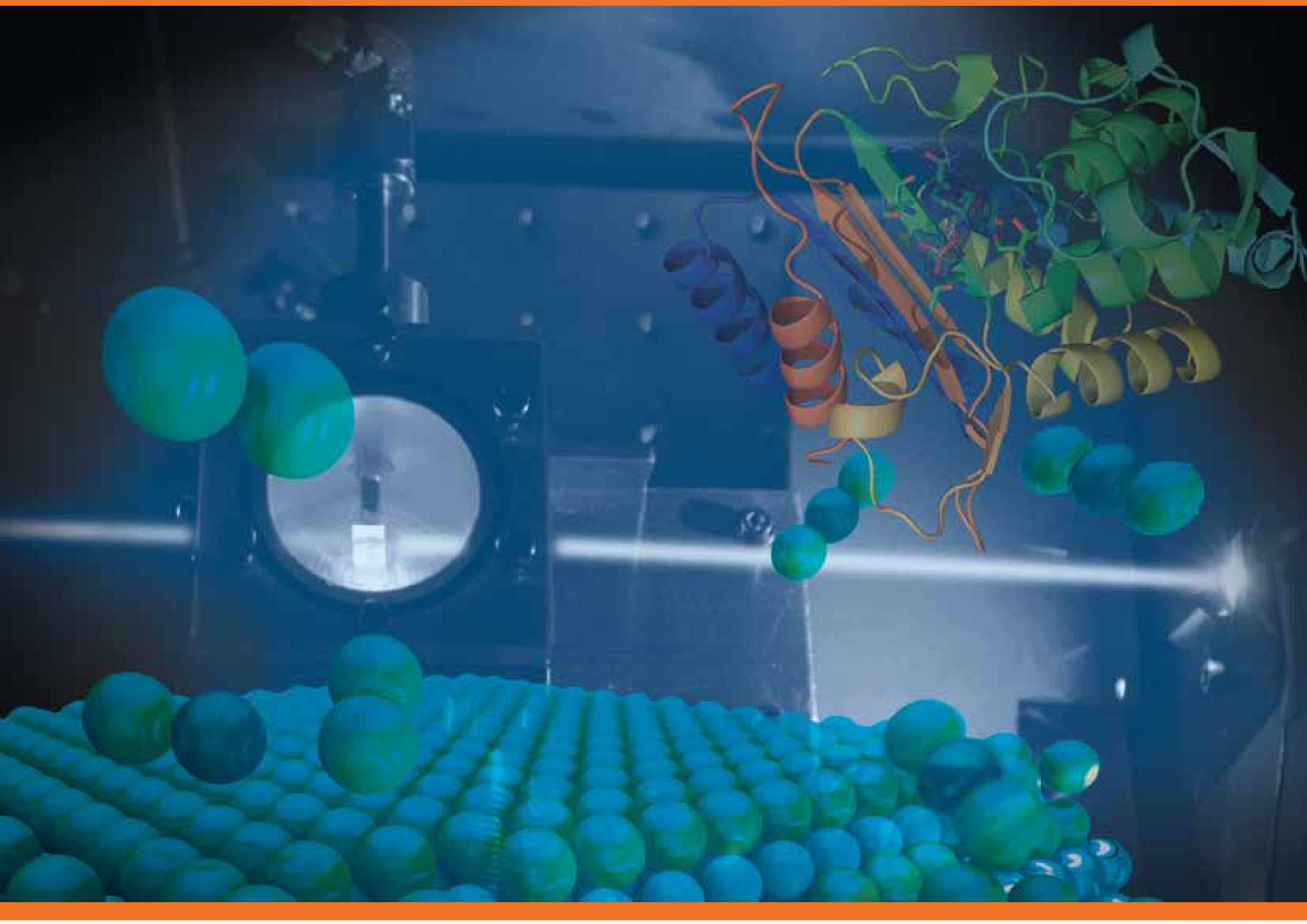
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Proposal for the Helmholtz Research Program

FROM MATTER TO MATERIALS AND LIFE

Research Field MATTER

Strategic Evaluation for the Fourth Period
of Program-oriented Funding, 2021 – 2027



C. PROGRAM *FROM MATTER TO MATERIALS AND LIFE*

Spokespersons

Prof. Dr. Thomas Stöhlker, GSI and HI Jena

Prof. Dr. Andreas Stierle, DESY

Participating Helmholtz Centers

DESY Deutsches Elektronen-Synchrotron

FZJ Forschungszentrum Jülich GmbH

GSI Helmholtzzentrum für Schwerionenforschung GmbH

HI Jena Helmholtz-Institut Jena

HZB Helmholtz-Zentrum Berlin für Materialien und Energie

HZDR Helmholtz-Zentrum Dresden-Rossendorf

HZG Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research

KIT Karlsruhe Institute of Technology

CONTENTS

1. OVERVIEW

The central mission of the Program *From Matter to Materials and Life* (MML) is to obtain unique insight into the properties of matter and materials over a wide range of length, time, and energy regimes for parameter spaces that are inaccessible on the laboratory scale, and thereby to contribute significantly to solving present and future grand challenges of society. For this purpose, the Program develops, constructs, and operates large-scale infrastructures for research with photons, neutrons, ions, and highest electromagnetic fields and carries out internationally unique, facility-oriented research, which opens up new fields of application and yields novel experimental opportunities for current and future user applications. A prominent example is our involvement in the recently commissioned European XFEL X-ray laser, which provides revolutionary novel research opportunities. The Program MML offers access to these facilities for a wide interdisciplinary national and international user community predominantly from the natural sciences, the life sciences, and engineering.

MML research deals with the structure, dynamics, and function of matter and materials, extending from fundamental research to applications. It is structured into the three central Research Topics *Matter – Dynamics, Mechanisms and Control* (MML-Matter), *Materials – Quantum, Complex and Functional Materials* (MML-Materials), and *Life Sciences – Building Blocks of Life: Structure and Function* (MML-Life). These Topics are closely linked to the four Facility Topics *Photon Facilities*, *Neutron Facilities*, *Ion Facilities*, and *Highest-Field Facilities*. Central research areas to be studied are related to matter under extreme and non-equilibrium conditions, the mapping of dynamical processes on atomic time and length scales, quantum, complex, and functional materials for new applications, and the decoding of complex biological structures and processes. This research is an integral part of the collaboration of MML with universities and other research institutions on the national and international level. For this purpose, science-driven development of methods, technology, and instrumentation (“enabling technologies”) within the Program is a *sine qua non* for internationally outstanding science. In particular with regard to accelerator and detector development as well as data management and analysis, our Program profits considerably from the synergies created by our close collaboration with the Programs *Matter and Technologies* (MT) and *Matter and the Universe* (MU) within the Research Field *Matter*.

Due to the profile of our facility-oriented research, our Program acts as a bridge between the large-scale facilities of the Research Field *Matter* and other Research Fields within the Helmholtz Association. The Program is engaged in all five Cross-Cutting Activities, organized across Research Fields, which embrace the areas of *Information and Data Management*, *Materials Research*, *Quantum Technologies*, *Structural Biology and Biological Processes*, and *Radiation Research* (see Volume I).

For the PoF IV period, the further development of coherent strategies for research with photons, neutrons, ions, and highest electromagnetic fields is of utmost importance. Correspondingly, upgrade plans to enhance our large-scale facilities for keeping them competitive on an international level and enabling forefront science play an important role. This requires long-term strategic planning. For this purpose, all current upgrade activities will go along with a national roadmap BMBF process and are linked to European roadmap developments.

1.1. Planned Resources

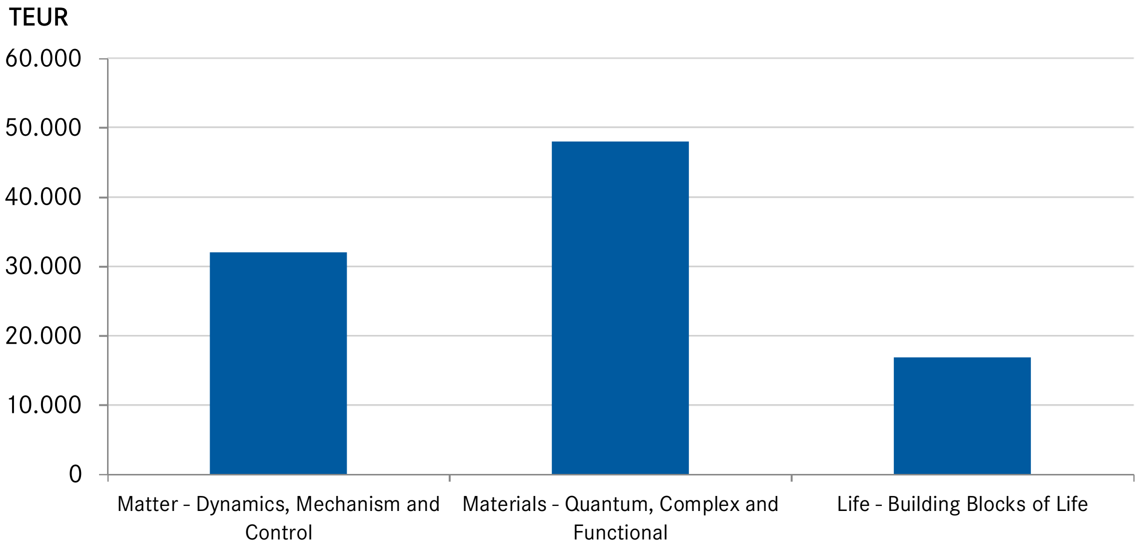


Figure 1: Program costs in 2021 by Topics. For details see Table 10.

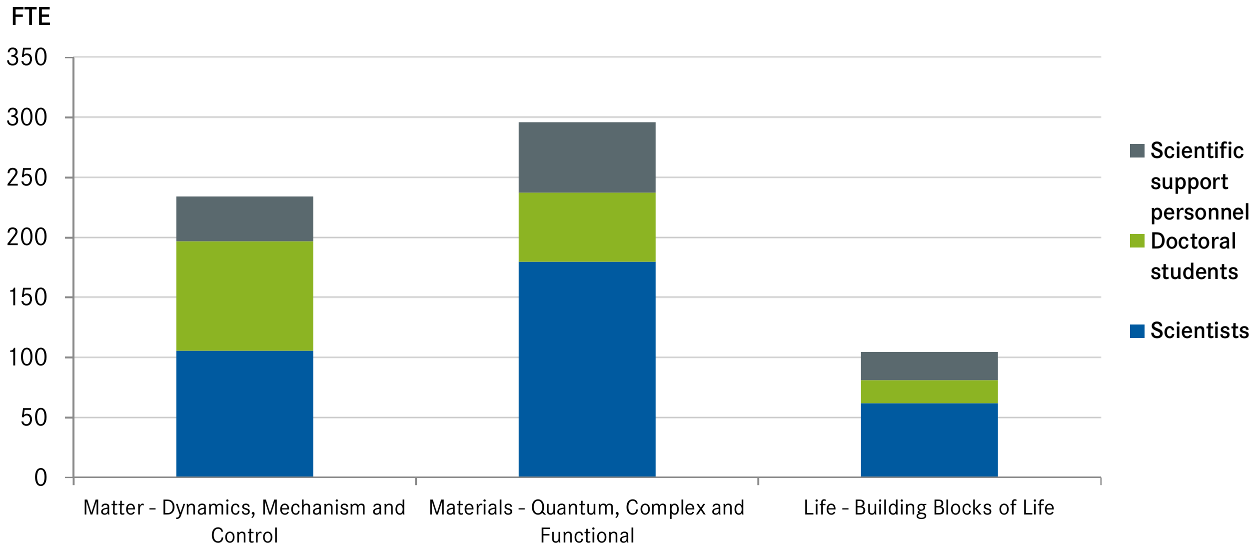


Figure 2: Foreseen personnel resource distribution for activities in the Program in 2021. For details see Table 10.

2. RESEARCH PROGRAM

In the following, we summarize and complement the objectives and strategy of the Program MML provided in the overview volume.

2.1. Objectives and Strategy

Within our Program *From Matter to Materials and Life* (MML), seven centers (DESY, FZJ, GSI, HZB, HZDR, HZG, KIT) have teamed up to explore the detailed structure and the electronic, magnetic, and chemical properties of matter and materials, as well as electronic, (bio-)chemical, and catalytic processes at all relevant length and time scales. Our research is based on the targeted exploitation of the analytical potential of our complementary, large-scale facilities, which provide a suite of probes for research: photons from storage rings and free-electron lasers (FELs), neutrons from research reactors and in future from accelerator-driven sources, intense ion beams, and highest electromagnetic fields. These form the backbone of a research infrastructure that is indispensable to meet the needs for analytical tools of our user community.

2.1.1. Challenges

The scientific challenges addressed by our Program are closely related to the following central subjects:

- **Matter under extreme and/or non-equilibrium conditions:** The properties and behavior of matter and materials at extreme temperatures and pressures and in interaction with strong external fields are mostly unexplored. It is hence a pressing question whether there are emergent functions under non-equilibrium conditions that can be utilized for future applications.
- **Mapping of dynamical processes on atomic time and length scales:** How can important processes in materials and at the surface of materials be mapped on the atomic time and length scale? Will it help to derive strategies on how to control material properties and processes on the level of single atoms, electrons, and spins?
- **Investigation of complex (functional) materials for new applications:** For the coming decades, complex, multifunctional materials and material systems such as heterostructures and nanosystems that blur the boundaries between metals, insulators, semiconductors, and organic-biological systems are expected to play a major role in technological developments. This requires novel interdisciplinary strategies for synthesis and for non-destructive *in-situ* and *operando* analyses.
- **Decoding of complex biological structures and processes:** Synchrotron and FEL studies provide crystal structures at highest resolution. In addition, the European XFEL opens up new possibilities for time-resolved studies at ultrashort time scales. With the revolutionary concept of serial femtosecond crystallography, the facility is expected to enable biological structures and processes to be recorded in native surroundings and in real time. In combination with the enormous success in the development of cryo-electron microscopy, a significant larger resolution range can be bridged, allowing for studies of more complex systems at higher resolution.

The **development, construction, and operation of complex infrastructure and large-scale facilities** for the national and international scientific community are a central part of the mission of our Program. A particular challenge is to pursue upgrade plans for our large-scale facilities for photons, neutrons, ions, and highest electromagnetic fields to maintain and enhance their world-leading capabilities in order to stay at the forefront of science. Within our Program and following a coherent strategy, corresponding plans have been developed.

More specifically, the upgrade plans for our large-scale facilities encompass the following:

- PETRA IV: fourth-generation synchrotron source at the diffraction limit (hard X-ray range)
- BESSY III: fourth-generation synchrotron source at the diffraction limit (VUV/soft X-rays)
- Dresden Advanced Light Infrastructure (DALI): IR/THz radiation sources in combination with laser and pulsed magnetic fields
- Vision MLZ2030: upgrade plan for the Heinz Maier-Leibnitz Zentrum (MLZ) with focus on hot neutrons
- Prototype High Brilliance Neutron Source (HBS): development and implementation of compact accelerator-operated neutron sources.

