can be understood as a pyramid of innovative technologies (see Fig. 13), which, starting from processes that are currently already being investigated, enables new innovation impulses through the implementation of further stages. The overarching goal of implementing an acceleration platform for material development is the increasing automation of the material development process, which is currently essentially characterized by manually conducted experiments and manually controlled simulations, along the lines of the automation of manufacturing within the Industry 4.0 concept. The final, still visionary, expansion stage of a material acceleration platform allows the fully autonomous exploration of materials according to specific criteria without human intervention (autonomous discovery).

To make this possible, the existing material data must first be systematically collected and semantically annotated (via ontologies) and made accessible. The currently implemented National Research Data Infrastructure (NFDI) will be able to make a significant contribution to this. A second stage is the development of predictive simulation methods for the prediction of material properties from their microscopic structure and taking into account the manufacturing process on the relevant time and length scales, supported by a small number of carefully selected experiments. The basis for this is the work in virtual material development that needs to be intensified in the current PoF period. The favorable cost-benefit ratio of computational approaches makes predictive simulations and "*digital twins*" key components of the future materials research strategy. The systematic application of such methods enables an innovation leap with reverse design, which enables the computational (i.e., data- and simulation-based) development of materials starting from (ideally) functional specifications.

The fourth stage of such a materials development platform is the implementation of predominantly autonomous robotics that largely automates both synthesis and characterization of the resulting materials. The development of these novel experimental apparatuses is one of the most important and elaborate challenges in the realization of MAP. Although such platforms have already been realized in individual cases, such as in pharmaceutical research, the goal of this initiative is the systematic development of an infrastructure that enables automated material synthesis and characterization for a variety of material classes in a modular fashion. The development of both the components and the overall systems offers considerable potential for innovation and transfer. The fifth stage of such a

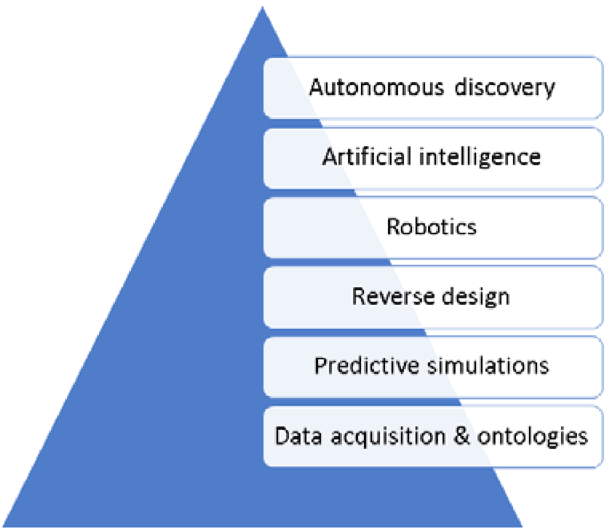


Fig. 13: Schematic representation of the elements of an acceleration platform for materials that build on one another (source: KIT).

material development platform involves extensive support of the material development process by robotics that integrates simulation, data analysis, and artificial intelligence into control strategies. In almost all applications, material development is characterized by very large search spaces that can only be searched in fractions, even by high-throughput methods. Therefore, systematic methods of model and AI-based algorithmic experimental design must be developed to replace human intuition based on iterative information acquisition through experimentation and simulation. In combination with the other components, the availability of these algorithms generates a unique selling point for the corresponding material development platform.

The sixth and final stage of the development of a material development platform implements an increasing reduction of the human intervention in algorithm-based material development to a complete automation in the sense of a self-learning, autonomous material development platform. The implementation of such an approach generates a further scaling potential in the application of the material development platform that moves beyond the fifth stage.

The goal of this step-by-step approach is to increase the speed of material development by one order of magnitude in each of the following stages

- Stage 1-2: Data acquisition and simulation
- Stage 3: Reverse design
- Stage 4: Robotics
- Stage 5 & 6: Autonomous, self-learning development platform,

So that the realization of this concept will lead to an increase of the search space in material development by a factor of about 1000 over a period of ten years.

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

- In the VMD JL, the Research Field Information, with the participation of DLR, is developing a virtual working environment for performing complex simulation and a hybrid, integrated data management system. These connected platforms are intended to make it possible to digitally link the elements of the process chain from materials to automated production, and to research new materials in a virtual process.
- Virtual material development and concepts for the virtualization of material development are being further developed in PoF IV in several centers.
- The Helmholtz Association is systematically pursuing the development of automated and increasingly self-guided experiments. For some applications (for example, biocatalysts or batteries), robotic systems for high-throughput experiments are already established or under construction. This work will be intensified and supplemented by a systematic cost-benefit analysis with a view to transfer to industry.
- In the participating institutes with a focus on materials research, the thermodynamic and/or *ab initio* simulation of materials and the necessary digital infrastructure will be further expanded in a targeted manner. The focus is on the application-oriented use and adaptation of these tools, their validation and feedback to the tool developers. In addition, AI-based tools for the evaluation of large amounts of data from materials analysis are being adapted or developed.
- Several centers are developing "*digital twins*", for example, for quantum materials, organic materials, and printed electronics, which also take into account the behavior of the material in the application.

LONG-TERM STRATEGIC GOALS

- An integrated, cross-facility virtual working environment for data and simulations that enables **cross-scale generation and use** of materials-specific data.
- High-resolution material analysis (see method platform "Correlative multi-method material characterization ") and AI-based analysis of data is established to validate simulation at all scales.
- **Acceleration of material development through virtual material design.**
- Use of AI methods as prescreening methods to target **multiscale simulations** and guide experiments.
- **Exascale and quantum** computing are available as tools for thermodynamic, kinetic, and *ab initio* simulation, allowing acceleration and enhancement of simulation quality. To enable and accelerate quantum mechanical material simulations, quantum computing (QC) will be a key contributor. The focus of the scientific work is on the development of the necessary QC/HPC platform, the quantum algorithms, and the integrated data management system including error correction. In addition to acceleration and quality improvement, this will also allow the search space for new materials, which is limited by human capacities, to be significantly expanded through QC and machine learning-based rapid screening. This can be used to find material compositions that remain invisible today. Due to its specific competence profile, the Helmholtz Association can take a leading position worldwide in this field.

- Methods for rapid production and testing/analysis of materials complement digitally accelerated material development. One focus here is also on new methods that allow faster testing/analysis with the aid of machine learning approaches.
- Development of a series of "*digital twins*" in the Joint Lab "*Virtual Materials Design*" (JL VMD, Research Field Information), which map processes from material design to material processing and application. They will exemplify how real material design can be significantly accelerated by virtual material design.

KEY FUTURE ACTIVITIES

- The virtual working environment for the targeted use of new digital tools to accelerate and increase the quality of material simulation and digital material development will be specifically expanded and made available. The focus will be on HPC-enabled non-commercial tools for simulating complex systems at the meso and macro scales, new methods of data management across centers, AI for big data analysis, and thermodynamic or *ab initio* simulation.
- A new **digital platform for accelerated assessment and prediction of material degradation** in complex environments will be based on artificial intelligence approaches to analyze large amounts of data collected by a robotic platform.

SELECTED INFRASTRUCTURE USE

- DLR is also developing the DLR Future Lab for Additive Manufacturing and Engineering **(FLAME)**, currently under construction, into a tool for rapid fabrication of new metallic alloys.
- Hereon is developing a robotic platform for rapid acquisition of large amounts of data on the interactions between materials and complex environments.
- KIT is developing a **robotics platform for high-throughput experiments** for battery materials and for organic synthesis.
- The partners involved in the JL VMD use the supercomputing centers of the Helmholtz Association.
- Neutron and synchrotron radiation are increasingly used for *in situ* characterization of new materials and their processing.

SYNERGIES

- Development of ab initio tools and use of HPC and quantum computing competencies.
- High-resolution analyses of materials.
- Exchange of workflows for virtual materials development in the Helmholtz Association and beyond.
- Use of techniques for correlative characterization.

ADDED VALUE / KNOWLEDGE TRANSFER FOR THE PRIORITY TOPICS.

- Faster availability of new materials and a broader range of new materials for the applications of the focus topics.
- Improved methods for rapid, high-resolution characterization.
- Expanded and faster digital incorporation of application-specific requirements.

Goal: Accelerated material development through virtualization and *digitalization*
Participating Research Fields: Information, Energy, Matter
Participating Centers: KIT, FZJ, HZB, HZDR, Hereon, DLR
Infrastrukturen: JSC, CSD, HDF, LSDF, HPC-KIT, KNMF, MBC, HTC/PTC, DiLAB, IBC, HLD, ELBE

METHOD PLATFORM "CORRELATIVE MULTI-METHOD MATERIAL CHARACTERIZATION"

SUMMARY

The Helmholtz Association operates a globally unique portfolio of excellent instruments for 2D and 3D characterization of materials with highest structural and chemical resolution, often providing complementary information. The platform for "*Correlative Multimethod Materials Characterization*" offers scientists working in different Research Fields of the Helmholtz Association, and external users, access to these state-of-the-art multiscale and multidimensional characterization techniques based on high-resolution microscopy, spectroscopy and scattering experiments. Characterization also often generates large amounts of data in a wide variety of formats, the aggregation of which is required for overarching analysis. The platform focuses primarily on research infrastructures and techniques embedded in the Research Field Information (among others Joint Lab "*Integrated Model and Data driven Material Characterization*", JL MDMC) and the Research Field Matter (Program MML and Topic "*Data management and Analysis*" in the Program MT). However, there are also bridges into the other Research Fields, for example, via the "*Helmholtz Imaging Platform*" (HIP). For the priority topics presented in this paper, this platform is of central importance and there are a number of interconnections with the "*Accelerated Materials Development*" platform.

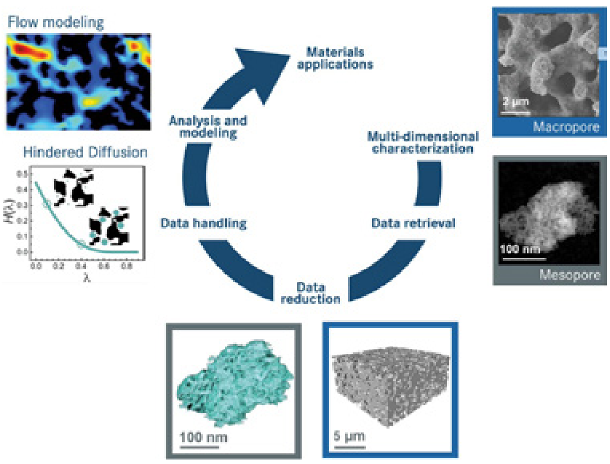


Fig. 14: Workflow example in the method platform (source: FZJ).

CURRENT ACTIVITIES AND MEDIUM-TERM GOALS IN POF IV

State-of-the-art materials characterization techniques with increasing emphasis on scale bridging through correlative and *in situ* and *operando* studies are making a critical contribution to progress in materials development and new technologies. The study of the same samples using a wide variety of methods, for example, combinations of X-ray or neutron imaging or of diffraction and scanning or transmission electron microscopy, are already realized in different forms in the Helmholtz Association:

- **KMNF** (KIT) offers users a portfolio of technologies in the field of micro- and nanostructuring and characterization, some of which are already used in correlative approaches and whose capabilities are being further developed (scanning probe methods, X-ray tomography, nuclear magnetic resonance, electron and ion beam analysis).
- DESY offers complementary investigations by synchrotron radiation experiments at **PETRA III** and **scanning probe methods or tomography** with a focused ion beam in the DESY NanoLab.
- At **ER-C** (FZJ), electron microscopy and scanning probe microscopy studies are combined to investigate structural, electronic and functional properties of materials. In addition, in collaboration with cooperating partners, electron microscopy and synchrotron beam-based characterization are used for correlative studies on identical sample sites and operando studies of the functional mechanisms of, for example, catalysts. Complementary methods for characterization of such samples are provided by neutron scattering experiments from **JCNS** (FZJ).
- **GEMS** (Hereon) focuses on correlative material science studies with emphasis on *in situ* and *operando* studies with synchrotron and neutron beams.
- GSI offers correlative studies of the effects of high-energy ion beams on materials (including under extreme conditions) using various **microscopic and spectroscopic characterization methods**.
- At HZB, the complementary synchrotron-based (**BESSY II**) and laboratory-based (**HZB CoreLabs**) characterization methods are available for science and industry. The focus of the laboratory methods is on scanning electron and ion microscopy as well as X-ray diffraction and imaging.

A major challenge is the volume of data generated by increasingly powerful characterization techniques. One of the major goals of the "*Correlative Multi-method Materials Characterization*" platform will therefore be to **develop approaches to relevant data selection, data reduction, and data analysis** that are capable of addressing the data rates and data volumes of modern experimental characterization techniques. Efforts will be made to increase the use of modern artificial intelligence-based methods in this field in the future.

The platform for "*Correlative Multimethod Material Characterization*" will initially focus on material characterization using the following techniques: Electron microscopy at ER-C in FZJ and KNMF at KIT, nuclear magnetic resonance at KNMF at KIT (also with combination of X-ray analysis) and synchrotron radiation-based studies at DESY, Hereon and HZB in combination with scanning probe microscopy and focused ion beam (FIB) nanotomography, also in combination with neutrons at JCNS in FZJ / GEMS (Hereon) at MLZ, and material modification with ion beams and their correlative in situ characterization at GSI and HZDR-IBC, as well as characterization of exotic material phases under extreme conditions and ultrafast processes at GSI, FLASH and European XFEL.

The materials-related workflow will be demonstrated initially for three specific materials challenges: a) corrosion and degradation of soft, hard, and hybrid materials systems, including their interaction with the environment, and the modification of materials under extreme conditions; b) dynamics of catalysts, including correlative studies performed with synchrotron-based characterization methods; c) ultrafast switching of nanoscale magnetic textures and resistive switching elements for brain-inspired computing applications. For each material, the work program includes three-dimensional, time-resolved in situ characterization over multiple length scales. Taken together, the experiments span spatial resolutions from the meter to the sub-nanometer range. Temporal resolution spans the range of hours to femtoseconds. Machine learning methods are further the basis for a complete and fast evaluation of large data sets from high-resolution 3D/4D analysis techniques as input for performing or validating cross-scale simulations.

During the PoF IV period, the "*Correlative Multimethod Material Characterization*" platform will progressively extend its scope to other techniques, including precision manufacturing technologies such as the development of optimized microfluidic/nanofluidic systems. In addition, application fields of other Research Fields will be included.

Targeted collaborations, such as those with scientists in the Matter and Technologies program, "*Detector Systems MT-DTS*" Topic, and the Research Field Information for the development of high-speed two-dimensional pixel array detectors for recording X-ray and electron signals with sub-100 ps temporal resolution, will be used to perform unique time-resolved measurements of magnetic and electronic dynamics under GHz or optical stimuli.

LONG-TERM STRATEGIC GOALS

This cross-domain research platform for materials characterization has the following goals:

- Establish a **cross-center, cross-program, and cross-topic experimental multi-method platform** that provides access to state-of-the-art techniques for modifying, and multiscale and multidimensional characterization of materials.
- Build a **data and information platform** focused on analyzing data from combined techniques obtained at high data rates and volumes to understand the complexity of materials, their structural evolution, and their interactions in complex systems.
- Develop workflows that link correlative materials characterization and analysis, with a special focus on correlative and *in situ/operando* studies using, for example, electron microscopy, NMR and/or X-rays, neutrons, or ions. This work is performed in close collaboration with researchers working on modeling and simulation in the "*Accelerated Materials Development*" platform and in data science.
- Establish joint **activities across research areas to develop modification and characterization techniques and data analysis tools**, such as joint development of (*on line*) visualization and image processing tools, standardization of samples, sample carriers and environmental conditions, or identification and comparison of artifacts from different methods.
- Extension of the scope of the multi-method and data/information platform to other characterization techniques as well as to other research areas of the Helmholtz Association.