2.1.2. Research Environment

The large-scale research infrastructures operated within our Program provide the central backbone for research on the structure, dynamics, and function of matter and materials at large-scale facilities for photons, neutrons, ions, and highest electromagnetic fields in Germany, and play an important role in the international landscape of large-scale facilities in these fields. All of our facilities are highly competitive if not world-leading in the international context, as has been confirmed in the recent scientific evaluations of the Helmholtz Centers. A unique aspect of our Program is that it provides a common, coherent approach to research, which utilizes the various complementary probes. In total, our Program serves about 7,000 external users annually from universities, research institutes and industry from Germany and abroad. Experiments are selected based purely on scientific merit, through a transparent peer-review proposal system. About 30–40% of the users come from outside Germany, mostly from Europe, but also from other continents. Similarly, German users and Helmholtz researchers make use of European and other international research infrastructures, such as ESRF and ILL, or e.g. SLS, Elettra, SOLEIL, Diamond, ISIS, SINQ, SACLA, LCLS, GANIL, IMP Lanzhou, as well as the EMFL high-magnetic-field facilities in Grenoble, Nijmegen, and Toulouse. In this environment, there is cooperation, but also a healthy competition between the research infrastructures for the most advanced experimental techniques in order to attract user experiments of highest impact. All research infrastructures ensure highest quality of the science program through the proposal review system mentioned before. Available beam time is typically overbooked by a factor of 2–3.

With regard to the international large-scale facilities ESS, European XFEL, and FAIR, in which the Helmholtz Association and the Program MML are strongly involved, large international user consortia and collaborations have been formed, such as the HIB consortia at the European XFEL and the APPA collaboration at FAIR. These collaborations are responsible for the design of experimental areas and for state-of-the-art instrumentation.

2.1.3. Objectives

The focus of research in MML is devoted to the analysis and modification of the structure, dynamics, and function of matter and materials based on the development and operation of large-scale infrastructures for photons, neutrons, ions, and highest electromagnetic fields. To cope most effectively with the scientific and technological challenges, the objectives of our Program activities are structured as follows:

- Topic ***Matter*** – *Dynamics, Mechanisms and Control*: In this research, the focus is on fundamental aspects of the structure and dynamics of matter and on its interaction with light. Our aim is to gain a deeper understanding of the mechanisms underlying the properties of matter and mainly use this knowledge to exercise a targeted control of these properties on a microscopic level and on ultrashort time scales. For details, see Section 2.2.1.
- Topic ***Materials*** – *Quantum, Complex and Functional Materials*: With this research, we tackle challenging problems in materials research by means of our large-scale facilities, which provide unique microscopic information over a huge range of space and time scales that are not accessible with laboratory methods. For details, see Section 2.2.2.

- Topic ***Life** Sciences – Building Blocks of Life: Structure and Function*: This research aims at understanding the building blocks and processes of life, from molecules up to organisms. To this end, by developing and employing MML-specific tools and techniques, we elucidate the structure, dynamics, and function of components on various hierarchical levels. For details, see Section 2.2.3.

A unique aspect of our Program is the user operation of our large-scale facilities (LK II; representing about three quarters of our resources), which addresses researchers at almost all science institutions, particularly universities, on the national and international level. The stable operation, professional on-site support, and dedicated experiment environments allow the analytical tools provided at these facilities to be used for many scientific disciplines from a broad user community. Our LK II Program activities comprise the development, construction, maintenance, and operation of a unique portfolio of complementary facilities. These activities are grouped according to our large-scale infrastructures for photons, neutrons, ions, and highest electromagnetic fields in four Facility Topics:

Photon Facilities: The research at brilliant synchrotron sources and free-electron lasers ranges from basic science to applied science and engineering. Photon sources with ultrashort pulses and high coherence allow new insights into static and dynamic effects on a wide range of length and time scales, into the atomic structure of partially ordered matter and into material properties relevant to nanoscience and technology. With the photon sources BESSY II, PETRA III, FLASH, and the contribution to the European XFEL, the Helmholtz Association provides first-class research infrastructures in Germany that cover the complete spectral range from the THz to the hard X-ray regime, attracting users from all over the world. With regard to the usable photon energies and the reachable time scales, the mentioned sources ideally complement each other. For PoF IV, important tasks and goals related to research at the photon facilities are:

- Operation of the existing facilities at the highest international level, also addressing new challenges such as further automated experiments and dealing with increased data rates due to improved detection schemes, the latter will be addressed in close cooperation with the topic DMA of the program MT,
- Leading involvement in the scientific use of the Helmholtz International Beamlines (HIB) at the European XFEL,
- Realization and start of operation of FLASH2020+ in the first part of PoF IV,
- Installation and operation of BESSY VSR technology.

Neutron Facilities: Thanks to the large accessible space–time window, neutrons provide a microscopic insight into highly complex matter and phenomena, thus enabling the understanding of the resulting functionalities. With the next-generation megawatt spallation sources, a neutron peak flux will be achieved that significantly surpasses existing sources and that will therefore significantly broaden the application of neutron methods. The investigation of matter with neutrons at the world's leading sources ESS, ILL, SNS, and FRM II are organized by the user platforms Jülich Centre for Neutron Science (JCNS/FZJ) and German Engineering Materials Science Centre (GEMS/HZG). For PoF IV, the main emphasis related to research at the neutron facilities is on the following subjects:

- Operation of the national facility at MLZ at the highest international level through a strengthened cooperation between FZJ, HZG, and TUM; implementation of the Vision MLZ2030, which includes among other measures an instrument upgrade program as well as a data management, automatization, and robotics strategy,
- Realization and commissioning of the instruments for the ESS,
- Construction and operation of a prototype for a HBS to demonstrate the potential of this novel type of facility and prepare for the construction of a full-fledged HBS.

Ion Facilities: The ion facilities of GSI and HZDR provide unique experimental capabilities for atom physics, plasma physics, materials science, and biophysics. The broad spectrum includes precision experiments on fundamental principles of physics in extreme electromagnetic fields, research on matter under extreme conditions, and applied research in microelectronics, information technology, space radiation protection, and nanoscience, as well as new medical techniques for particle beam therapy. The facilities and ion beams available at HZDR and GSI are complementary with respect to instrumentation and ion energies and go far beyond standard ion beams existing at universities and in the semiconductor industry.

For PoF IV, particular emphasis is placed on:

- Operation of the Ion Beam Centre (IBC) for controlled modification and structuring of materials on the nanometer and sub-nanometer scale,
- Development of high-resolution, standard-free chemical analysis for resource technology,
- Operation of the facilities HITRAP, CRYRING, M-Branch, and PHELIX, including the experimental area at SIS18,
- Construction of the Atomic Physics, Plasma Physics and Applied sciences (APPA) experimental area at FAIR and first experiments in FAIR Phase 0 applying advanced FAIR instrumentation.

Highest-Field Facilities: Thanks to new technological developments in recent years, electromagnetic fields of so far inaccessible magnitude have become experimentally feasible. They enable the investigation of matter in highest electromagnetic fields, as available in the form of ultrahigh magnetic fields at the Dresden High Magnetic Field Laboratory (HLD) and through high-intensity photon pulses at accelerator-based infrared and terahertz sources (ELBE), at the high-power laser systems DRACO, PENELOPE (HZDR), and PHELIX (GSI), as well as at HIBEF, coupled with brilliant X-rays at the European XFEL. Major goals and activities foreseen for PoF IV are:

- Operation and further development of the HLD and its European integration,
- Operation and development of ELBE for the coupling of ultraintense lasers with accelerators and beam-driven strong field sources (FELBE, THz, DRACO, PENELOPE); development of the Helmholtz beamline HIBEF at the European XFEL, establishment of new laser-based sources for X-ray and particle beams and of a pulsed-field materials science experimental station.

2.1.4. Strategy

In a coherent approach, all MML groups at the seven Helmholtz Centers team up to tackle the objectives and challenges of our research activities. Bringing together our expertise both in performing state-of-the-art experiments with the four probes at hand (photons, neutrons, ions, and strong fields) and in providing comprehensive user support allows us to address major challenges of modern society and creates otherwise not possible synergies. This is worldwide unique. Close exchange and collaboration with the other two Programs within the Research Field *Matter*, MU and in particular MT, is of great relevance for our research program. As an example, the new Topic Data Management and Analysis of the Program MT (MT-DMA) is of utmost importance for experiments dealing with unprecedented data rates, as expected for instance at the European XFEL. Our research and the associated facilities also complement and support activities related to other Helmholtz Research Fields and are in the focus of our involvement in the Cross-Cutting Activities *Information and Data Management*, *Materials Research*, *Quantum Technologies*, *Structural Biology and Biological Processes*, and *Radiation Research*. It is worth noting that for research within MML, support and guidance by theory is crucial to the success and development of our Program.

A central part of the mission of our Program is the **development and operation of complex infrastructures and large-scale facilities** for the national and international scientific community. A particular challenge is to pursue upgrade plans for our large-scale facilities to maintain and enhance their world-leading capabilities in order to stay at the forefront of science. Within our Program and following a coherent strategy, based on a stringent science case, corresponding plans have been developed for research with photons, neutrons, ions, and high electromagnetic fields. More specifically, the major upgrade plans for our large-scale facilities encompass the following:

Photon Facilities: New concepts for the magnet design of synchrotron radiation storage rings have triggered a revolution in the achievable source performance worldwide, and at the same time, FELs are also continuously progressing towards improved and better beam properties. With regard to this technological progress and in order to ensure the future competitiveness of the synchrotron and FEL radiation sources within Helmholtz on an international level, a national photon science roadmap process has been initiated, with the aim to establish a coordinated national strategy for the entire photon energy and beam parameter range required by the diverse user communities. This roadmap process will be carried out in close consultation at the European level within the framework of a roadmap process of the League of European Accelerator-based Photon Sources (LEAPS). In order to place the larger of these projects on the national BMBF roadmap for large-scale facilities, conceptual design reports (CDR) and technical design reports (TDR) will be compiled. For PETRA IV (a fourth-generation synchrotron source at the diffraction limit in the harder X-ray range) the CDR is already completed and the TDR should be available in the first year of PoF IV. If approved, its realization would be finished towards the end of the PoF IV period. For BESSY III (a fourth-generation synchrotron source at the diffraction limit for the VUV/soft X ray range), a CDR will be completed by the middle of the PoF IV period at the latest and a corresponding TDR in the second half of PoF IV. Furthermore, during the course of PoF IV, scenarios for the further development of the European XFEL towards a continuous pulse sequence (CW operation) and a second set of additional beamlines are to be worked out in close coordination with the European XFEL management and Council as well as at the European level within the framework of LEAPS.

Neutron Facilities: After the shutdown of the BER II reactor, MLZ remains the only national neutron facility. A development plan called Vision MLZ2030 has been worked out, which will be implemented in PoF IV and which guarantees that MLZ will strengthen its position within the internationally leading group of neutron facilities. A central component of the neutron strategy is the development and realization of compact accelerator-driven neutron sources (CANS), which will be optimized for brilliance and thus allow complementary experiments to the ESS. Thanks to their scalability, they will find a wide range of applications. This novel concept is to be evaluated based on a CDR and TDR submitted by the middle of PoF IV. On this basis, the construction of a prototype is to be decided within PoF IV in coordination with the funding bodies. Within the framework of a German–Russian cooperation, a contribution is to be made to opening up the PIK reactor for research with neutrons. This new task will have to be fulfilled beyond the current timeframe of PoF IV. These activities will be reconciled with the other European players through the League of advanced European Neutron Sources (LENS).

Ion Facilities: During the PoF IV period, the IBC at HZDR will concentrate on commissioning a low-energy ion laboratory and start providing beam, as well as the 1 MV tandem accelerator to strengthen both research activities and user operation in accelerator-based mass spectrometry. At GSI, the focus will be on the installation of the MML experimental facilities (storage rings and caves) and the implementation of novel FAIR instrumentation. The latter will also be used for experiments at the current GSI facilities (FAIR Phase 0).

Highest-Field Facilities: HZDR is currently developing a new research infrastructure called DALI, which will combine pulsed magnetic fields, high-intensity laser systems and high-frequency THz beam systems under one roof. A TDR should be available in the first year of the PoF IV period. DALI will also be part of the planned national photon science roadmap.

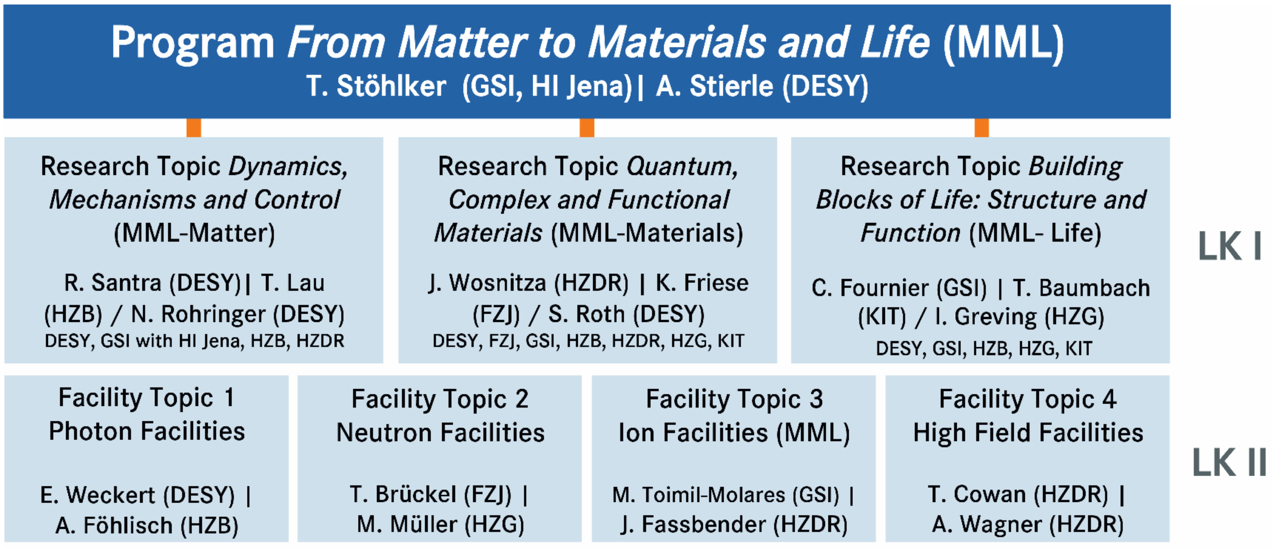
2.2. Structure of the Program

The Program structure is shown in Figure 3. Research (LK I) within the Program MML is structured in three Research Topics. This research addresses the most important scientific and technological challenges associated with the use of photons, neutrons, ions, and highest fields and is the prerequisite for an expert user service as well as for the development of new methods and instrumentation in accordance with user demands. Based on the intensive cooperation between the Helmholtz Centers, research activities are concentrated on the Topics listed in Table 1 and the related Facility Topics.

Table 1: Research Topics and Facility Topics of the Program MML.

Research Topic	Related Facility Topics	Participating centers
Matter – Dynamics, Mechanisms and Control	Photon Facilities, Ion Facilities, Highest-Field Facilities	DESY, GSI/HI Jena, HZB, HZDR
Materials – Quantum, Complex and Functional Materials	Photon Facilities, Neutron Facilities, Ion Facilities, Highest-Field Facilities	DESY, FZJ, GSI, HZB, HZDR, HZG, KIT
Life Sciences – Building Blocks of Life: Structure and Function	Photon Facilities, Neutron Facilities, Ion Facilities	DESY, GSI, HZB, KIT, HZG

The four Facility Topics (LK II) and the participating centers are grouped as follows: ***Photon Facilities***: DESY, HZB, HZG; ***Neutron Facilities***: FZJ, HZG; ***Ion Facilities***: GSI, HZDR; ***Highest-Field Facilities***: HZDR



Program *From Matter to Materials and Life* (MML)
T. Stöhlker (GSI, HI Jena)| A. Stierle (DESY)

Research Topic *Dynamics, Mechanisms and Control* (MML-Matter)
R. Santra (DESY)| T. Lau (HZB) / N. Rohringer (DESY)
DESY, GSI with HI Jena, HZB, HZDR

Research Topic *Quantum, Complex and Functional Materials* (MML-Materials)
J. Wosnitza (HZDR) | K. Friese (FZJ) / S. Roth (DESY)
DESY, FZJ, GSI, HZB, HZDR, HZG, KIT

Research Topic *Building Blocks of Life: Structure and Function* (MML- Life)
C. Fournier (GSI) | T. Baumbach (KIT) / I. Greving (HZG)
DESY, GSI, HZB, HZG, KIT

LK I

Facility Topic 1
Photon Facilities
E. Weckert (DESY) |
A. Föhlisch (HZB)

Facility Topic 2
Neutron Facilities
T. Brückel (FZJ) |
M. Müller (HZG)

Facility Topic 3
Ion Facilities (MML)
M. Toimil-Molares (GSI) |
J. Fassbender (HZDR)

Facility Topic 4
High Field Facilities
T. Cowan (HZDR) |
A. Wagner (HZDR)

LK II

Figure 3: Structure of the Program MML with the respective Topic spokespersons indicated.

2.2.1. Topic Matter – Dynamics, Mechanisms and Control

Executive Summary

The Topic MML-Matter explores fundamental aspects of the dynamics of matter, identifies the underlying mechanisms, and, based on the resulting insights, pursues microscopic control strategies. As the most fundamental of the Topics of the Program, MML-Matter provides the conceptual and methodological backbone for all scientific activities employing cutting-edge large-scale facilities involving photons, ions, and high fields.

Strategy

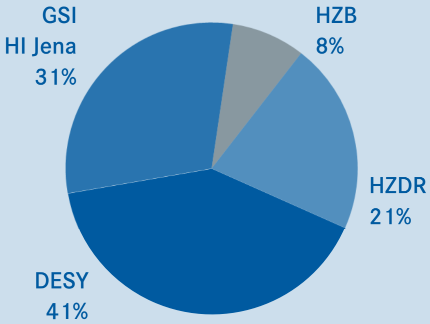
In PoF IV, MML-Matter will focus on the following three research directions (Figure 4): (i) **fundamental processes in strong fields**, with expected benefits for example to structural imaging, (ii) **observation and steering of real-time dynamics**, exploring new opportunities in chemistry and biology, and (iii) **matter under extreme conditions**, providing new insights for example into geo- and astrophysics.

Facts and Figures

Participating centers:
DESY, GSI/HI Jena, HZB, HZDR

Spokespersons:
Robin Santra, DESY
Tobias Lau, HZB
Nina Rohringer, DESY

Core-funded scientists: 105 FTE (2021)
Core-financed costs: 32,01 MEUR (2021)



Contributions of the centers to the topic *Matter*:
total core-funded personnel in 2021.

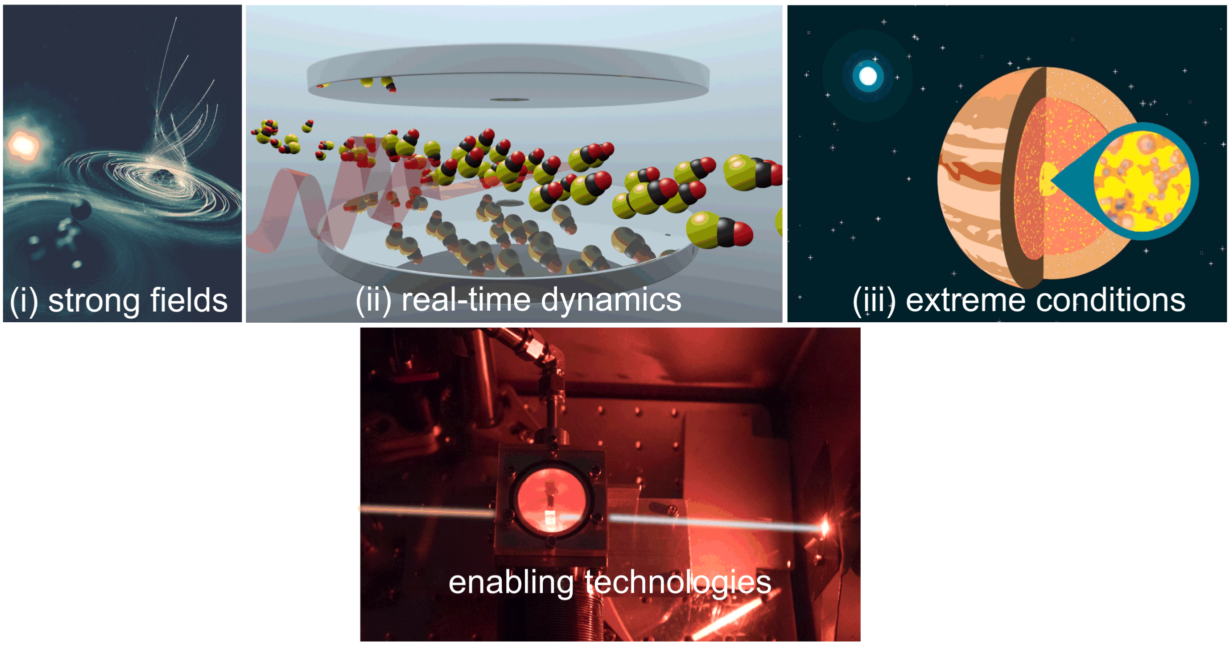


Figure 4: The three PoF IV research directions of the MML Research Topic Matter – Dynamics, Mechanisms and Control and their shared foundation of enabling technologies.

Strategic Goal of the Topic

(i) Fundamental processes in strong fields: Our present understanding of the electromagnetic interaction and of the coupling of light with matter is formulated within the framework of **quantum electrodynamics** (QED), which lays the conceptual basis for other field theories. However, our current knowledge of QED in the domain of **strong fields** is very limited and constitutes a profound challenge for both experiment and theory. Experimentally, paramount options include the study of vacuum birefringence by means of non-linear scattering of X-rays by intense laser light and, complementarily, measurements of Lamb shift, hyperfine structure, and *g*-factor of bound electrons for the heaviest highly charged ions. This is also true for detailed experimental studies of dynamic and non-linear processes in the strong-field limit, such as correlated multiphoton, multielectron ionization, and fundamental scattering and impact phenomena for electrons as well as for photons. In addition, the combination of ultrahigh-intensity lasers with the European XFEL will allow us to explore polarization effects in most extreme fields and to test models for relativistic plasma dynamics as well as fundamental QED theory.

Another promising field of research at X-ray free-electron lasers such as the European XFEL is **femtosecond- and Ångstrom-resolved structural imaging** of individual biological molecules interacting with their environment (see Section 2.2.3). A major challenge remains the fact that the strong X-ray fields required result in **ultrafast electronic modifications** of the sample, which need to be accounted for when reconstructing molecular structures from X-ray scattering data. Furthermore, short-wavelength free-electron lasers offer the potential of transferring non-linear spectroscopic techniques from the visible spectral domain to the X-ray region. **Non-linear X-ray techniques** could give detailed, chemically relevant information on electronic structure. The challenge is to isolate and quantify the underlying effects in the presence of competing processes. In addition to non-linear interactions, the quantum properties of X-rays are playing an increasingly important role in the decoding of matter. One direction is imaging with non-classical X-rays at sub-atomic spatial resolution beyond the diffraction limit. Moreover, new high-field THz and CW positron sources will enable the filming of transient states and dynamic phenomena.

(ii) Observation and steering of real-time dynamics: (Bio-)chemical systems are driven by the transfer of energy, electron, and mass (e.g. hydrogen atoms) through and between molecules. A deeper understanding of such processes is a prerequisite for designing novel functionalized materials for energy harvesting, the control of chemical processes at the fastest time scales, or improved pharmaceuticals. To this end, we address the basic scientific question of how to identify, and ideally control, the **governing principles of molecular functionality** on a fundamental molecular level. To control rate and selectivity in chemistry, we will identify and isolate **intermediate or transient species of molecular processes** to characterize electronic and spin states as well as their modification by solvation, with the aim of understanding governing principles and mechanisms as a prerequisite for targeted control of reaction pathways. This will involve studying and affecting physicochemical transformations on the driving energetic and temporal scales that govern these fundamental phenomena.

The use of **coherent light to induce and steer the motion of electrons** in matter is a cornerstone in photonics and drives technological innovation. A mechanistic understanding of charge and energy transport at the quantum level plays an important role in the design of future molecular electronics and functional nanostructured devices. One of our goals is to monitor and steer **electronic wave packets in molecular building blocks of life**, with element and site specificity, on their natural time scale by means of tailored soft X-ray FEL pulses. Such research must go hand in hand with the **development of advanced laser technology** that can simultaneously handle high pulse energies at high average power, i.e. high repetition rate, beyond current commercial systems, to enable ultrastrong fields and progress in observing and controlling real-time dynamics in matter, often in concert with high-repetition-rate FELs. We will demonstrate unique prototype laser systems that are applied to various strong-field processes and also transfer technology through spin-off companies to the commercial sector.

(iii) Matter under extreme conditions: Exotic states of matter for which **extreme temperatures, pressures, and fields** prevail are ubiquitous in the universe and present in the atmospheres, on surfaces, and in the interiors of a whole variety of stars and planets. In the deep Earth, the volatile cycle has an essential influence on the Earth’s atmosphere, as it impacts the concentration of e.g. CO_2 and H_2O released/recycled through volcanism and subduction. More extreme phenomena include highly charged nuclei produced during stellar explosions, the existence of metallic hydrogen, the helium–hydrogen de-mixing processes expected inside gas giants, or the ejecta from recently observed neutron star mergers. Such states of matter can be generated under steady-state conditions by powerful beams of heavy ions, or alternatively by intense optical or X-ray laser pulses in a strongly transient regime. It remains a veritable challenge to design precision experiments to create and characterize such samples in the laboratory.

Conducting research on exotic states of matter inevitably requires **dedicated advanced instrumentation**, such as novel lasers, spectrometers, polarimeters, detectors, and ion traps. For lasers, the challenge is to overcome limitations in pulse energy, temporal contrast, average power, carrier envelope phase control, pulse shaping, and spectral coverage from the THz to the ultraviolet wavelength range. High-power, well-synchronized and controlled laser sources will be required in so far unexplored spectral regions via frequency conversion. Spectral accuracy and sensitivity at acceptable detection efficiency are the major goals in the development of spectrometers and polarimeters.

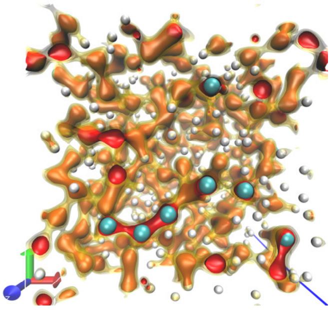


Figure 5: *Ab-initio* simulation of complex chemical processes in a carbon–hydrogen mixture at warm dense matter conditions.

Laboratory studies of stellar and planetary environments require multidisciplinary research on plasma, atomic, molecular, nuclear, and radiation physics. Investigating ionization and transport mechanisms in dense plasmas is of specific importance to shed light on astrophysical processes and plasma acceleration schemes. Phase diagrams of material mixtures (Figure 5) at planetary conditions are key for classifying the rising number of confirmed exoplanets and directly related to magnetic field generation in planetary liquid cores. Both the underlying **hydromagnetic dynamo effect and the magnetorotational instability** (MRI) are crucial mechanisms for the interaction of flows and magnetic fields. In planetary/stellar environments or accretion disks, these processes are hardly accessible to numerical simulations. Large-scale liquid-metal experiments will complementarily enhance our understanding of both effects. The Sun is the benchmark for all stellar models, which underlines the importance of the unresolved **solar abundance problem**. To probe element abundances in the solar core, new studies of solar fusion reactions are needed in addition to plasma physics and fluid dynamics research. The experimental activities require support from extensive theoretical studies of extreme pressure and temperature conditions as well as related non-equilibrium processes.

Competences

(i) Fundamental processes in strong fields: Substantial know-how has been gained for **experiments with stored and cooled high-*Z* ions** interacting with atomic targets, electrons, or photons. Prominent examples are the magnetic moments (*g*-factors) of H- and Li-like ions, such as $^{40}Ca^{17+}$ measured in Penning traps with unprecedented accuracies, also leading to the most precise value of the electron mass. Furthermore, hyperfine splittings in Bi^{82+} and Bi^{80+} were measured at the ESR storage ring, revealing a disagreement with theory by seven standard deviations [1], thereby stimulating further research activities. For the dynamics in strong fields, differential aspects of the electron coupling to the radiation field were investigated by means of electron and photon spectroscopy.

The observation of birefringent QED vacuum requires **sensitive polarimeters** to measure an ellipticity of the order of 10^{-12}. Previously, the purity of X-ray polarimeters was enhanced by three orders of magnitude by means of channel-cut silicon crystals, which were further improved by using diamond crystals and by reducing the divergence of the X-ray beam. This technology was established as a standard technique at PETRA III and the European XFEL (e.g. [2]).

Theory has advanced in recent years regarding the **description of fundamental processes in strong fields**. This includes the development of many-body techniques for the strong-field regime as well as computational tools for ionization dynamics triggered by high-intensity X-rays. In PoF III, we developed the world's first and so far only **first-principles electronic-structure tool** capable of describing the pronounced and ultrafast modifications of molecules exposed to high-intensity X-ray pulses. This development laid the foundation for the discovery of a new molecular ionization enhancement mechanism [3]. Another milestone achieved was the first demonstration of chemically relevant information in **stimulated X-ray emission spectroscopy** of transition metal compounds at an X-ray free-electron laser. Despite the ultrahigh X-ray intensity required for this technique, which implies strong, ultrafast modification of the electronic degrees of freedom, we were able to demonstrate that chemical information such as the oxidation state of the metals was preserved. Furthermore, in first experiments, we were able to show that **quantum correlations of photons** in completely incoherent light can be used for structure determination [4].