ESSENTIAL FUTURE ACTIVITIES

- Extend the collaboration between the Research Fields Information and Matter to other Research Fields to develop optimized approaches to challenges requiring modular solutions for high-level knowledge extraction from data generated at large-scale facilities using complementary techniques, and for access to these solutions.
- **Data analysis and modeling** will be performed in col-

laboration with the "*Accelerated Materials Development*" platform. Here, the Jülich Center for Supercomputing (JSC) will also be involved, complementing the central data platform concept at both the hardware and software levels.
- **Development of AI approaches** for real-time and automated data acquisition and analysis to optimize workflows.
- Optimize ptychographic and spectroscopic techniques for studies of weakly scattering materials and chemically sensitive signals.
- Development of new approaches for sample transfer between different measurement methods.
- Development of correlative characterization methods for the study of materials under extreme conditions of pressure, ion and laser irradiation, and temperature.
- Collaboration with the Helmholtz Imaging Platform (HIP) to develop multidimensional online visualization tools.

In line with FAIR data principles, the platform will drive data accessibility, standardization of data formats, and definition of best practices. In addition, a standard for electronic laboratory notebooks for multi-method characterization of a sample will be developed.

SELECTED INFRASTRUCTURE USE

- The multi-method platform is initially based on several infrastructures: The Ernst Ruska Center for Microscopy and Spectroscopy with Electrons **(ER-C)** at FZJ and the Karlsruhe Nano Micro Facility for Information **(KNMFi)** at KIT, **PETRA III** (DESY) with the **DESY NanoLab**, **GEMS** (Hereon), **BESSY** (HZB), **MLZ** (FZJ), **ELBE, HLB, IBC** (HZDR), experimental stations at **UNILAC, SIS-18** and **CRYRING** (GSI/FAIR), **European XFEL** and the Jülich Center for Research with Neutrons **(JCNS)** at FZJ and **MLZ**.
- In addition, developments within the planned InnoMatSy platform (*in Situ* Innovation Platform for Multifunctional Materials Systems, see Chapter VI) will be used to complement activities of the "*Correlative Multimethod Materials Characterization*" platform.

SYNERGIES

Helmholtz Association examples include collaborations with the "*Accelerated Materials Development*" platform, the Jülich Supercomputing Center, or initiatives such as **InnoMatSy** and Helmholtz Energy Materials Characterization Platform (**HEMCP**) and the Energy Materials In-Situ Laboratory Berlin (**EMIL**). For imaging methods, collaboration with the Helmholtz Imaging Platform (HIP) is planned. On the topics of data management and analysis, a large number of networks exist in the Research Field Information and beyond. The platform contributes to major national and international initiatives such as NFDI and others.

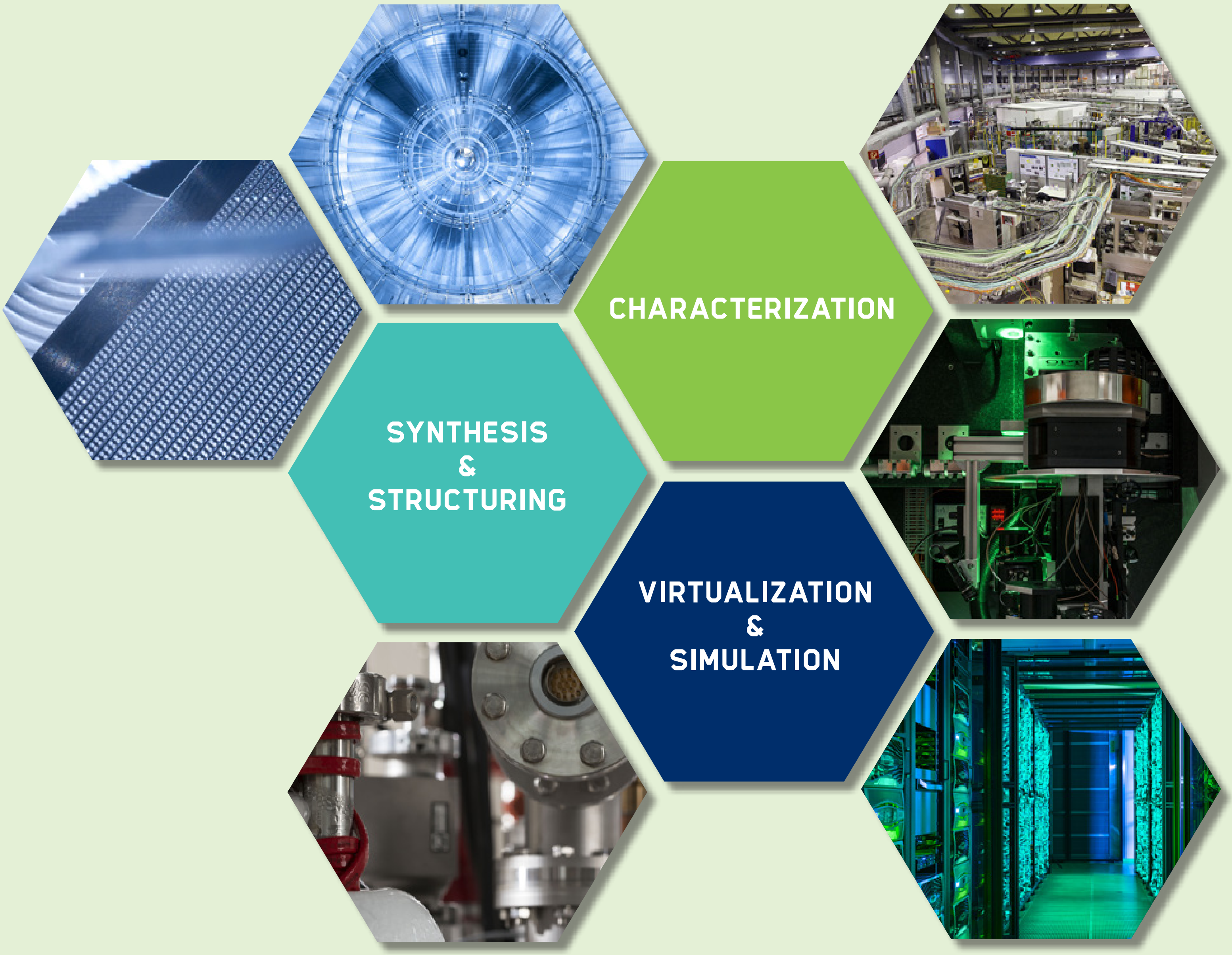
The joint position paper **ARIE** (highlights how a common, complementary approach of analytical research infrastructures in Europe will help address the societal challenges of the "*Horizon Europe Missions*" framework program. Links with European materials characterization platforms such as **NFFA** (Nano foundries for fine analysis), as well as the **ES-TEEM3** (Enabling Science and Technology through European Electron Microscopy)network will be strengthened. Within **LEAPS** (League of European Accelerator-based Photon Sources), **LENS** (League of advanced European Neutron Sources) and **RADIATE** (Research And Development with Ion Beams – Advancing Technology in Europe), methodological developments for synchrotron, neutron and ion facilities are bundled in a European context. Another synergy effect is the combination of know-how in characterization and modeling with applications and data science.

ADDED VALUE / KNOWLEDGE TRANSFER FOR THE KEY TOPICS

The platform for "*correlative multi-method material characterization*" offers methods with which questions from the focal topics of lightweight construction, hydrogen, batteries, life and health research and sustainability can be addressed, and knowledge transfer is ensured. The cross-Reseach Field experimental method platform presented here is essential to establish a powerful data and information base for the "*digital twin*". By means of a generic approach, the understanding of the structure and behavior of complex material systems and their functions will be developed and validated for the creation of cross-scale and cross-process models of material science and biological systems. Thus, "*use cases*" can be used to develop predictive material simulations together with the "*Accelerated Material Development*" platform. Systematic material screening based on the platform's multi-method approach can be used to efficiently explore the development of novel approaches and the use of new material combinations in information technology and for photovoltaic materials. Combinatorial *in situ* and *in operando* methods allow direct insights into the elementary processes occurring during the operation of battery materials. In addition, they provide important insights for the development of more efficient materials for hydrogen technology. The combination of methods allows spatially resolved investigation of the biocompatibility of materials in health research and direct assignment of failure mechanisms of lightweight materials. Correlative analysis methods are therefore essential to investigate, understand, and improve the new materials of the various focus areas.