The recent demonstration of highly efficient THz harmonic generation [5] illustrates the unique capabilities at ELBE to study high-field THz-driven dynamics with sub-cycle time resolution. We have recently demonstrated the potential of ELBE for breakthrough results by studying the non-linear THz response of graphene [5]. ELBE offers unique capabilities for exploring high-field THz-driven dynamics using narrowband THz pulses in conjunction with sub-cycle time resolution. The pulse repetition rate of ELBE's the quasi-CW positron sources can be matched to a wide range of sample-specific positron annihilation lifetimes. The high-average current mode allows for performing *in-situ* matter manipulation and dynamic defect-related studies with the upcoming AIDA facility.

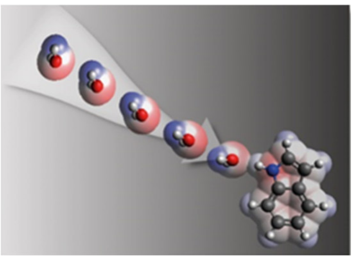


Figure 6: Formation of a bond between a biomolecular building block and water.

(ii) Observation and steering of real-time dynamics: We have unique capabilities of preparing **highly controlled samples of molecular systems** that are ideally suited for ultrafast imaging approaches. This includes individual structural isomers of small biological molecules and their microsolvated aggregates, which allows us to add e.g. water molecules one by one (Figure 6). Furthermore, we have developed experimental protocols to fix arbitrary molecules in space that enable us to look at **ultrafast dynamics directly in the molecular frame**. These systems are exploited in chemical reaction kinetics studies of individual species and in ultrafast atomic-resolution imaging of the structural dynamics. Here, we combine our expertise in table-top laser self-diffraction experiments and novel imaging approaches at X-ray facilities with the strong control to provide unprecedented insight into the workings of prototypical molecular systems.

We build on our unique photon science method developments to address **governing principles of molecular functionality**. We intentionally cross boundaries between atomic, molecular, and condensed matter to elucidate transitions and couplings that drive molecular dynamics, all the way to phase changes and switching phenomena. We investigate native-state electronic structure, most notably to interrogate **highly radiation-sensitive and photoexcited materials in elemental X-ray–matter interactions**. Our unique sample preparation capabilities offer size and composition control at the atomic level, allowing us to selectively investigate isolated, cryogenic, highly dilute gas phase metastable transient species [6] as well as micro-, interfacially, and fully solvated species [7]. Our compact femtosecond-pulse, mid-infrared to soft X-ray sources and BESSY VSR will augment these competences.

In PoF III, we developed novel optical parametric convertors and light wave synthesizers. We also devised a flexible cryogenic picosecond laser technology based on Yb:YAG at the 1 J level with average powers approaching the 1 kW level. **High-energy THz pulses** were used to observe the molecular polarizability anisotropy of liquid water and to demonstrate THz acceleration and 6D phase space manipulation of femtosecond electron bunches [8]. THz accelerators combined with nanostructured field-controlled emitter arrays have the potential for **compact, fully coherent, attosecond-duration X-ray sources**. Generation of extremely short pulses down to the attosecond domain inevitably calls for sophisticated techniques for time characterization, generally based on the detection of charged particles. We developed a novel approach for the **reconstruction of attosecond light transients** based on an all-optical technique [9]. The method was successfully demonstrated for table-top sources, and it will soon be extended to FELs.

(iii) Matter under extreme conditions: In the area of **ion–plasma interactions**, accurate measurements of ion energy loss at velocities near the Bragg peak have shown that traditional stopping-power models fail in this regime, highlighting the need for a detailed description of ion–electron collisions [10]. By modeling the generation of warm dense plasmas by ion irradiation, we demonstrated that iron is driven to conditions predicted in the **cores of super-Earth planets**. Diagnosing samples at such densities is enabled by laser-produced, highly penetrating secondary sources. Exploiting the ultrahigh contrast of the PHELIX laser, we were able to show that laser–matter interaction at intensities reaching 10^{21} W/cm^2 exhibit the predicted transition to the **relativistic transparency regime**.

Concerning instrumentation, we demonstrated the **coherent combination of femtosecond laser pulses**, thereby achieving several performance records. The novel high-repetition-rate and ultrashort-pulse fiber lasers provide unique performance, exceeding 1 kW average power in the infrared regime, and enable secondary sources with mW average power in the XUV as well as Watt-level super-octave sources in the mid-infrared regime [11].

The **HIBEF user consortium** brings several high-energy-density (HED) drivers and diagnostics to the European XFEL. To advance the implementation of HIBEF, relevant science has been performed at predecessor facilities. At LCLS, first dynamic *in-situ* measurements of chemistry relevant to the interiors of giant planets were performed applying an unprecedented set of single-shot X-ray diagnostics [12]. Moreover, it was shown that X-ray scattering techniques can resolve the **femtosecond evolution of nanoscale structures** in relativistic laser–matter interaction [13]. Our architect role in studying liquid-metal flows and magnetic fields during the last two decades now culminates in DRESDYN, which will soon run two large-scale liquid-sodium experiments dedicated to **dynamo action in a precession-driven flow** and to two different variants of the MRI [14 The underground Felsenkeller laboratory ion beam now offers the energy range needed to comprehensively address **solar fusion**, as well as neutron sources for the s-process, where ELBE's neutron and gamma-ray beams as well as CRYRING provide complementary approaches. The experimental studies are strongly linked to theoretical competences in quantum simulations of extreme conditions, non-equilibrium quantum many-body theory, and quantum field theory beyond standard perturbation theory.

Objectives and Approach

(i) Fundamental processes in strong fields: For precision tests of strong-field QED, the new CRYRING and HITRAP facilities will open unparalleled research opportunities. One prominent goal is to measure the ground-state Lamb shift in the heaviest one-electron ion (U^{91+}) by applying novel, high-resolution magnetic microcalorimeters [milestone RT1-1]. An unsurpassed precision is envisaged, which will challenge the QED theory for the most fundamental atomic system. These studies will be complemented by first measurements of the magnetic moment of the bound electron in heavy hydrogen-like ions at HITRAP (Figure 7). For few-electron ions, an additional approach will be provided by novel, portable XUV sources. At HESR, due to the relativistic velocities, laser frequencies are upshifted by more than an order of magnitude and the pulse duration is reduced by the same amount. This will allow, for the very first time, **multicolor, pump–probe experiments for atomic states in few-electron heavy ions** [RT1-2]. Further activities will be related to the intersection of atomic, plasma, and astrophysics. Using the FAIR storage rings, emphasis will be given to new mechanisms for nuclear excitations such as two-photon excitation and exotic decay processes.

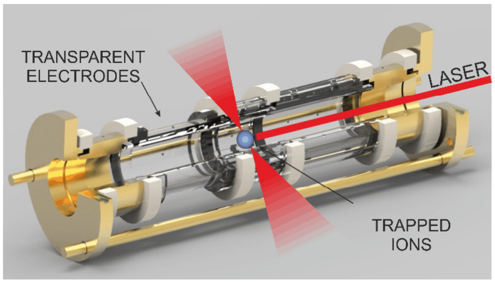


Figure 7: Precision laser spectroscopy of ions in a Penning trap.

Concerning **vacuum birefringence studies**, X-ray polarimeters with unprecedented sensitivity and high-resolution X-ray monochromators will be developed and implemented at the HIBEF station of the European XFEL [RT1-3]. In these experiments, focusing of the X-ray beam is mandatory in order to cross-correlate the X-ray pulse with an infrared or optical beam. Therefore, the combination of polarimetry and focusing optics will be an essential tool for such pump–probe experiments with high temporal resolution limited by the duration of both laser pulses. At first, this laser pump/X-ray probe technique, together with the X-ray polarimeter developed in MML-Matter, will be applied for **high-energy-density experiments** at the European XFEL. Afterwards, the detection of the vacuum birefringence in strong laser fields will be approached.

Theory will be advanced by combining field and (effective) many-particle methods to overcome limitations of low-order perturbation approaches and to describe **electronic processes in strong Coulomb and laser fields** [15]. Investigations of non-linear photon–matter interaction processes in the presence of strong nuclear fields will also be pursued. Furthermore, we aim at supporting diffractive imaging experiments using high-intensity X-rays and *ab-initio* studies of X-ray-generated solid-density plasmas. Structural imaging of individual biomolecular systems using X-ray FELs requires the ability to quantitatively describe the **dynamical transformations triggered by high-intensity X-ray pulses**. To this end, we will enhance our first-principles molecular electronic-structure tool [3] by incorporating relativistic and resonance effects. Then, we will develop a hybrid methodology, combining first-principles electronic structure with force-field-based ideas, which will enable predictive calculations on systems containing tens of thousands of atoms. Building on this, we will pursue a multiscale approach [RT1-4] to capture the spatial scales covered by focused X-ray FEL beams (volumes containing 10^{12} atoms or more).

Non-linear X-ray spectroscopy could become a novel technique at X-ray FELs to unravel electron motion in chemical reactions. In PoF IV, we will target two non-linear techniques: (1) A quantitatively predictive theory will guide proof-of-principle experiments of non-linear X-ray spectroscopy based on stimulated electronic X-ray Raman scattering. (2) We will assess the potential of non-linear X-ray/visible wave-mixing techniques such as X-ray/optical sum-frequency generation or parametric down-conversion in order to directly image and probe valence electronic changes in chemical reactions. In addition, we want to develop new methods to generate and use **non-classical (entangled) states of resonantly scattered X-ray photons**. Due to their long decay times, the narrow-band resonances of Mössbauer isotopes play a key role, because they can be manipulated dynamically during their lifetime. The pulsed excitation of the nuclei generates a highly entangled state of the emitting nuclei, so that non-classical properties can also be expected for the emitted radiation.

At ELBE, new high-field THz methods will be developed towards potential applications. Ideally suited to the high duty cycle, THz angle-resolved photoelectron spectroscopy (ARPES) and liquid-jet techniques will access high-field THz-driven dynamics in complex organic molecules and record **femtosecond “movies” of THz-driven changes** to the electronic structure [RT1-5]. Using pulsed positron beams, positron annihilation lifetime, and Doppler-broadening spectroscopy uniquely combined with *in-situ* material characterization and modification (laser annealing, layer deposition, ion implantation) will reveal information about **defect evolution and dynamic processes** with picosecond time resolution.

(ii) Observation and steering of real-time dynamics: Based on our unique highly controlled samples, the selection of individual molecular species, and the approaches for fixing them in space, we will use advanced imaging methods to unravel the **electronic, structural, and chemical dynamics of well-defined complex molecules** and even well-defined molecular aggregates [RT1-6]. Utilizing available facilities ranging from intense mid-infrared lasers for self-diffraction through ultrashort UV and XUV pulses (table-top, FLASH, European XFEL) for electron and ion imaging to powerful short X-ray pulses (European XFEL) for diffractive imaging will enable us to provide a comprehensive picture of the complete inner workings of specific molecular systems.

We will conquer sample complexity using the selectivity of X-rays in science-driven research with advanced X-ray methods. We aim for breakthroughs in determining **electronic structure in native states** with the lowest possible radiation dose on highly controlled samples [RT1-7]. In concert with first-principles theoretical spectroscopy, excited states, their kinetics and dynamics, and associated potential energy surfaces will be identified at selected atomic sites in extended bonding networks. **Targeted modification of molecular electronic and spin states** will be studied using stepwise ligand changes around metal centers. Complementary studies of gas- and solution-phase species will allow us to isolate the effects of **solvation and its influence on dynamic behaviors**. An in-depth understanding of increasingly complex aqueous solutions and associated solute and solvent effects [7] will be garnered using multidimensional soft X-ray techniques. To determine the governing molecular principles of chemical rate and selectivity, we will study elemental charge migration and reactive chemical phenomena as well as photoactive sites that drive and control efficient phase and state transitions [RT1-8]. We will address nuclear, electronic, and spin dynamics of molecules and clusters by developing time-resolved, gas-phase X-ray magnetic circular dichroism spectroscopy. We will investigate

bulk and interfacial aqueous-phase reaction dynamics using femtosecond- and picosecond-time-resolved soft X-ray spectroscopies with potential field control of associated pathways.

We will demonstrate parametric sub-cycle optical waveform synthesizers and apply them to the longstanding problem of how to **trigger chemical reactions from the ground state** [RT1-9]. Combined with high-flux attosecond water window radiation sources driven by high-average-power mid-infrared laser systems, we provide a unique toolset to study ultrafast chemical processes beyond photo-driven chemical reactions and in aqueous environment. The technology will be adapted to demonstrate advanced laser systems needed for upcoming high-repetition-rate facilities such as FLASH2020+. Using site-selective absorption of extremely short-pulse (from few femtoseconds to attoseconds) soft X-ray radiation, the **light-activated electron dynamics in biochemically relevant molecules** will be mapped with extremely high temporal and spatial resolution [RT1-10]. By comparing the results obtained in isolated molecules with those obtained in molecules embedded in a solvent (such as water), the **environment-induced modifications of the charge dynamics** will be revealed. By applying ultrashort femtosecond and even sub-femtosecond soft X-ray pulses generated by FELs, such as FLASH, and laser-driven photon sources, we will disentangle the electronic response from the characteristic motion of the molecular backbone in building blocks of biochemical compounds such as peptides and proteins.

(iii) Matter under extreme conditions: In PoF IV, we will study the stability of volatile-bearing Earth materials to significantly improve the understanding of the Earth's volatile cycle and its role in driving plate tectonics. The main approach will be to study the stabilities of volatile-bearing phases through crystallographic structure analysis at conditions of the Earth's interior using high-pressure devices at the PETRA III beamlines.

Plasma physics will benefit from unprecedentedly high ion beam intensities available from the SIS18 synchrotron. On the one side, intense proton pulses will now allow for imaging of the density distribution in dynamic events at a few-percent precision level, using the proton microscope PRIOR. This precision is crucial for stringent tests of equation-of-state or conductivity models in the **warm dense matter regime**. On the other side, heavy-ion heating and expansion of lead will enable us to explore the exotic phase diagram around the liquid–gas phase boundary, now reaching all the way up to the critical point [RT1-11]. Here, the newly built laser beamline of the PHELIX facility will result in a worldwide unique combination, enabling state-of-the-art pump–probe X-ray diagnostic capabilities for the exotic matter states created by the intense heavy-ion beams. First experiments will address **optical properties and ionization potential lowering in strongly coupled plasmas** as well as the investigation of phase transitions and superheating by X-ray diffraction. In order to further enhance diagnostic capabilities, emphasis will be given to the development and optimization of ultraintense, laser-driven secondary sources of X-rays and particles. This includes investigations of novel schemes and advanced target design for HED-research at the APPA cave of FAIR [RT1-2].

As an enabling technology, we are developing tailored laser sources to serve specific experimental needs. **High-repetition-rate and high-photon-flux XUV laser sources** will be employed for precision and ultrafast spectroscopy on atoms, molecules, and highly charged ions by combining them with traps, storage rings, FELs, and dedicated end-stations. Moreover, we intend to qualify table-top XUV imaging for studies of ultrafast electron and spin dynamics on smallest (sub)-femtosecond temporal and nanometer spatial scales.