Goal: Cross-Research Field platform for correlative multi-method material characterization and data reduction
Participating Research Fields: Information, Matter, Energy, Health
Participating Centers: HZDR, DESY, KIT, FZJ, HZB, Hereon, GSI-FAIR
Infrastructure: PETRA III, FLASH, European XFEL, ER-C, BESSY II, KNMF, JCNS, GEMS, IBC, LSDF, JARA-CSD, HPC-KIT, DiLAB, UNILAC, CRYRING, SIS-18, KARA, ELBE, HLD

VI. RESEARCH INFRASTRUCTURES AND LARGE-SCALE EQUIPMENT



Interdisciplinary materials research in the above-mentioned Research Fields is based on the large-scale infrastructures described below, many of which are also available to researchers beyond the Helmholtz Association.

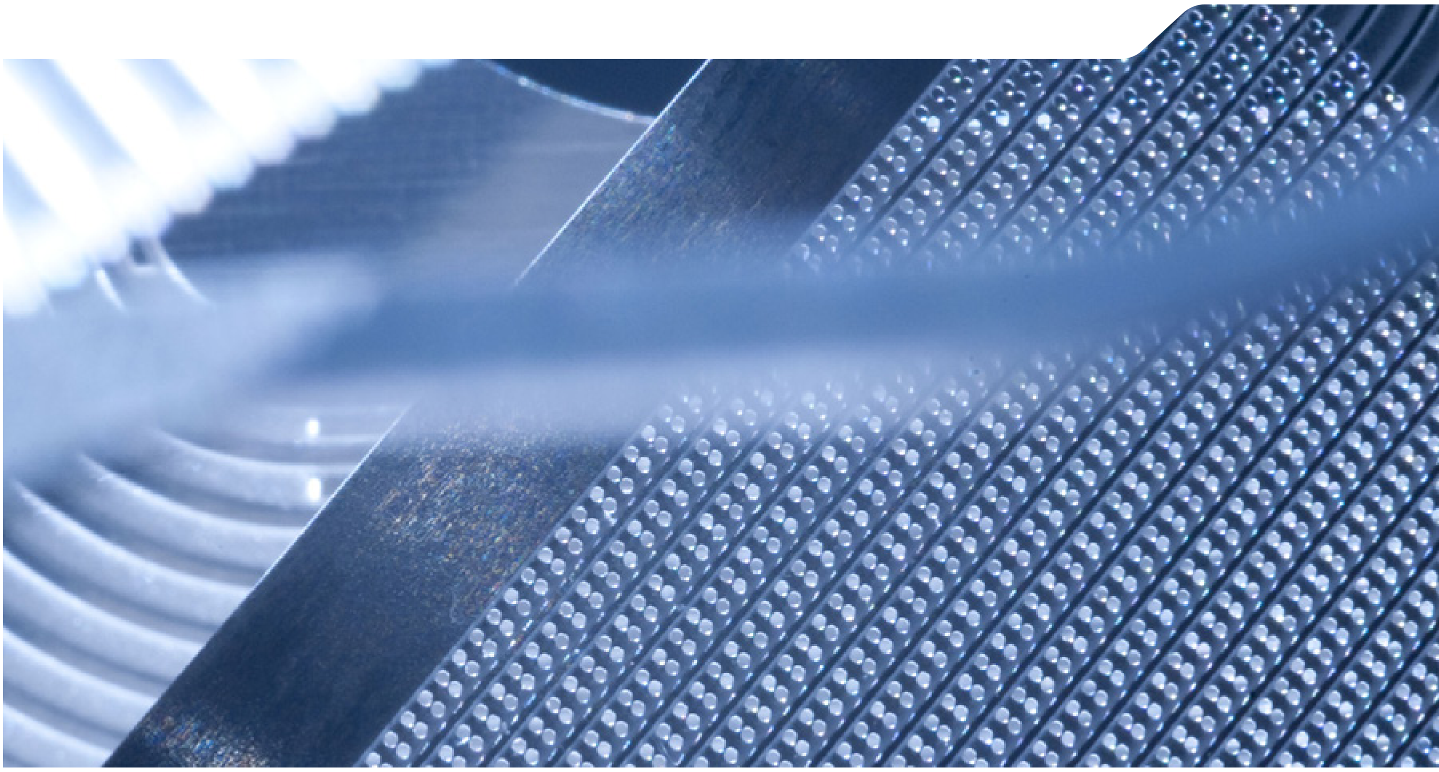
SYNTHESIS AND STRUCTURING OF MATERIALS

Helmholtz Nano Facility (HNF): The HNF at FZJ is a state-of-the-art large-scale clean room facility with a variety of processing tools for nanoscale materials structuring. With an interdisciplinary approach that combines electrical engineering and physics with chemistry and biology, it provides tools for processing a wide range of inorganic materials such as silicon, III-V semiconductors, superconductors, topological insulators, graphene, metals, and oxides. Future capacity expansion to meet the needs of the research areas of quantum and neuromorphic computing is also planned.

Helmholtz Quantum Center (HQC): With the HQC, a central technology laboratory of the Helmholtz Association is established in Jülich to meet the scientific and technological challenges of building a European quantum computer. The Helmholtz Quantum Center combines basic research, theory and development in quantum computing, from quantum materials to complete quantum computing systems. Research on materials for qubits is combined with fabrication of devices and systems for quantum computing and co-design of hardware and software. The HQC is under construction and is expected to be operational in early 2025.

Karlsruhe Center of Optics & Photonics (KCOP): The KCOP at KIT is a clean room infrastructure under construction that will enable application-relevant basic research as a multidisciplinary research platform in the field of optics and photonics. Research in the KCOP addresses major challenges in the research areas of information processing and data transmission, efficient and sustainable energy systems, life sciences and medical technology. The investment measure is currently being implemented and is expected to be operational from 2024.

Helmholtz Energy Materials Foundry (HEMF): HEMF is a large-scale collaborative R&D platform dedicated to the synthesis of new materials for energy conversion and storage applications. It is operated as an international user facility for academic and industrial partners. The scientific focus is on materials and applications in solar cells, solar fuels, fuel cells, batteries, thermoelectrics and thermochemistry. The project started on January 1, 2016, and involves HZB (lead), DLR, FZJ, HZDR, Hereon, KIT, and GSI.



Biomedical Engineering Center (BMT): Translational biomaterial research with a focus on multifunctional polymer biomaterials and soft actuators is carried out in the Hereon Biomedical Engineering Center. For this purpose, among other things, clean room laboratories have been created to enable the qualified production of biomaterials. Translational research focuses on the first application in humans, which is carried out at the Berlin-Brandenburg Center for Regenerative Therapies (BCRT), the joint clinical translational center of Hereon and Charité, and, if necessary, with the involvement of other clinical institutions, such as the Ernst-von-Bergmann-Klinikum.

Future Lab for Additive Manufacturing and Engineering (FLAME): This DLR research platform brings together the 3D printing activities at DLR. In this context, a park of modern 3D printers for printing metals, polymers and ceramics has been built up in recent years, which will be supplemented by the end of 2020 with further machines primarily for metallic 3D printing. Based on these process technologies, new powders, new 3D-specific alloys, rapidly solidified alloys, reinforced and unreinforced polymers and hybrid materials are being developed, for example.

NanoLab: The DESY NanoLab provides access to high-resolution material characterization and structuring methods that are used for sample preparation and their complementary analysis for experiments at the DESY light sources. Through the DESY NanoLab marker technology, correlative multi-method investigations can be performed on the beamlines of the synchrotron radiation and FEL sources as well as on laboratory measurement facilities on materials at the nanometer scale. In addition, DESY NanoLab operates a dedicated electrochemistry laboratory for the study of electrochemical and electro-catalytic processes in energy conversion.

Magnesium Innovation Center (MagIC): The research focus of MagIC at the Hereon is on the development of magnesium-based materials for diverse applications (for example, in the transport and medical sectors). The center concentrates primarily on the areas of new alloy development with a focus on wrought magnesium alloys, their processing, and corrosion and surface protection.

Polymer and Hydrogen Technology Center (PHTC): The center at the Hereon was established to further develop photoelectrochemical hydrogen production and hydrogen storage, as well as to promote upscaled polymer synthesis and the transfer of membrane-based separation technologies to industrial applications.

CHARACTERIZATION OF MATERIALS

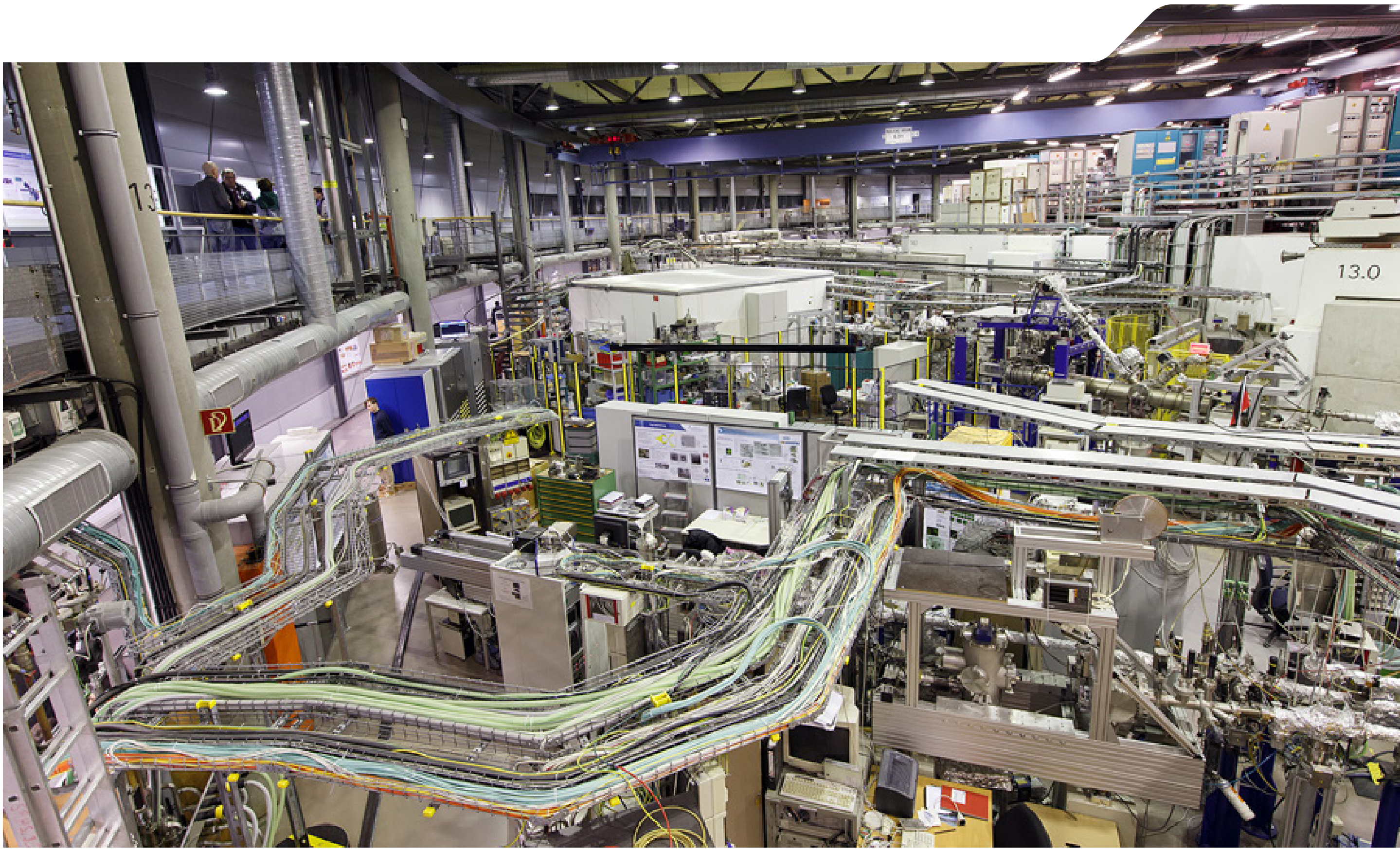
BESSY II: The synchrotron radiation source BESSY II, operated by HZB, is a highly recognized source of extremely brilliant soft and medium X-rays worldwide. The user community has at its disposal at BESSY II unique instruments for high-resolution spectroscopy, microscopy and time-resolved experiments as well as innovative sample environments for in situ and operando measurements. The main focus of the use of BESSY II is materials research, from fundamentals to applications, major societal challenges such as sustainable energy supply, quantum technology, energy-efficient information technology and health. With its 37 experimental stations, BESSY II has an outstanding productivity in international comparison.

PETRA III: The high-energy synchrotron radiation source PETRA III operated by DESY is one of the most brilliant storage ring X-ray radiation sources in the world. As one of the most powerful light sources of its kind, it offers scientists excellent experimental opportunities with X-rays of particularly high brilliance over a wide photon energy range. Its main applications lie within the medium to hard X-ray range with the possibility to reach a photon energy of over 200 keV. This is of particular benefit to researchers who want to study very small samples or require highly focused, very short-wavelength X-ray light for their analyses. This makes it possible to characterize materials with subμm spatial resolution in a spatially resolved manner using a variety of different techniques. The high-energy radiation also makes it possible to use complex sample environments for *in situ* or *operando* studies under relevant process or operating conditions, or to analyze the interior of samples or complete workpieces. In the final stage, 27 beamlines with more than 60 experimental stations will be realized at PETRA III.

Karlsruhe Research Accelerator (KARA): The electron storage ring KARA at KIT serves for the development of new accelerator technologies and as a synchrotron radiation source. Various beamlines and laboratories are operated at KARA, which are used for *in situ, in vivo* and *in operando* characterization of materials, nanostructures, and biological processes, among others.

Free-electron laser (FLASH): Since 2005, FLASH, the world's first free-electron laser in the soft X-ray range, has been generating extremely intense, ultra-short pulsed X-ray laser flashes at DESY in Hamburg. The extremely short pulses in the 10 fs range make it possible to study ultrafast processes or non-equilibrium states in matter. This makes it possible, for example, to break down reaction paths in atomic resolution. Due to the energy range of FLASH, mainly spectroscopic measurement methods are used here. Due to the high pulse repetition rate, which is unique worldwide in this photon energy range, even highly diluted sample systems or those with an extremely small but highly precise useful signal can be investigated. The knowledge gained from such experiments extends our fundamental understanding of the structure and dynamics of matter on the atomic scale and can be used to develop new materials, for example, for catalytic processes, and drugs.

European XFEL: The European XFEL generates ultrashort laser light flashes in the X-ray range. XFEL enables investigations in a unique and broad range of applications. As with FLASH, the extremely short pulses enable investigations of dynamic processes on time scales down to below 10 fs. Thus, the main application of the European XFEL is the investigation of ultrafast processes that cannot be studied with traditional synchrotron radiation sources. Due to the higher photon energies at the European XFEL compared to FLASH, diffractive experiments are able to advance simultaneously in time and space into atomic dimensions. In this way, detailed images of cell components, individual protein molecules and viruses and their dynamic behavior help in the fight against disease and the targeted design of drugs. The access to the exact structure of nanomaterials and their atomic dynamics made possible by the XFEL will enable the development of novel, functional materials for the future, for example, for more effective solar modules and fuel cells as well as for future data storage devices.



Materials research with neutrons: Research on matter with neutrons at world-leading sources, including ESS (commissioning 2023), ILL, SNS and FRM II, is organized via the user platforms "*Jülich Centre for Neutron Science*" (JCNS, at FZJ) and "*German Engineering Materials Science Centre*" (GEMS, at Hereon). The JCNS uses neutrons as microscopic probes to study condensed and biological matter, builds and operates neutron scattering instruments for this purpose, and makes them available to a large user community at leading neutron sources. A key role is played by the Heinz Maier-Leibnitz Center (MLZ) as the national user facility.

German Engineering Materials Science Centre (GEMS): With GEMS, the Hereon operates instrumentation for the investigation of materials with synchrotron radiation (at PETRA III, DESY) and neutrons (at MLZ). The instruments are also explicitly made available to external users from universities, other research institutions and industry for their work with a focus on *in situ* experiments.

Ion Beam Center (IBC): The IBC of the HZDR is concerned with the modification and analysis of materials, in particular thin films and surfaces, using ions in a wide energy range (eV to MeV). The focus includes novel 2D materials, doping and defects in semiconductors, magnetic films, synthesis of new phases, and analytics using a variety of ion techniques. A nanofabrication clean room facility is also part of the IBC.