HIBEF at the European XFEL will soon enable worldwide unique experiments with intense lasers in combination with the X-ray FEL source [RT1-12]. From 2020, precise imaging of laser-driven instabilities in relativistic solid-density plasmas as well as experiments addressing ionization potential depression models will be performed with X-ray scattering techniques. Dynamic compression experiments will clarify the **role of metallic hydrogen for phase separation processes inside giant planets** and study the **synthesis of high-performance materials through the warm dense matter state**. The precession-driven experiments at DRESDYN aim at demonstrating **dynamo action in a homogeneous bulk of fluid**, bringing experimental dynamos closer to the reality of planetary interiors. First tests with water are planned for 2020, the sodium experiments will start in 2021 [RT1-13]. While the helical and azimuthal versions of the MRI have been demonstrated, experimental evidence of the standard MRI is still elusive and will be demonstrated at a new large-scale liquid-sodium experiment. This facility is versatile enough to study combinations of the different versions of the MRI with the Tayler instability starting in 2022. Rayleigh–Bénard (RB) convection is a paradigm for the flow in planetary and stellar interiors. The combination of large Rayleigh numbers and small Prandtl numbers will be addressed in a large convection experiment. A smaller setup will test whether weak tidal forces synchronize the helicity of non-axisymmetric flow components, which could explain the synchronization of the solar dynamo with the alignment cycle of the planets. Using the new Felsenkeller laboratory, **leading hydrogen-burning reactions** will be studied from solar to asymptotic giant branch star energies, including $^{3}He(\alpha,\gamma)^{7}Be$, $^{2}H(p,\gamma)^{3}He$, $^{14}N(p,\gamma)^{15}O$, and $^{12}C(p,\gamma)^{13}N$. For the s-process, neutron source reactions, α-widths (Felsenkeller), neutron widths (nELBE), and γ-widths (γELBE) of relevant levels in Ne and Mg isotopes will be studied. The $^{12}C(\alpha,\gamma)^{16}O$ reaction, which affects the abundances of many chemical elements, will be accessed at helium burning energies. Related **theory developments** will encompass quantum simulations of warm dense matter and new models for strong-field regimes such as polarization effects, electron–positron pair creation, multiphoton emission, and its back-reaction onto the electrons. Moreover, non-equilibrium phenomena in strongly correlated quantum many-body systems, especially under the combined influence of strong magnetic fields and electromagnetic radiation, will be studied.

Expected Results

The sketched work program translates into a number of milestones that are well suited for monitoring the progress of the Topic. These are shown in the following table.

Table 2: Overview of milestones for the Topic MML

	Milestone	Year
RT1-1	Obtaining highly accurate experimental results on bound-state QED in the extreme fields of high-*Z* ions, which challenge theory	2024
RT1-2	Using intense SIS100 beams to create novel extreme states of matter and probing atomic lifetimes on the femtosecond scale for cooled relativistic ions	2026
RT1-3	Obtaining first results on birefringent QED vacuum at the European XFEL	2025
RT1-4	Developing a quantitatively predictive computer simulation of X-ray FEL-induced dynamics in complex matter	2027
RT1-5	Recording femtosecond “movies” of high-field THz-driven dynamics of the electronic structure in complex organic molecules	2026
RT1-6	Unraveling the concerted ultrafast transfer of electrons, protons, and atoms across bonds in prototypical biomolecules and the influence of (micro-)solvation	2025
RT1-7	Determining electronic structure properties of functional aggregates in their native states using novel soft X-ray methods	2027
RT1-8	Characterizing elemental chemical steps and interactions on the level of atomic constituents and on relevant time scales for archetypal reactions	2027
RT1-9	Realizing multi-mJ sub-cycle optical wave form synthesizers to trigger chemical reactions	2026
RT1-10	Demonstrating, using FLASH and table-top lasers, the control of the chemical reactivity of biomolecular building blocks on the electron time scale	2027
RT1-11	Performing first experiments employing laser-driven X-ray probing to dense strongly coupled plasmas produced by heavy-ion heating	2023
RT1-12	Performing first lighthouse experiments at the European XFEL to investigate transient non-equilibrium processes of dense plasmas and phase transitions in warm dense matter	2022
RT1-13	Demonstrating the homogenous dynamo effect in a precessing flow of liquid sodium	2024

Synergies and Collaboration

The research structure of the Topic MML-Matter is designed to encourage and support the cooperation among the participating Helmholtz Centers, while providing a framework for individual research accomplishments.

(i) Fundamental processes in strong fields: DESY, HI Jena, and HZDR work together in research direction (i) to develop polarimeters with utmost purity for the detection of the birefringence of the vacuum in laser fields of extreme intensities. New simulation tools for describing the impact of high-intensity X-ray pulses on complex matter will be tested through experiments in collaboration with MML-Life. Additional synergies with MML-Life are expected in the area of non-linear X-ray spectroscopy and in biological imaging applications of non-classical X-rays. Defect-related studies with positrons are intimately linked to MML-Materials, with a strong connection to memristive and magnonic materials for spintronics. Within the Wolfgang Pauli Center for Theoretical Physics (WPC), DESY and HI Jena theorists working in research direction (i) exchange methodological insights with MU-Theory. This includes organizing joint workshops on intersectional subjects.

(ii) Observation and steering of real-time dynamics: DESY and HZB cooperate in research direction (ii) on the real-time investigation of molecular reactivity in water. This collaboration is implemented within the framework of the newly founded Centre for Molecular Water Science (CMWS). This pan-European cooperation with more than 30 partners will achieve a molecular understanding of water and its consequences for life and technology. The CMWS brings together the Helmholtz Centers DESY, GFZ, HZB, HZG, and GSI/HI Jena. Also relevant to research direction (ii) is the collaboration of HZB and DESY within the hRIXS consortium at the European XFEL, which studies chemical dynamics, among other things. The development of advanced light sources, including lasers and attosecond FELs will be guided by the precise light characteristics needed for understanding the response of matter at extremely short time scales.

(iii) Matter under extreme conditions: A key collaborative structure within research direction (iii) is HIBEF. The HIBEF user consortium connects the Helmholtz partners HZDR, DESY, and GSI/HI Jena with a large international network of leading institutions to study extreme conditions at the European XFEL. Plasma physics experiments at FAIR will enable complementary studies at significantly longer time scales and larger sample volumes. For managing the amount of expected data, there will be strong exchange with MT-DMA. Joining high-intensity lasers with the European XFEL will inform the physics of plasma acceleration techniques that are pursued in MT-ARD (e.g. ATHENA). The liquid-metal experiments with geo- and astrophysical background are naturally linked with phase diagrams of planetary interiors and nuclear reactions in the solar interior. The close cooperation with the HZDR liquid-metal activities in the Research Field Energy will be continued. The astronuclear experiments are synergetic to s- and p-process nucleosynthesis studies at GSI, including CRYRING and ESR, to HIBEF plasma studies, and to DRESDYN.

Within MML-Matter, various **advanced laser technologies**, going far beyond what is commercially available, are under development and are closely tied to the science goals that are addressed at the participating Helmholtz Centers. All centers benefit from the individual developments through the joint innovation pool project ECRAPS in the areas of compact XUV sources, high-energy and high-power lasers, laser-based electron acceleration, FELs and their science applications, and data analysis. This allows for a continuous flow of information and exchange among the centers. The advent of laser-driven high-photon-flux XUV sources recently enabled table-top coherent imaging with a few-ten-nanometer axial and lateral resolution. Future applications of this new imaging technology are envisioned for the field of materials research, e.g. for the analysis of nanostructures (MML-Materials).

The **MML-Matter management board** currently consists of Robin Santra and Nina Rohringer for DESY, Thomas Stöhlker and Jan Rothhardt for GSI/HI Jena, Tobias Lau and Alexander Föhlisch for HZB, and Dominik Kraus and Thomas Cowan for HZDR. The members of the management board communicate and exchange ideas with all MML-Matter scientists in the participating centers. It is foreseen that during PoF IV, the management board will hold a teleconference at least four times a year (more often if urgent issues need to be discussed). In addition, once a year there will be a MML-Matter conference at one of the four Helmholtz Centers participating in the Topic. All principal investigators, postdoctoral researchers, and Ph.D. students funded through MML-Matter are expected to participate in this conference. The purpose of the conference is not only to create awareness of the breadth and depth of research activities within MML-Matter, but particularly to identify and foster new collaborative projects. To this end, there will be, one or more goal-oriented brain-storming sessions at each of these conferences.

Infrastructures

The major infrastructures used by MML-Matter are APPA@FAIR, AXSIS, BESSY II, BESSY VSR, CRYRING@ESR, DRESDYN, ELBE, ESR, European XFEL, Felsenkeller, FLASH, HESR@FAIR, HIBEF, HITRAP, JETI200, PETRA III (IV), PHELIX, POLARIS, PRIOR, SIS18, UNILAC, plus various laser laboratories at the participating centers. For more information, please see the table of infrastructures in Chapter 3.2. and the description of LK II in Volume III.

Opportunities and Risks

The proposed research has the potential to provide **important new insights into the fundamental properties of matter**. The research program is based on the **unique large-scale MML research infrastructures** (see above) as well as on most sophisticated instrumentation. The planned developments of methods and detector techniques as well as the construction of these devices pose risks in reaching the envisioned performance parameters. The key facilities, the European XFEL and FAIR, will enable unparalleled opportunities for our research program. However, FAIR is scheduled to deliver first beam in 2025, and thus there is a risk of schedule delays during the currently ongoing construction phase. As some of the other key infrastructures will also start full operation in PoF IV, there is the risk of delays during commissioning. As of now, HIBEF is partially operational, and commissioning of the Felsenkeller accelerator has started in collaboration with TU Dresden. The liquid-sodium experiments at DRESDYN will operate at the edge of technical feasibility, which implies significant risks for a successful accomplishment. Any significant delay in the implementation of the BESSY VSR technology for full user operation would pose a risk to the scientific goals associated with picosecond time-resolved soft X-ray spectroscopy, which could only partly be lifted by the availability of X-ray FEL and laser-based sources.

2.2.2. Topic Materials – Quantum, Complex and Functional Materials

Executive Summary

The development of tailored advanced materials is key to the solution of many of the grand challenges of society, starting from renewable-energy concepts over quantum materials for information technologies to biocompatible materials for medical applications. Tackling some of the most urgent challenges in materials research withlarge-scale facilities, which provide unique macro- and microscopic information over a huge range of space and time scales, holds the potential for fundamental discoveries and truly disruptive technology advancements. The most challenging questions in research on quantum, complex, and functional materials in all forms from the nanoscale to workpiece materials pose demanding requirements on our large-scale facilities and lead to an ever-ongoing improvement of our analytical instruments, feeding back to ever-improved materials characterization.

Strategy

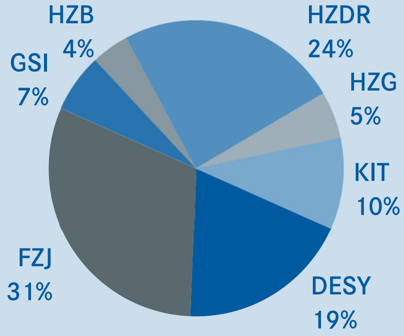
The Topic MML-Materials aims at achieving fundamental discoveries and truly disruptive technology advancements in materials design through the unique information that can be acquired by making full use of our large-scale facilities. The interplay of this materials research aspect with the focused improvement of our large-scale instruments is the hallmark of our research program, which is fully embedded in the strategies of the Helmholtz Cross-Cutting Activities *Materials Research* and *Quantum Technologies*. Taking advantage of the combination of photon, neutron, ion, and highest-field facilities, complemented by modern data management methods and theory support, together with the distinguished system competence of our personnel, makes our Topic unique and puts us in a clear leadership position.

Facts and Figures

Participating centers:
DESY, FZJ, GSI, HZB, HZDR, HZG, KIT

Spokespersons:
Joachim Wosnitza, HZDR
Karen Friese, FZJ
Stephan Roth, DESY

Core-funded scientists: 179 FTE (2021)
Core-financed costs: 48,055 MEUR (2021)



Contributions of the centers to the topic *Materials*: total core-funded personnel in 2021.

Strategic Goal of the Topic

Within the Topic MML-Materials, the distinctive portfolio of the MML large-scale facilities is utilized to study fundamental properties of condensed matter, with the aim to reach an in-depth understanding on the atomic level and, based on this understanding, facilitate the rational design of novel functional materials and their use in unprecedented applications. The development of tailored advanced materials is key to the solution of many of the grand challenges of society, starting from renewable-energy concepts over quantum materials for information technologies to biocompatible materials for medical applications. To develop new materials with specific functionalities, one of the next challenges is the combination of various materials into more complex structures, for instance in heterostructures. To design tailored materials for specific applications in various geometries, from the nanoscale to bulk to functional workpiece materials, an in-depth understanding of structure and excitations at the atomic level must be attained, and the detailed knowledge of production processes must be continuously increased.

Within the Program MML, these goals are reached with our LK II facilities as a central pillar, which provide photons, neutrons, ions, and high fields as well as a worldwide unique variety of state-of-the-art synthesis and analytical instruments. With them, we tackle the mentioned urgent societal grand challenges, by applying tools that provide unparalleled macro- and microscopic information over a huge range of space and time scales. The gained knowledge is in turn fed back into the ever-ongoing improvement of our analytical instruments. These two aspects, together with the excellent competence and expertise of our personnel, make our Topic unique on a global scale, placing us in a worldwide leadership position. The advancement of experimental techniques provides exclusive tools for other Helmholtz Programs focused on specific materials research aspects as well as for users from science and industry, thus fulfilling the key mission of the Helmholtz Association.

Novel and smart materials with custom-designed functionalities for information, quantum, energy, and chemical technologies are characterized by an increasing complexity, frequently with various competing degrees of freedom. For the development of suitable materials, the comprehensive exploration and understanding of their quantum-mechanical and entropy-driven properties are a prerequisite. This goal will be achieved during PoF IV by the following main measures: (i) further extending our high-end large-scale facilities, allowing *in-situ* studies of targeted synthesis and modification on the atomic level, (ii) enlarging the access to all relevant spatial, momentum, time, and energy scales with improved resolution, (iii) developing *operando* methods for materials systems and devices relevant for technological applications, (iv) developing and extending the existing infrastructure to enable worldwide unique investigations under extreme conditions, such as high fields, pressure, spatial, energy, and temporal resolution, (v) employing machine learning and advanced tools of artificial intelligence in close collaboration with the Topic MT-DMA to obtain the ultimate possible information from multidimensional data sets, (vi) further extending the existing cooperation within MML in order to make use of multiple complementary probes, and (vii) working closely with high-performance simulation and theory groups to develop models and improve *ab-initio* methods to enhance their predictive power.

Competences

The continuous developments of the leading materials research competences of the MML centers clustered in this Topic were recognized by the excellent to outstanding marks of the scientific evaluation. Within the PoF III period, the overall competences were particularly strengthened by the inclusion of the HZDR research activities in materials research and the synergetic possibilities offered by the corresponding LK II facilities ELBE, IBC, and HLD. In the following, the distinct competences of the participating partners are exemplified by selected highlights of the pioneering materials research performed in MML – often obtained in close collaboration among the different centers and with a leadership role in international cooperation.