GSI/FAIR Facilities: At the GSI accelerator facilities, high-energy ion beams (MeV-TeV) are used to study microscopic and macroscopic interaction processes with matter, to fabricate nanostructures, and to test the radiation hardness of materials and components at beam branches specifically designed for materials research. Experiments in atomic, bio- and plasma physics as well as in materials research are performed at GSI's current accelerator and storage ring facilities (UNILAC, SIS18, ESR with CRYRING and HITRAP). In the coming years, experimental stations will also be available at the FAIR accelerator facilities, which will offer, among other things, the possibility to investigate the behavior of materials under multiple extreme conditions (particle and laser radiation, high pressure and temperature).

High-field magnetic laboratory Dresden (HLD): The HLD at the HZDR conducts modern materials research in high magnetic fields. Experiments in high fields offer researchers unique opportunities to gain fundamental knowledge about the matter surrounding us, because they allow material properties to be influenced in a targeted and, above all, controlled manner in a unique way. Primarily, electronic properties of metallic, semiconducting, superconducting and magnetic materials are investigated. Special attention is given to exotic superconductors, strongly correlated electron systems, low-dimensional and frustrated spin systems, and nanostructured materials.

Electron Linear Accelerator for Beams of High Brilliance and Low Emittance (ELBE): Different types of secondary beams, both electromagnetic radiation and particles, are produced with the ELBE radiation source at HZDR. High-intensity coherent infrared and THz radiation is used for nonlinear and time-resolved spectroscopy as well as microscopy of materials. Positrons enable the analysis of defects, especially vacancies and small voids in a wide variety of materials.

Highest field NMR spectroscopy: By means of solution and solid state NMR spectroscopy at HMGU, FZJ and KIT, biological material structures, such as amyloid fibrils, the self-assembly of macroscopic structures by liquid/liquid phase separation (LLPS), as well as nanocarriers and carrier systems are studied *in vitro* with near atomic resolution. Biological structures can be studied in particular also the interfaces between inorganic and biological materials in native state (without chemical modification). In the solid state, enormous increases in sensitivity can be achieved by transferring the magnetization of electrons to nuclear spins using DNP (dynamic nuclear polarization).

Ernst Ruska Center for Microscopy and Spectroscopy with Electrons (ER-C): For the characterization of novel materials and devices, the ER-C of FZJ offers the (inter)national scientific community several transmission electron microscopes of the highest performance class. For the ER-C 2.0, five novel instruments of the next generation and highest performance class will be acquired in the next years, covering in a coordinated way user operations from classical solids to nanomaterials and soft matter to biomolecules and cell structures.

Karlsruhe Nano Micro Facility (KNMF): The KNMF at KIT is a research infrastructure for the characterization of functional materials, components, and systems on the micro- and nanoscale. Since 2008, this facility has provided users from academia and industry with access to sophisticated and unique technology and equipment as well as process chains necessary for materials engineering and in the development of information systems. The expertise of researchers at KNMF helps users solve their application-oriented problems. This makes the KNMF a platform for collaboration between users and KIT scientists, who can thus address the major challenges in the field of information. For PoF IV, this will be restructured to KNMF for information (KNMFi) and supplemented by the focus on digital materials analysis.

Energy Materials In-situ Laboratory (EMIL@BESSY II): EMIL is a worldwide unique laboratory infrastructure at the synchrotron light source BESSY II, dedicated to X-ray analysis of the growth and properties of energy materials in real time (*in situ*) and in full functionality (*in operando*), laying the foundation for detailed optimization of materials and structures for energy conversion. EMIL includes analytical and industrially relevant deposition facilities in an integrated ultra-high vacuum system that enables rapid layer-by-layer deposition and characterization. HZB and the Max Planck Institutes Fritz Haber Institute (FHI) and Chemical Energy Conversion (CEC) are involved.

Center for X-ray and Nanoscience (CXNS): The CXNS is an interdisciplinary center for research with X-ray light to solve problems in materials and nanoscience. Research topics such as the investigation of optimized materials for energy conversion processes and transport, sensor technology, imaging X-ray methods or scanning probe microscopy and nanostructuring are bundled under the CXNS umbrella. The CXNS is a cooperative project of DESY, jointly operated with the Hereon, the Christian-Albrechts-Universität zu Kiel (CAU), the Leibniz Institute of Crystal Growth (IKZ) and the Hamburg University of Technology (TUHH).

Helmholtz Energy Materials Characterization Platform (HEMCP): The central access research platform provides analytical methods for the characterization of energy materials in 4D as well as *in situ* information on structural, electrical and chemical properties. HEMCP brings together a unique collection of instruments and analytical methods from seven research institutions (FZJ, DESY, DLR, HZB, HZDR, Hereon, KIT) under one virtual roof, offering a wide range of possibilities for research questions on materials for energy technologies.

VIRTUALIZATION AND SIMULATION OF MATERIALS

A major goal is the development of strategies for the virtualization of materials and material development on the basis of model- and data-based material design. Generic issues arise here, particularly with regard to the *digitalization* of materials science, which can only be addressed across programs. Two essential aspects of *digitalization* are the virtualization of material development, i.e., the provision of methods and tools for the computer-aided design of materials, and the comprehensive acquisition and use of material data with regard to composition and microstructure, properties and manufacture, and changes due to use. Among other things, the activities of the cross-sectional activity of the Research Field Information "*Virtual Materials Design*" contribute to this by developing and validating new methods for computer-aided material and process development. This establishes the anchor point in the Helmholtz Association for the development of new materials, in which the concept of the "*digital twin*" is further developed and broad use is made possible. This contributes to technology-oriented material developments in the Helmholtz Association.

The complementary expertise from all Research Fields and the research results obtained through a common approach to material design are used for a wide variety of application areas. To this end, we are developing a cross-scale modeling platform incorporating high-performance, user-friendly simulation methods and data-driven approaches. Important goals here are the development of a virtual research environment for the implementation of cross-scale simulation methods and for the exchange of data, methods and software for virtual material design. This also includes the development of improved and hardware-near algorithms and the use of the Helmholtz Association infrastructures:

Supercomputing Facility (JSC): FZJ has strengthened its position as a leading European center of excellence for Tier 0/1 supercomputing. It drives technology development in exascale computing, collaborates with scientists from a wide range of scientific and technical disciplines to open up new possibilities for gaining knowledge through co-design of computing technology and application, and manages various e-infrastructures for the international community. It operates a modular supercomputer of the highest performance class. It will take this concept to the exascale performance level and also combine it with advanced modular (post-von Neumann) architectures integrating different technologies (in particular components that exploit neuromorphic and quantum effects). In this context, the development of an open Innovation Hub for research in quantum annealing and quantum computing is currently envisaged.

Helmholtz Data Federation (HDF): With the HDF, a nationwide federated research data infrastructure is being developed in Germany that is open to the entire national science system. An initial set of scientific use cases covers most of the research disciplines in the Helmholtz Association Research Fields. The HDF represents a national building block for the realization of a European Open Science Cloud (EOSC). Launched in 2017, the HDF comprises three elements: Innovative software technologies for research data management, excellent support and collaborative research with users, state-of-the-art storage, and analysis hardware. Partners are KIT (coordinator), AWI, DESY, DKFZ, FZJ and GSI.

Large Scale Data Facility (LSDF): Since 2010, KIT has been operating the LSDF; an infrastructure that provides data storage, archiving, and analysis capacities for a wide range of scientific research conducted at KIT and in Baden-Württemberg (for example, hydromechanics, structural biology, astrophysics). The LSDF is connected to the Tier-2 supercomputer ForHLR at KIT to efficiently enable data-intensive computing. A total of about 10 PB capacity is available for storing and archiving research data.

High-Performance-Computing-Systeme (HPC): KIT operates innovative HPC systems for so-called capability and capacity computing. For efficient data-intensive computing and smart data analyses, these are closely linked to the LSDF. The supercomputer ForHLR is a Tier-2 supercomputer with 1.4 PetaFlop/s performance; it uses an innovative, energy-efficient water cooling concept that was recently awarded the German Data Center Prize 2017. It will be complemented by the HoreKa supercomputer starting in fall 2020.

Interdisciplinary Data and Analysis Facility (IDAF): DESY operates a very large system for simulation, as well as analysis, storage and archiving of large amounts of data. This system, with more than 60,000 cores of the latest technology and supported by GPGPU special processors, is connected to an extensive multi-level storage structure that allows high-performance analysis of experimental data at PETRA III and FLASH. DESY is a partner of HDF and actively participates in the development of modern cloud concepts for the communities through a variety of projects. In the future, artificial intelligence methods will be increasingly used to analyze correlative data in particular.

FUTURE RESEARCH INFRASTRUCTURES

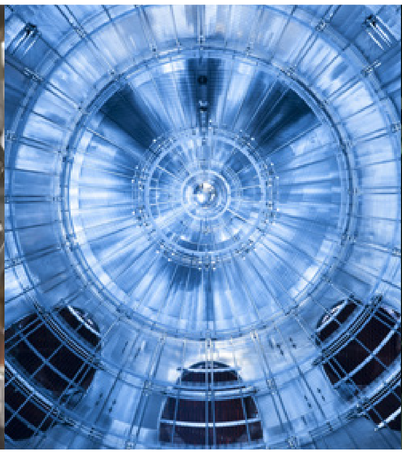
In addressing global societal challenges, large-scale research infrastructures such as accelerator and experiment facilities, as well as supercomputers, play an important role in scientific progress. Their development, construction and operation are one of the important core elements in the mission of the Helmholtz Association and thus offer a unique advantage to Germany as a center of science. International visibility is further enhanced by appropriate user operation for national and international researchers.

The Helmholtz Association is currently developing the Helmholtz Roadmap for expansion investments in large research infrastructures for the next ten years. The large-scale research infrastructures that are in the planning phase and relevant for materials research are listed here. These include photon and electron accelerators for the generation of neutrons, data infrastructures, characterization methods such as electron microscopy, NMR technology as a new focus, as well as dedicated application laboratories.

The list of planned large-scale research infrastructures below, but also the plans in the participating Helmholtz Centers for research infrastructure in general, show that the challenges of modern materials science require a continuous development of research facilities and large-scale equipment. On the one hand, the resolution limits are being pushed to ever smaller dimensions and time increments while, on the other hand, ever larger material systems can be characterized under real conditions. At the same time, these trends are associated with ever-increasing amounts of data, which must be analyzed and stored efficiently. The planned research infrastructures create the corresponding conditions and thus maintain the efficiency and top position of materials research in the Helmholtz Association. An essential building block here is also the comprehensive user operation that the Helmholtz Centers make possible for the national and international materials research community.

PETRA IV: The PETRA IV project at DESY comprises the expansion of the synchrotron radiation source PETRA III into a source with ultra-small emittance, which is to reach the physical limits of the focusability of synchrotron radiation in the photon energy range up to 10 keV. (diffraction-limited radiation). As with PETRA III, the main application range of PETRA IV will be in the hard X-ray energy range. With the targeted beam properties, PETRA IV will become the ultimate X-ray microscope for biological, chemical and physical processes under realistic *in situ/ in operando* conditions, enabling their investigation on length scales from atomic dimensions to millimeters and process-relevant time scales. This will enable new breakthrough investigations in many areas of science and industry, from basic research to industrial applications. Important contributions to the major societal challenges are made in areas of health, energy, earth and environment, transport and information technology. The analytical capabilities of PETRA IV are essential for the development of novel materials structured on the nanoscale or atomic scale with tailored functions.

BESSY III: With its focus on spectroscopic methods, the synchrotron radiation source BESSY III enables the realization and optimization of highly efficient materials and systems for the conversion, storage and utilization of energy as well as for energy-efficient information technologies. As a next-generation source, BESSY III allows unique insights into the interaction of light with matter, the transport of electrons and ions through interfaces, and catalytically as-



sisted chemical reactions. In combination with dedicated sample environments, BESSY III allows *in situ/in operando* investigations from the nano to the macro dimension and from extremely short time scales to steady states. As the leading facility for soft X-ray radiation in Europe, BESSY III at the Adlershof Technology Campus will create unique opportunities for research and industry in Germany as a science and high-tech location.

FLASH2020+: The FLASH2020+ project is a modernization of the existing FLASH FELs in the soft X-ray range with respect to a better and faster tunability of photon energy and better defined spectral properties of photon pulses. As FELs in the soft X-ray range, the two FLASH FELs are predestined for the investigation of electronic as well as magnetic properties on ultrashort time scales ranging to below 10 fs. Examples include fast chemical reactions or non-equilibrium states. The high pulse repetition rate made possible by the use of a superconducting linear accelerator also allows the analysis of highly dilute systems or those with an extremely small useful signal.

Dresden Advanced Light Infrastructure (DALI): The DALI radiation source based on superconducting electron accelerators comprises the worldwide unique combination of a high-field radiation source for the terahertz (THz) spectral range and the mid-infrared as well as a free-electron laser for wavelengths in the vacuum ultraviolet (VUV). As successors to the ELBE radiation source, these sources allow the experimental investigation of dynamic processes with femtosecond time resolution at extremely high pulse energies and repetition rates. In combination with positron secondary radiation, a system for ultrafast electron diffraction, and dedicated user laboratories for physics, materials science, chemistry, biology, and medicine, DALI creates the conditions for excellent cutting-edge research by national and international user groups from different scientific disciplines.

High Brilliance Neutron Source (HBS): The development of the high brilliance accelerator-driven neutron source HBS) serves to realize the next generation of neutron sources in Germany and worldwide. The project is being advanced at Jülich Research Center with the goal of providing a prototype facility by 2028. With its intense focused neutron beams, the HBS will contribute to neutron analytics to unlock the spatial structure and its dynamics on nanostructured or biological materials to develop new materials and functionalities in areas ranging from quantum materials to energy storage. Through dedicated target stations and instruments, HBS will complement large international facilities such as the European Spallation Source ESS in the future and provide users with sustainable access to neutrons as a national neutron source.

ACcelerator-Driven multipurpose ion beam Complex (ACDC): The ACDC will expand the ion energies available in Germany and thus close the currently existing gap between HZDR (low energies) and GSI (highest energies). The expansion of the available ion energies and the provision of neutrons with ACDC strengthens the focus on important questions of society: With the establishment of unique high-energy accelerator mass spectrometry, current questions of climate change and environmental protection are addressed. In addition, the research portfolio will be expanded to include the field of radiation biology and, with the use of ion post-acceleration, extended to radiation medicine. In the field of materials research, new processes for low-loss high-performance components for electromobility and smart grids will thus be further developed.

The **Karlsruhe Nuclear Magnetic Resonance Facility (KNMR)** will be an incubator for novel and outstanding materials research to enable imaging and processing along the entire NMR value chain. Here, the focus will be on advancing instrument technology and methodology as well as correlative characterization methodology with evaluation algorithms and in situ/operando techniques for the life sciences. The KNMR serves as a collaboration platform and user facility for industry and academia alike. For the digitalization of materials science, the KNMR will be able to make an important contribution to the national and international research landscape and shape it in the long term.

With **ER-C 2.0**, a national research infrastructure for high-resolution electron microscopy is being established at the Ernst Ruska-Centrum (ER-C) at the Jülich Research Center. With novel, internationally pioneering next-generation instruments covering user applications from classical solids to nanomaterials and soft matter to biomolecules and cell structures, the ER-C will be further developed into a unique infrastructure for high-resolution characterization of atomic and molecular structures. The establishment of a modern data management system is an integral part of the concept and will include aspects of data security, the safeguarding of the rules of good scientific practice and the generation of transferable metadata as well as the possibility for subsequent evaluation of the measurement results by independent expert groups.

The **International Fusion Materials Irradiation Facility - Demo Oriented NEutron Source (IFMIF-DONES)** is a research infrastructure based on an accelerator-driven neutron source to simulate the neutron spectrum in a fusion reactor and its effects on the materials used. It will be used to characterize, validate, and qualify these materials for the first fusion demonstration reactor, DEMO. IFMIF-DONES was included in the European ESFRI roadmap in 2018; preparatory work is already underway in Granada, Spain. Synergies are possible, for example, with medical accelerator applications, as well as with respect to hydrogen diffusion through damaged materials. The realization of the facility will bring valuable data on liquid metal corrosion and erosion of structural materials relevant for high temperature storage processes. Among other things, KIT will contribute its fusion materials laboratory for the necessary follow-up investigations with cross-scale characterization and modeling methods and thus secure its leading position in the development & qualification of energy materials internationally in the long term (construction approx. 10 years with approx. 30 years of operation). This results in direct synergies to the MTET program, Topic 4 (HT3: Gas Turbine, Concentrating Solar Thermal, Thermal Storage) and Topic 3 (Chem. Energy Carriers). Furthermore, this engagement strengthens the cooperation with German industry.