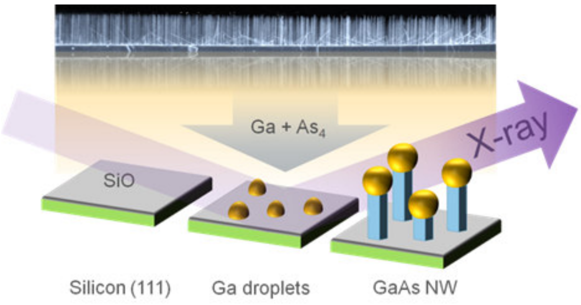


Figure 8: Growth of crystalline GaAs nanowires visualized by *in-situ* X-ray characterization schematically shown in the lower part. Top: Electron microscope view of the nanowires.

Our combined expertise ranges from sophisticated synthesis methods of novel materials to the characterization of their physical and chemical properties from macroscopic to atomic length scales and from application-relevant time scales to ultrafast processes.

Using highly brilliant synchrotron radiation, particularly **growth processes** of nanostructures under harsh conditions of elevated temperatures and reactive gases can be followed *in-situ* at the atomic scale. Based on time-resolved ***in-situ* X-ray structure characterization** during molecular-beam epitaxy at PETRA III, we were able to directly monitor the growth of tiny crystalline GaAs wires in a unique way (Figure 8). Such wires are broadly used for daily-life applications, such as infrared remote controls or high-frequency devices in cell phones, as well as for solar cells in space applications [1]. In another *in-situ* growth experiment, we monitored the evolution of the morphology of a gold layer with **time-resolved grazing-incidence small-angle X-ray scattering** during sputter deposition at PETRA III [2]. The study opened up new opportunities to improve the fabrication of tailored metal–polymer nanostructures for plasmonic-enhanced applications such as organic photovoltaics and sensors. Using **high-energy heavy-ion beams** at GSI, novel hierarchical and self-supporting threedimensional networks of pure ZnO and TiO_2-coated ZnO nanowires were synthesized [3]. Thanks to their excellent mechanical stability, applications in sensing, catalytic, and piezoelectric devices are envisioned. By using so-called Shack–Hartmann sensors for hard X-rays, a **new macroscopic time-resolved imaging scheme** was developed that allows for unrivaled contrast sensitivity on the nanoscale [4]. This technique now enables a better understanding of the fundamental mechanisms of structure formation and a controlled manipulation of the resulting materials.

We investigate **magnetic and electronic correlations of quantum materials** by combining a number of different probes available at the MML large-scale facilities. Using **polarized neutron scattering** – a technique in which JCNS with its outstations at MLZ, ILL, and SNS concentrates world-leading expertise – we could unravel how the magnetization of an all-oxide-based transition-metal antiferromagnetic multilayer structure can be switched layer by layer in a controlled way [5]. This microscopic insight into switching phenomena adds functionalities for new applications in antiferromagnetic spintronics. Magnetocaloric materials form the basics of cooling technologies that promise energy savings of up to 30% compared to present-day non-environmentally friendly compressor-based technologies. We now reached a breakthrough in the understanding of the inverse magnetocaloric effect, in which the material is cooling in an applied magnetic field, contrary to the usual heating observed for most materials. First exhaustive characterization of the underlying dynamics of the effect using **inelastic neutron scattering** at MLZ and ILL revealed that it is caused by increasing fluctuations of the magnetic moments in the applied magnetic field [6]. Spin waves offer intriguing perspectives for information technology, since ohmic losses as in conventional electronics do not occur. We could prove for the first time that spin wave control is possible using natural anisotropic features of magnetic order in an interlayer exchange-coupled ferromagnetic bilayer by employing **scanning transmission X-ray microscopy** at BESSY II to image the generation of spin waves and their propagation [7]. Further on, we demonstrated the long-time predicted existence of one-dimensional excited states in quantum spin chains, so-called Bethe strings [8]. Utilizing **THz spectroscopy and high magnetic fields**, these many-body excitations were evidenced in $SrCo_2V_2O_8$ crystals in which the Co ions form the spin chains (Figure 9). This groundbreaking result is of key relevance for a number of modern research subjects such as quantum magnetism and its application in quantum information as well as for string theory in particle physics.

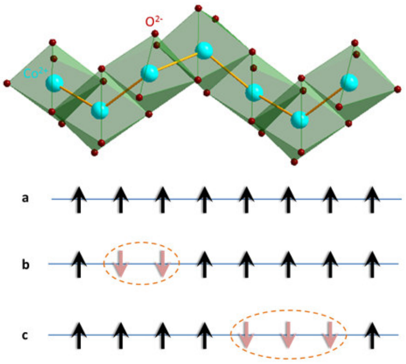


Figure 9: Crystalline structure of $SrCo_2V_2O_8$ with observed magnetic excitations in the Co spin chains.

We performed first science benchmark experiments at the ESRF using **X-rays in pulsed magnetic fields** up to 30 T [9]. Using X-ray magnetic circular dichroism, we were able to follow the rotations of the magnetic moments of Ho and Fe in the ferrimagnet $HoFe_5Al_7$ individually through a field-induced phase transition. These findings provide unique microscopic insight into the magnetization process of a strongly anisotropic ferrimagnet. The **Femtoslicing X-ray** facility at BESSY II (HZB) is a worldwide unique research instrument for ultrafast magnetic-dynamic studies with femtosecond temporal resolution. Using this infrastructure, we revealed that antiferromagnetic order can be changed much faster than that of ferromagnetically aligned magnetic moments [10]. This discovery led to the suggestion to combined ferro- and antiferromagnetically arranged spins to design materials for faster and more energy-efficient magnetic memories.

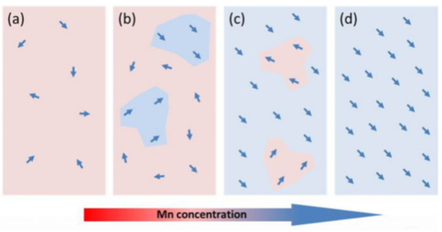


Figure 10: Schematic picture of the evolution of magnetic order from para- to ferromagnetic in (Ga,Mn)As with increasing Mn concentration.

The interplay between the concentration-dependent metal–insulator transition and magnetism was studied in detail in resulting dilute ferromagnetic GaAs and InAs Mn-ion-implanted semiconductors (Figure 10) [11]. Complementary to the high-energy ions at GSI, low-energy ions are available at the IBC, allowing the **implantation of magnetic ions** such as Mn. Combined with pulsed-laser annealing, this materials synthesis technique has the advantage that neither do magnetic ions exist on interstitials nor are As antisites present in the samples, in contrast to films produced by widely used molecular-beam epitaxy. In another pioneering experiment, we investigated graphene at the ELBE **free-electron laser** in a time-integrated **four-wave mixing experiment** in the mid-infrared spectral range [12]. We found that, in an applied magnetic field, graphene features a giant resonantly enhanced optical non-linearity caused by the non-equidistantly split Landau levels. The possibility to tune the resonance frequency by the magnetic field makes this optical non-linearity attractive for applications.

We possess strong expertise in the **characterization of complex and functional materials**, especially *in-situ* and *operando* under real-world application conditions. For the optimization of materials-engineering processes, we developed a portable friction stir unit, designed for use in high-photon-energy synchrotron beamlines. It enables ***in-situ* studies of microstructural evolution** processes during friction stir welding in workpiece materials such as Al and Ti alloys as well as steel. The real-time capability allowed us to study *in-situ* the coarsening and dissolution of hardening nanoprecipitates during friction stir welding in an Al alloy developed for aircraft construction, using small-angle X-ray scattering at PETRA III [13]. These results allowed us to evaluate a model for the friction stir welding process.

To improve catalyst performance, an atomic-scale correlation of the nanoparticle surface structure with its catalytic activity under industrially relevant *operando* conditions is essential. We were able to investigate the surface properties of Pt–Rh nanoparticles using **X-ray diffraction combined with *in-situ* mass spectrometry** during near-ambient-pressure CO oxidation at PETRA III (Figure 11). This approach opens the door for an in-depth characterization of nanoparticle-based catalysts under operational conditions with unprecedented atomic-scale resolution [14]. By use of **small-angle neutron scattering** at MLZ combined with thermodynamic measurements, we showed that the dynamics in crystalline self-assembled, complex materials can be predicted from their amorphous state [15]. Molecular exchange processes are important equilibration and transport mechanisms in both synthetic and biological self-assembled systems such as micelles, vesicles, and membranes. Still, these processes are not entirely understood, in particular the effect of crystallinity and the interplay between cooperative melting processes and chain exchange. Similar experimental approaches can be applied to understand the properties and interactions in other molecular structures.

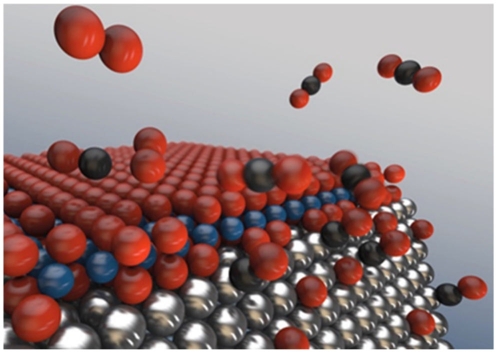


Figure 11: Oxygen (red) deposition on the surfaces, but not on the edges and corners of Pt–Rh nanoparticles. Edges thus increase the efficacy of catalysts.

Further on, we demonstrated that the structural sensitivity and accuracy of the established **X-ray standing-wave technique** can also be applied at the **high-repetition-rate free-electron laser** FLASH [16]. This opens up the possibility to obtain unprecedented structural information of adsorbate and surface atoms with picometer spatial and femtosecond temporal resolution. This technique will substantially contribute to a fundamental understanding of chemical reactions at catalytic surfaces and the structural dynamics of superconductors. As a backbone for future X-ray microscopy experiments, we further develop and manufacture **high-performance X-ray optics**, such as high-diffraction-efficiency and high-numerical-aperture multilayer Laue lenses and blazed gratings [17]. We demonstrated hard X-ray focusing to a world-record spot size below 10 nm, which is a prerequisite for future high-resolution X-ray materials-imaging applications.

Objectives and Approach

The comprehensive and fundamental understanding of the relationship between structure and physico-chemical properties is a prerequisite for the rational design of novel and smart materials. Combining challenging materials research with the mission to advance the already unique analytic capabilities of our LK II research infrastructures towards improved resolution in space, momentum, energy, and time, towards studies under multiple extreme conditions, and towards *in-situ* and *operando* techniques is the hallmark of our Topic. Together with advanced data management and theory support, we expect to provide a breakthrough in basic understanding and tailoring of a wide range of quantum, complex, and functional materials. Gaining full insight into these materials from the nanometer scale to the bulk will enable us to obtain the full picture from synthesis to function. In the following, we summarize the main objectives and approaches in our comprehensive materials science research, starting with the fundamentals and continuing with nanostructured functional materials over complex engineering to soft-matter materials.

Our objective with respect to **quantum materials** is to elucidate exotic superconducting, orbital, and magnetic order and excitations using our large-scale facilities. Thereby, the focus will be laid on quests for dynamical signatures of fractionalization and emergent quasiparticles and on tuning quantum critical systems to their critical point. We will put special attention on the interplay between band structure topology and electronic-correlation effects in systems such as magnetic Weyl and other topological materials – candidate materials for future quantum technology. Furthermore, the influence of geometrical frustration (for instance, in kagome and honeycomb-lattice materials) on the magnetic ground state and emergent collective phenomena will be elucidated.

These studies require the further development of the experimental infrastructure at our LK II facilities to enable experiments over the widest possible parameter range as well as an intense interaction with theory. In particular, we will develop wide-angle polarized neutron diffraction and inelastic neutron scattering under synergetic extreme conditions of high magnetic field, pressure, and ultralow temperature [milestone RT2-1]. The unique possibilities offered by the HIBEF installation at the European XFEL will be complemented by a dedicated materials science beamline that will enable unrivaled element-sensitive X-ray diffraction experiments in record high magnetic fields up to the range of 60 T. We plan first pioneering investigations, such as studies of magnetic-field-induced metal–insulator transitions for 2024 [RT2-2].

A further objective is the comprehensive investigation of novel **magnetic functional materials** allowing for the optimized design, synthesis, and modification of advanced devices for future information technology. Here, we investigate these magnetic materials in particular with respect to their magnetization dynamics. Low damping and highest achievable frequencies are addressed in order to increase the energy efficiency in spintronic, spin-orbitronic, and magnonic applications as well as for antiferromagnetic spintronics. We use ion beam technology to tailor and fabricate such magnetic devices, high-field facilities to investigate their basic properties in magnetic fields, and photon and neutron facilities to image the magnetic functionality and elucidate the magnetic order. A major focus lies on the understanding and applicability of non-trivial, 3D magnetization configurations in the field of curvilinear magnetism. The mutual interplay between optics, magnetics, and plasmonics is utilized to achieve uniquely new functionalities. Furthermore, flexible magnetoelectronics is promoted for smart augmented-reality applications. A specific goal is to advance the development of antiferromagnetic spintronics, chiral magnetism, and superconductivity in heterostructures towards future possible quantum-technology devices by gaining an in-depth understanding of interface phenomena through e.g. 3D layer-resolved neutron magnetometry and advanced small-angle neutron scattering with polarization analysis.

Additional relevant functional materials to be studied are semiconductor nanowires and other nanostructures, 2D materials such as graphene and transition-metal dichalcogenides, topological insulators, and Weyl semimetals. Wherever applicable, our goal is to demonstrate functionality of electronic nanodevices, using our unique ion-beam-assisted nanofabrication and -characterization tools. We will use ion beams to synthesize novel functional materials or modify and tailor their electronic and magnetic properties with *in-situ* control and analysis. This comprises hyperdoping of semiconductors, novel semiconductor alloys, for instance GeSn, as well as complex oxides whose properties are modified through ion-induced strain and/or defects. Specific defects in SiC and Si will be employed for applications in quantum technology. Activities within milestone RT2-3 will utilize our ion beam facilities to realize novel ultrathin nanostructured devices with atomic precision.

The **investigation of novel materials on the nanoscale and on ultrafast time scales** in order to understand and tailor functional dynamics of correlated quantum materials is a challenging subject that we will tackle. We intend to use ultrafast and THz radiation sources to investigate quantum, complex, and functional materials on the nanoscale by scanning near-field infrared microscopy (SNIM), under high pressure in newly developed low-temperature diamond anvil cells, and on ultrafast time scales to study the dynamics of low-energy electronic, vibronic, and magnetic excitations. FLASH with its unique possibility of providing intrinsic synchronization between THz and soft X-ray FEL pulses is ideally suited to studying the influence of low- and high-energy THz pump stimuli in order to reach a solid understanding and control of the dynamic response of ferromagnetic materials toward these classes of electromagnetic radiation [RT2-4]. Effects of strong THz fields in materials will be tackled in collaboration with the Topic MML-Matter.

We will also focus on **ultrafast non-equilibrium dynamics in quantum and functional materials**, in particular the flow of spin angular momentum and energy by time-resolved X-ray magnetic circular dichroism and magnetic diffraction, which was recently extended towards depth resolution. As one of our milestones [RT2-5], we will address processes occurring on atomic length scales as well as those in tailored nanostructures in order to ultimately optimize materials design for applications and novel functionalities.

Furthermore, our objective is to develop functional and quantum **materials based on nanoparticles and polymers** that are compatible with biotechnology and wet-chemical processing. Potential applications are in spin- and straintronics-tailored permanent magnets, flexible electronics, and drug delivery. We will investigate the correlations between (nano-)structure and (optical, electronic, magnetic) function down to single nanoparticles with atomic resolution, using advanced X-ray optics approaching the physical limits and X-ray imaging such as ptychography and coherent diffraction imaging. As milestone RT2-6, we will combine small-angle scattering from different probes, such as surface- and interface-sensitive grazing-incidence X-ray and neutron scattering, with advanced simulation methods for retrieving the complex, hierarchical real-space structures. Particular efforts will focus on a maximal integration of synchrotron technology and novel computational methods to enable high-throughput solutions for the digitalization of materials structures and properties, including their evolution during fabrication, processing, and operation, as a basis for materials modeling and virtual materials design.

Our goal is to reach an **in-depth understanding of the structural and compositional evolution during the production and operation** of functional and advanced structural materials that allows the dedicated development of new materials for special components and applications. To this end, our research activities will focus on the method development and utilization of unique *in-situ* and *operando* approaches for the characterization of the structure, dynamics, and function of real-world materials and devices for information technologies (thin films, nanostructures, interconnects, printable electronics), transport technologies (lightweight devices, injection nozzles, aerospace shields), and energy conversion (such as solar cells, heterogeneous catalysts, batteries, electrolyzers, hydrogen-storage tanks). Using the synchrotron and neutron radiation facilities available in MML, novel spectroscopy, scattering, and imaging approaches will be employed. This includes laminography of extended 2D specimens as well as *in-situ* and *operando* investigations of complex, hierarchical materials on all length scales down to the atomic level and towards ultrashort time scales, using nanofocused beams at synchrotrons.

We plan to **investigate the early stages of the nucleation phase** during physical vapor and spray deposition of metals on organic surfaces, as well as under high-pressure synthesis conditions. We expect to obtain millisecond and sub-millisecond time resolution for investigating transient and order phenomena during the formation of grainy colloidal, opaque, and industrially relevant coatings. Moreover, with the ongoing quest for miniaturization, the investigation of single nanoscale devices becomes inevitable, as well as the study of their *operando* behavior in real time. We plan to investigate the structure–function correlations for single nanoparticles and nanowires by pushing coherent diffraction imaging towards atomic resolution. Concerning high photon energies, grain mapping under *operando* conditions is one of the challenging future plans [RT2-7]. New research has commenced on the *in-situ* characterization of mechanical properties of materials via stress–strain measurements at simultaneously high pressures, temperatures and in corrosive environments. Today, alloy and process improvements should be knowledge-based, requiring full time-resolved microstructure characterization. As milestone RT2-8, we will perform *operando* analyses of production processes, such as selective laser melting, utilizing high-energy synchrotron radiation of highest temporal resolution.

Our research concerning the in-depth understanding of **catalysts and chemically active materials under *operando* conditions** addresses key questions in heterogeneous catalysis, such as the quest for the active phase and the promotion of selectivity, durability, and lifetime. As milestone RT2-9, we will perform single-nanoparticle X-ray imaging under *operando* catalytic reaction conditions with nanometer resolution, which would allow a direct correlation of changes in activity and the atomic structure of the catalyst material. To achieve this aim, we will push X-ray optics, such as multilayer Laue lenses, as well as coherent diffraction imaging and scanning X-ray imaging techniques to their limits. We plan to make best use of the extreme brilliance of upcoming high-energy fourth-generation storage rings, such as the ESRF EBS. In the field of heterogeneous catalysis and beyond, one of the dreams is to track electrons and nuclei simultaneously during chemical reactions in momentum and real space at the intrinsic time scales of the systems under investigation. We plan to achieve this goal by a combination of time-resolved surface-sensitive spectroscopy and scattering methods at the European XFEL and FLASH. The spectroscopic information obtained from such systems in optical pump/X-ray probe experiments can be directly compared to time-resolved gas phase experiments performed in MML-Matter. We will realize pump–probe experiments for photocatalytic reactions as milestone RT2-10.

Another objective is to **identify materials for alternative refrigeration technologies and information technology applications** that show caloric effects. The focus of our research is on the coupling between different order parameters to enhance caloric efficiency and extend functionalities. For these investigations, a multidimensional parameter variation (field, pressure, temperature, composition, etc.) utilizing elastic and inelastic neutron and synchrotron scattering as well as high-magnetic-field experiments is of key importance to tune the entropy changes and understand spin–lattice and charge–lattice coupling on a microscopic level.

Important objectives related to ion beams concern the **response of materials to high-energy particle irradiations**. This subject is essential to understand transient and long-lasting radiation damage processes and develop figures of merit and lifetime estimates [RT2-11]. We will also focus on irradiation effects in material simultaneously exposed to extreme pressures in diamond anvil cells and expect to reach new thermodynamic pathways in the phase diagram and stabilize new material phases [RT2-12].

In the field of **complex soft-matter materials**, our overarching theme is to fundamentally understand the relation between molecular and colloidal structure and interactions, as well as the self-assembly pathways into different topologies (micelles, vesicles) and superlattices (liquid crystals, quasicrystals). This knowledge is used to design and assemble polymers and colloids over large length scales to obtain responsive and functional structures and devices as well as direct nanoparticle growth into desired shapes and sizes. We will functionalize nanoparticle surfaces with polymers for the controlled fabrication of highly ordered polymer nanocomposites. The *in-situ* observation of the formation of bio-inspired materials from well-defined nanoscale building blocks is another challenge in materials science that we are going to address in the future [RT2-13]. New characterization methodologies over wide spatial and temporal ranges will be developed, taking advantage of the high-brilliance neutron and X-ray beams at our LK II facilities. Complemented by advanced modeling and simulation tools, this will serve to find new strategies for the design of soft materials.

A key objective is to reveal **how environmental conditions affect the structure and dynamics of macromolecules** such that these fold into defined conformations, or how they induce liquid–liquid phase separation. Synthetic protein mimics are investigated as model systems to understand the influence of charges, hydrophobic moieties, and hydrogen bonds on structure, dynamics, self-assembly, and ion conduction. This forms a direct link to the activities in the Topic MML-Life. We will develop new methods for time-resolved experiments that allow for the detection of fast temperature and concentration jumps based on microfluidic techniques and the investigation of nanoscale structural evolution and phase transitions by use of *in-situ* neutron, X-ray, and light scattering. All that will allow us to reach milestone RT2-14, the establishment of a fundamental understanding and control of macromolecular conformation and liquid–liquid phase separation.

Expected Results

The sketched work program translates into a number of milestones that are well suited for monitoring the progress of the Topic. These are shown in the following table.

Table 3: Overview of milestones for the Topic.

	Milestone	Year
RT2-1	Establishing synergistic extreme conditions for neutron scattering to investigate/tune spin-based materials	2025
RT2-2	Performing first pioneering materials science investigations at HIBEF using high pulsed magnetic fields	2024
RT2-3	Utilizing the targeted extensions of the ion beam facilities to design novel ultrathin nanostructured devices with single-atom precision	2023
RT2-4	Utilizing THz pump–probe schemes for the excitation and analysis of novel magnetic materials	2024
RT2-5	Fully characterizing the ultrafast non-equilibrium dynamics of spin and orbital angular momentum and energy transfer in a magnetic material	2026
RT2-6	Achieving in-depth characterization of nanoparticle assemblies by use of small-angle scattering and newly developed simulation methods	2026
RT2-7	Demonstrating grain mapping under *operando* conditions	2024
RT2-8	Performing *operando* production process analysis using high-energy synchrotron radiation of highest temporal resolution	2025
RT2-9	Performing single-nanoparticle X-ray imaging under *operando* catalytic reaction conditions	2026
RT2-10	Realizing pump–probe experiments for photocatalytic reactions involved in energy conversion	2022
RT2-11	Developing figures of merit for radiation hardness of functional materials exposed to high-dose environments	2025
RT2-12	Stabilizing and characterizing high-pressure phases created by ion irradiations under high pressures	2027
RT2-13	Performing *in-sit*u observation of the formation of bio-inspired materials from well-defined nanoscale building blocks	2023
RT2-14	Establishing the fundamental understanding and control of macromolecular conformation and liquid–liquid phase separation	2027

Synergies and Collaboration

Within the Topic MML-Materials, numerous **collaborations** exist between the centers, as well as with other Topics, Programs, Research Fields, and cooperation partners worldwide. The large-scale facilities of MML in particular have bridging functions to the national and global materials science community. Our access to fundamental materials properties provides unique information for stringent tests of simulation and *ab-initio* theory, and is thus always underpinned by corresponding collaborations with theory groups.

The synergetic merger of the Helmholtz materials science competences based on large-scale infrastructure within MML-Materials has led to various collaborations between the Helmholtz Centers as well as to personnel exchange. Often a combination of experimental techniques, using ions, photons, neutrons, and high fields, underpinned by theory, is needed to fully characterize and understand novel materials. This is documented by the large number of common projects and publications in all fields of materials science research exemplified above. Beyond that, within the Program MML there are strong links with the Topics MML-Matter and MML-Life, as well as, naturally, with all the Facility Topics. For instance, strong cooperation exists with MML-Matter in the field of non-linear and ultrafast THz spectroscopy and high-field research as well as on advancing pump–probe schemes for ultrafast experiments and developing nanostructured targets for high-energy-density experiments. In addition, strong cooperation has been established with the Program MT. This concerns accelerator- and detector-related materials science questions, *inter alia* for the performance improvement of radio frequency cavities. The increasing amount and complexity of data collected in materials science experiments at the LK II facilities lead to an obvious link to the new data management Topic MT-DMA. Interactions with MML-Life are most strongly given through the soft-matter research activities and include studies using X-rays and neutrons on biological systems, investigations of transport processes through ion-track-based nanochannels in polymers, and the application of heavy-ion microprobes for the investigation of radiation effects in living cells.

Due to the high interdisciplinarity of the materials research activities within MML-Materials and the relevance of the MML LK II facilities for materials synthesis and characterization, we maintain strong links to virtually all Helmholtz Research Fields. This is also documented in the Helmholtz cross-cutting activities Materials Research and Quantum Technologies, with the MML-Materials portfolio being a significant part of the activities listed in these documents. A further example is the installation of a new research infrastructure (In-Situ Innovation Platform for Multifunctional Materials Systems, InnoMatSy) which is planned across several Research Fields.

Cooperation with universities and other research institutes, both in Germany and worldwide, is decisive to MML-Materials research. Numerous groups are embedded in collaborative research activities such as DFG-funded SFBs (CRCs), graduate schools, and clusters of excellence (AIM in Hamburg and ct.qmat in Dresden).

The materials science research within MML-Materials is embedded in a very broad and highly interdisciplinary global scientific community. Our researchers work closely together with cooperation partners from all over the world, performing experiments at the MML LK II facilities and at facilities abroad (e.g. the outstations of JCNS at ILL or ORNL).

The **management** of MML-Materials will be done in a similar way to the other Topics within MML. The management board, consisting of one designated person per center and the Program speakers, will meet at least four times per year (or more often if needed), either via teleconference or in person. New ideas and requests from the scientists will be discussed during these meetings, and flexible solutions for the implementation of new ideas will be found. The management board members will communicate the results of these meetings to all MML-Materials scientists within the seven cooperating Helmholtz Centers. This includes, for example, proposals to the Matter Forum. In order to deepen existing and foster new MML-Materials collaborations across Helmholtz Centers, a yearly workshop involving all scientists and students of the Topic will be held. Our doctoral students will organize their own Topic-wide Ph.D. days that will encourage cooperation between the centers. The students will present their results and have ample time for scientific discussions and exchange of new ideas.

Infrastructures

The research addressed in the work program of MML-Materials relies heavily on the MML large-scale LK II infrastructures (see Volume III). The continuous science-driven development and implementation of targeted instrumentation at these facilities is a prerequisite to maintaining and extending the world-leading position of our materials research. In addition to the large-scale facilities, access to various laboratories provided by the participating Helmholtz Centers is key to some of our research. For example, laboratory methods available at JCNS are complemented by an advanced sample preparation platform using the Helmholtz Nano Facility, NMR characterization (Biomolecular NMR Centre), high-resolution electron microscopy (Ernst Ruska Centre), short-time-scale photon experiments (JuSPARC facility), all the way to simulations (Jülich Supercomputing Center JSC). Synchrotron-radiation-based methods are combined with microscopy and nanostructuring methods at the DESY NanoLab located at the Center for X-ray and Nano Science (CXNS).

Opportunities and Risks

Within the Topic MML-Materials, the planned establishment of uniquely new experimental infrastructures at the MML LK II facilities and the advancement of existing ones will enable further **opportunities** for outstanding research. The combination of the scientific expertise of our staff with the large-scale infrastructure, together with our cooperation with national and global partners, will enable, in a unique way, a faster throughput from gaining a fundamental understanding of material properties to first devices and final disruptive applications. The unique scientific and infrastructure environment will foster the potential of young researchers by attracting them at an early stage of their careers to the large-scale facilities. On the other side, there is the **risk** of a delayed realization of the scheduled, highly demanding research due to unforeseen challenges, such as delays in the planned infrastructure developments. Although the development of high-performance computing with deep-learning algorithms for automated high-throughput data analysis offers great opportunities, there is always the risk of delays in the provision of adequate hardware and software tools.

2.2.3. Topic Life Sciences – Building Blocks of Life: Structure and Function

Executive Summary

The Topic MML-Life aims to achieve a deeper understanding of living systems. Our mission is to enable unique studies of building blocks and organizational levels of life, by exploiting the unrivalled potential of large-scale facilities. The participating centers (which were recently joined by GSI) develop unique methods and instrumentation to examine such structures and (bio-)chemical processes on molecular and (sub-)cellular levels up to whole organisms, and to study their response to the environment. Another goal is to transfer particular knowledge to medicine and aerospace.

Strategy

The Topic MML-Life will develop cutting-edge methodologies and instrumentation for the life sciences, employing the unique beam properties of high-brilliance free-electron lasers (FELs), synchrotron radiation sources, and sources of high-energy charged particles. Special emphasis will be dedicated to: crystallographic methods, including serial and high-throughput crystallography for extensive compound screening; X-ray spectroscopy, microscopy, and tomography for highest energy, spatial, and temporal resolution; pipelines for correlative, hierarchical, and highly automated high-throughput imaging combined with artificial-intelligence (AI)-based data analysis; and biomedical application of high-energy heavy ions.