In-Situ Innovation Platform for Multifunctional Materials Systems (InnoMatSy): The Hereon is planning an *in-situ* innovation platform for multifunctional materials systems. Together with other centers, InnoMatSy will form a cross-material, cross-functional and cross-application characterization infrastructure combined with data storage, Big Data strategies and software tools. In terms of a feasibility study, InnoMatSy will be used to elucidate changes in metabolic functions in the environment of degradable metallic implants in living organisms. In the long term and with the involvement of other centers, this will be used to improve the combination of *in situ / operando* process sample environments in laboratories with synchrotron radiation, neutrons, electron microscopy and nuclear magnetic resonance spectroscopy with computer simulations. This innovative platform for systematically integrated and multifunctional material systems will significantly accelerate model- and simulation-based development of material systems and, most importantly, allow validation of "*Dynamic Digital Twins*" describing the ongoing process during materials processing and application.

4D-CAT – Bridging the innovation gap in catalyst research for electro-, photo- and thermocatalysis: Electro-, photo- and thermo-catalytically effective functional materials are essential elements of efficient process chains of the energy transition for the production of chemical intermediates and high-value energy carriers. Power-to-X process technologies in which CO_2 is used catalytically as a C source for the production of basic chemicals and synthetic fuels, the electrification of chemical syntheses and the development of photocatalytic syntheses are the central drivers of new technologies for closing material cycles. For catalysis, this results in the need to accelerate innovation cycles from material design to industrial application. This need is addressed by the planned infrastructure 4D-CAT via the 4 dimensions "*Design from Nano to Macro*", "*Operando*", "*Theory*" and "*Lab to Fab*".

CeRI^2: The resource-efficient circular economy plays a prominent role in the German government's high-tech strategy and the EU's raw materials initiative. Energy-efficient resource technologies are a key element in this. These technologies often use turbulent multiphase flows for resource recovery. Key processes in such multiphase flows, such as the adhesion of recyclable particles to bubbles, remain largely misunderstood. The optical lack of transparency of such multiphase flows with high solid and gas content hardly allows measurements with classical techniques. CeRI2 addresses both of these problems. It investigates the micro- and mesoscopic length scales of multiphase flows relevant for the recovery of valuable materials. It develops measurement techniques for these flows and tools for process intensification. Process optimization relies heavily on the incorporation of artificial intelligence methods.

FlexiPlant: Building a sustainable circular economy requires a completely new approach to processing raw materials. Technologies must be able to process complex raw materials with maximum efficiency. This can only be achieved through consistent *digitalization* and networking of adaptive and flexible resource technologies. Research on such technologies in Europe has so far been conducted on a laboratory and small-scale technical scale. There is no research infrastructure that makes it possible to test the technologies on a pilot scale, and to test their networking at the same time. FlexiPlant will uniquely enable the development and networking of adaptive and flexible resource technologies, as well as their transfer to industrial use.

ACDC: ACcelerator-Driven multipurpose ion beam Complex (HZDR)
AFM: atomic force microscope (HZDR)
AMANDA: Autonomous Materials and Device Application (FZJ)
AWI:Alfred Wegener Institute
BCRT: Berlin-Brandenburg Center for Regenerative Therapies
BESSY II: Berlin Electron Storage Ring
BMBF: Federal Ministry of Education and Research
BMT: Biomedical Technology Center (Hereon Teltow)
CCA: Cross-cutting Activity
CSD: Center for Simulation and Data Sciences (FZJ)
CRYRING@ESR: first large-scale facility of the FAIR accelerator facility (GSI, Helmholtz Institute Jena)
CT: Computed Tomography
CXNS: Center for X-ray and Nano Science (DESY)
DALI: Dresden Advanced Light Infrastructure (HZDR)
DESY: German Electron Synchrotron
DiLAB: Digital Design and Fabrication Lab (Hereon)
DLR: German Aerospace Center
ELBE: Electron Linear Accelerator for Beams of High Brilliance and Low Emittance (HZDR)
ELISE: Evolutionary Light Structure Engineering (AWI)
EM: Electron Microscopy
EMIL: Energy Materials in-situ Laboratory Berlin
ER-C: Ernst Ruska Center (FZJ)
European XFEL: European X-ray laser in Schneefeld near Hamburg
EuU: Earth and Environment
FLAME: Future Lab for Additive Manufacturing and Engineering (DLR)
FLASH: Free Electron Laser in Hamburg (DESY)
FZJ: Research Center Jülich
GEMS: German Engineering Materials Science Centre
GSI/FAIR: GSI Helmholtz Centre for Heavy Ion Research/Facility for Antiproton and Ion Research
HDF: Helmholtz Data Federation
HGF: Helmholtz Association
HEMF: Helmholtz Energy Materials Foundry
HEMCP: Helmholtz Energy Materials Characterization Platform
Hereon: Helmholtz Centre Hereon (formerly Helmholtz Center Geesthacht, HZG)
HLD: High Field Magnetic Laboratory Dresden
HIPS: High Impact Polystyrene
HMGU: Helmholtz Center Munich
HNF: Helmholtz Nano Facility
HPC: High Performance Computing (KIT)
HQC: Helmholtz Quantum Center (FZJ)
HTC/PTC: Hydrogen Technology Centre and Polymer Technology Centre (Hereon)
HZB: Helmholtz Center Berlin
IBC: Ion Beam Center (HZDR)

ICT: Information and Communication Technologies
IDAF: Interdisciplinary Data and Analysis Facility (DESY)
IFMIF-DONES: International Fusion Materials Irradiation Facility - Demo Oriented NEutron Source (KIT)
IMI: Innovative Medicines Initiative
InnoMatSy: In-Situ Innovation Platform for Multifunctional Materials Systems (Hereon)
ITN: Innovative Training Networks
IVF: Initiative and Networking Fund of the Helmholtz Association
JARA-CSD: Jülich Aachen Research Alliance-Center for Simulation and Data Science (RWTH Aachen, FZJ)
JCNS: Jülich Centre for Neutron Science (FZJ)
JL: Joint Lab (cross-sectional activity of the Research Field Information)
JSC: Jülich Supercomputing Centre (FZJ)
KARA: Karlsruhe Research Accelerator (KIT)
KCOP: Karlsruhe Center of Optics and Photonics (KIT)
AI: Artificial Intelligence
KIT: Karlsruhe Institute of Technology
KIT-BaTec: Battery Technology Center Karlsruhe
KNMFi: Karlsruhe Nano Micro Facility for information
LSDF: Large Scale Data Facility (KIT)
LRV: Aeronautics, Space and Transport
MagIC: Magnesium Innovation Center (Hereon)
MAP: Materials Acceleration Platform
MBC: Magnesium Biomaterials Centre (Hereon)
MDC: Max Delbrück Center for Molecular Medicine
MDMC: Integrated Model- and Data-driven Material Characterization (Joint Lab of Research Field Information)
MLZ-FRM II: Research Neutron Source Heinz Maier-Leibnitz
MOF: Metallic Organic Framework
MRI: Magnetic Resonance Imaging
MTC: mechanical-chemical-thermal test facilities (DLR)
NanoLab: nano laboratory (DESY)
NextGenBat: Next Generation Batteries (RWTH Aachen)
NFDI: National Research Data Infrastructure
NMR: nuclear magnetic resonance
PEM electrolysis: proton exchange membrane electrolysis
PET: positron emission tomography
PETRA III / IV: German Electron Synchrotron (DESY)
PHTC: Polymer and Hydrogen Technology Centre (Hereon)
PoF: Program-oriented Funding
PVcomB: Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin
QC/QT: Quantum Computing / Quantum Technology
RF: Research Field
SIS-18: Heavy Ion Synchrotron (GSI)
UNILAC: Universal Linear Accelerator (GSI)
VMD: Virtual Materials Design (cross-sectional activity of the Research Field Information)

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