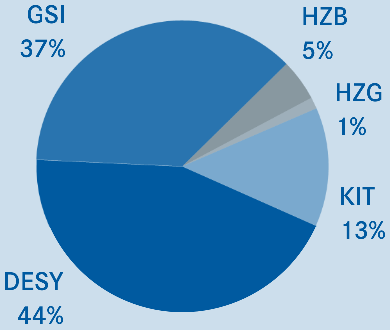
Applying the methods to dedicated studies from molecular to organism level, this Topic is accordingly structured into four mutually linked research themes: (i) structure and interaction of subcellular and molecular components, (ii) morphology of higher hierarchical levels, (iii) response of biological systems to external stressors and stimuli and their interaction, and (iv) translational research.

Facts and Figures

Participating centers:
DESY, GSI, KIT, HZB, HZG

Spokespersons:
Claudia Fournier, GSI
Tilo Baumbach, KIT
Imke Greving, HZG

Core-funded scientists: 62 FTE (2021)
Core-financed costs: 16,82 MEUR (2021)



Contributions of the centers to the topic *Life Sciences*: total core-funded personnel in 2021.

Strategic Goal of the Topic

Structure and interaction of subcellular and molecular components: Accelerator-based X-ray photon sources will be used for time-resolved spectroscopy and imaging to resolve the properties and functioning of biological molecules, their macromolecular complexes, and soft matter. The ultimate goal is to delineate the underlying rules governing the interactions of constituents that may generate biological function. Starting from the smallest entity among the building blocks of life, we will study the structure, dynamics, and functionality of water for a better understanding of its behavior in complex physical and chemical environments. Furthermore, we aim at identifying universal concepts that govern the structures and organizations of biological macromolecules up to soft condensed matter. This information will also be used for tailoring new materials and synthetic procedures for the fields of energy and health. High-throughput tools will be developed for accelerated structure-based screening of effector compounds (e.g. drug precursors or other biologically active compounds). This will enable the robust structural investigation of up to 1,000 substances per target protein in one week by single-crystal X-ray diffraction, and it will open entirely new avenues for early drug discovery research in many directions, with a large and significant societal impact.

Morphology of higher hierarchical levels in relation to genetics and the environment: We develop synchrotron techniques both for cell and tissue imaging and for full animal imaging. To this end, we focus on vertebrate model organisms such as fish and frog, which provide indispensable strategies for testing paradigms about development and disease, and on arthropods such as insects, which fulfill key functions in our ecosystems. We will build AI-supported 3D imaging and analysis pipelines for comparison of quantitative morphological and morphometric data from huge numbers of individuals, e.g. for phenotype–genotype correlation, as well as dose-efficient *in-situ, in-vitro,* and *in-vivo* 4D cine-tomographic pipelines to elucidate morphodynamics.

Response of biological systems to external stressors and stimuli and their interaction: We will develop techniques to study the response and interaction of molecules, tissues, and organisms with their environment while they are being subject to external stressors and stimuli. One major focus will be stress by ionizing radiation, in particular charged particles, which represent both a risk for the population exposed and an opportunity to treat cancer.

Translational research: The strategic goal is to improve radiotherapy in oncology and to develop solutions to protect astronauts during space travel. Heavy-ion cancer therapy pioneered at GSI within a pilot project for carbon ion cancer treatment and by HZB for proton therapy in Germany will be developed in the upcoming PoF IV funding period.

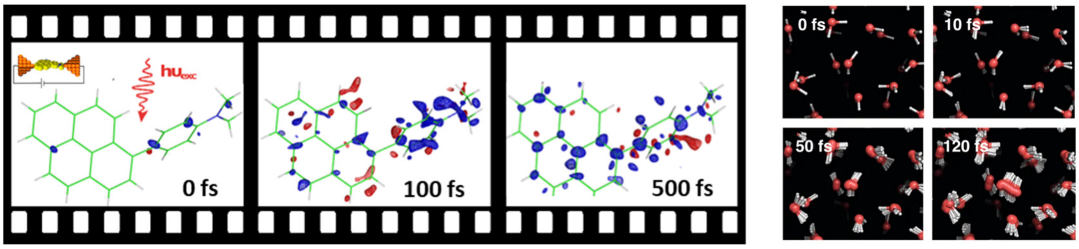


Figure 12: Structure and interaction of subcellular and molecular components. Left: Optical electron transfer reaction tracked at atomic resolution (electron density decrease in red; increase (blue)) [1]. Right: Molecular dynamics simulations of molecular water (comparison to XPCS) [2].

Competences

X-ray spectroscopy and diffraction: In PoF III, the Topic MML-Life was extended, and strong competences in utilizing high-flux X-ray sources, such as synchrotrons and FELs, were created for studying the structure, dynamics, and energetics of various systems that make up the building blocks of life (including water, soft condensed matter, and biochemical systems). Pioneering studies of complex chemical and biochemical reactions, followed in real time and at atomic resolution, were developed and carried out using novel "molecular-movie" methods of ultrafast diffraction and multidimensional X-ray spectroscopy (X-ray emission spectroscopy and inelastic X-ray scattering). These studies gave new mechanistic insights into biochemical reactions relevant to solar-energy and materials research (Figure 12 left [1]).

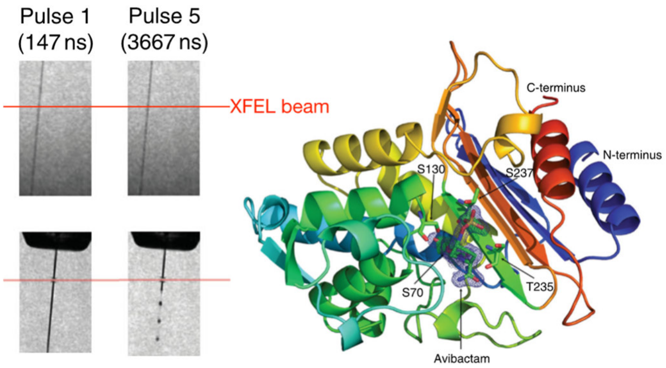
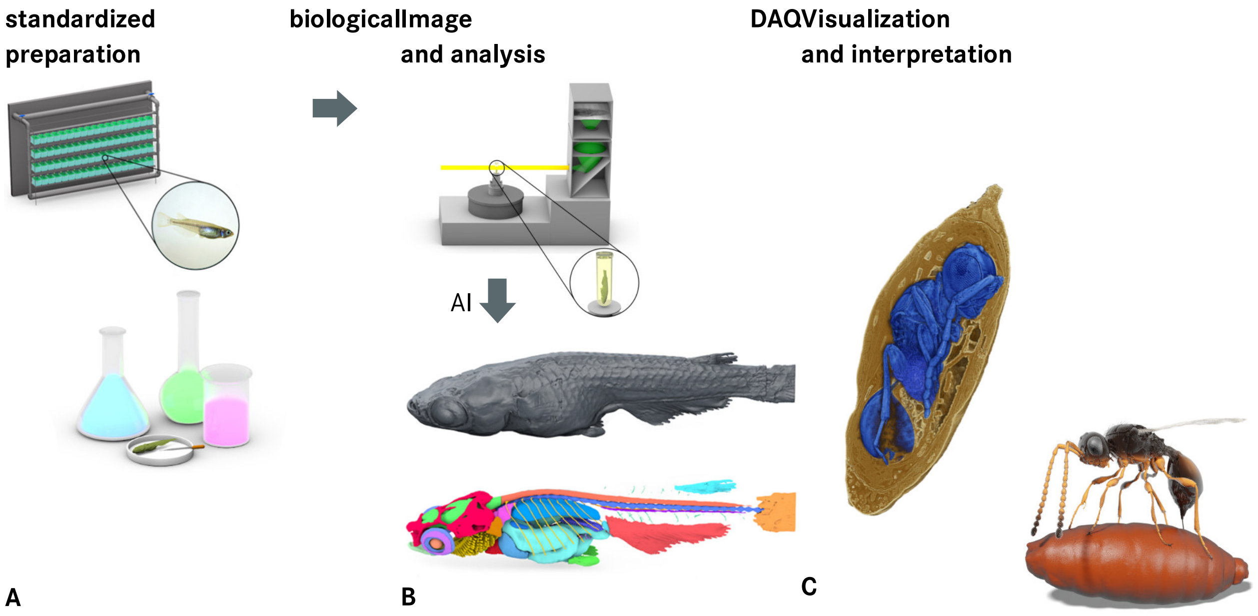


Figure 13: Serial crystallography (at the European XFEL) of beta-lactamase and inhibitor [3].

New understandings of nanoscale soft-matter systems and their intrinsic dynamics were obtained using our development of X-ray correlation spectroscopy techniques pioneered in MML-Life. This was applied to the study of real-time dynamics of water on the nanoscale – from picoseconds to milliseconds, answering long-standing open questions about the anomalous phase properties of liquid water (Figure 12 right, [2]). All these approaches have recently been extended to fully utilize the MHz rates of the European XFEL experiments in order to vastly improve our analysis of ultrafast chemical reactions and of structures and functional dynamics of water and soft condensed matter. The development of X-ray FELs, together with our understanding of how femtosecond-duration pulses allow the collection of diffraction patterns and images, enabled us to elucidate macromolecular structure and dynamics at room temperature as well as at length scales down to those of interatomic distances and at time scales of molecular responses. The recording of atomic-resolution "molecular movies" of photoactive proteins have revealed the sub-picosecond isomerization of a chromophore that triggers signaling reactions, and 3D views of the structural kinetics of drug binding in real time. Serial diffraction measurements of non-crystalline materials, such as single amyloid fibrils [3, 4], may help to understand their formation and interactions. Our demonstration of serial crystallography at the MHz pulse rates of the European XFEL to eleucidate the structure of β-lactamase and its inhibitor [3] (Figure 13) will allow us to progress beyond model systems to elucidate detailed structural dynamics in the process of photosynthesis. Our development of rapid sample delivery systems, the use of detector systems developed in the Topic MT-DTS, and the analysis of high-rate diffraction data also vastly expanded the scope of macromolecular crystallography with high-brightness synchrotron radiation, and these techniques are currently being adopted by at least eight other facilities around the world. For the screening of biological and biochemical effector compounds by single-crystal X-ray diffraction, nearly full automation of the experiment is required. In PoF III, HZB laid the groundwork for making compound screening feasible by X-ray crystallography at BESSY II. Such studies were impossible less than a decade ago. In PoF IV, we will optimize the technology and infrastructure to the extent that all samples provided by users in the sample Dewar at the beamline can be analyzed with no or very minimal user intervention [milestone RT3-1].

X-ray biological imaging techniques optimized for imaging cells up to full organisms have been investigated and implemented at different facilities with the development of complex experimental setups for parallel-beam imaging and X-ray microscopy combined with 3D X-ray tomography and laminography. The portfolio covers soft and hard X-ray techniques with resolutions from micrometers down to a few nanometers employing various contrast modalities (absorption, scattering, phase, spectroscopic). This instrumentation include stations at the GEMS and DESY PETRA III beamlines; the ultrafast-imaging technologies and the LAMINO - stations and hard X-ray microscopes developed at KIT; and, for ultrahigh sub-cellular resolution, the soft X-ray microscopes at HZB. All are complemented by electron and optical microscopy in order to incorporate super-resolution microscopy into X-ray microscopy.



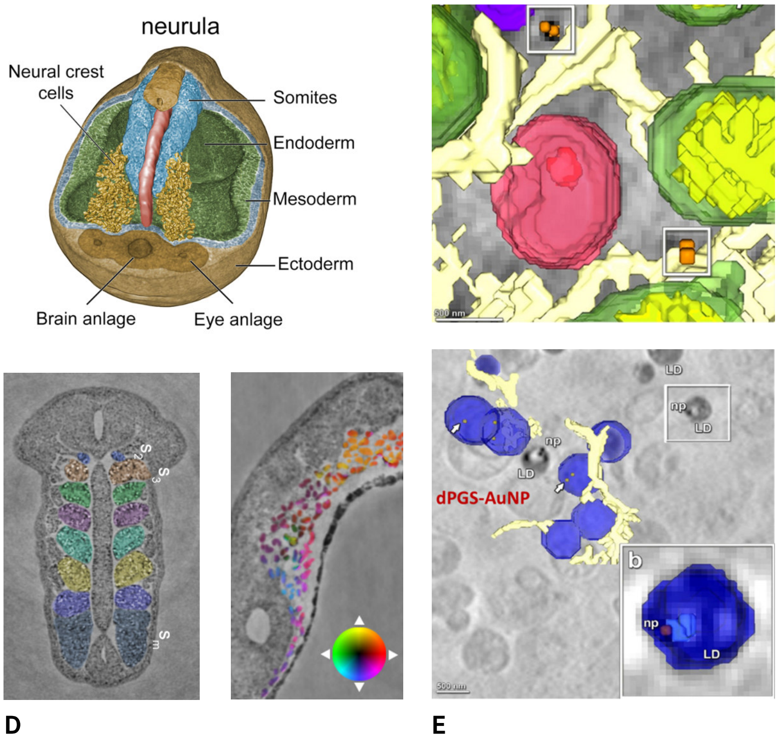


Figure 14: Morphology of higher hierarchical levels. Schematic illustration of morphological imaging pipelines.

A: Standardized biological preparation.

B: High-throughput DAQ, image reconstruction, and AI-based automated analysis in a medaka fish [7].

C: Visualization of parasitation of a host pupa by a parasitoid wasp and its interpretation [6]. Imaging goes down to the cellular level, e.g. *in-vivo* imaging of tissue and cell migration in *Xenopus* (D), and molecular scale e.g uptake of nanoparticles (E).

Nanoscale X-ray imaging yields unprecedented views into native cellular structures (Figure 14 E). By combining iterative X-ray spot scans (SXM) and focused ion beam milling (FIB), we will develop FIB-SXM at BESSY II. Together with the Topic MML-Materials (see Section 2.2.2), we developed a new concept of X-ray microscopy of cells for PETRA IV. **High-throughput data acquisition** is a prerequisite for large specimen series. Central elements are the virtual laboratory syris, the UFO high-performance computing framework, and the dedicated control system CONCERT. **Segmentation** is a bottleneck for large series and stimulated new semi-automated segmentation algorithms based on random-walk principles. Exemplary **pipelines for morphological imaging** of cells up to complex organisms have been established (Figure 14). Applications comprise zoology, paleontology, and biomimetics, with manifold morphological studies on extinct and extant insects and other invertebrates [5, 6]; developmental biology, with phenotype–genotype studies of vertebrate embryos (Figure 14 D) and adult model organisms (Figure 14 A, B, [7]); biomaterials and tissue engineering; and initial research for uptake of nanoparticles as active ingredients into isolated cells. First screenings of very large sample series enabled spectacular discoveries, even from 30-million-year old specimens, and revealed interactions, e.g. between parasitic wasps and their hosts, as well as important biological, morphological, and ecological information (Figure 14 C, [6]).

Ion accelerators for biology and medicine: The accelerator facilities we use offer the opportunity to irradiate living cells, tissue, and organisms with protons and heavy ions at energies from a few MeV/u up to 1 GeV/u. Cutting-edge biology infrastructures (including tissue culture laboratories and animal facilities) allow local groups and external users to perform ion radiobiology experiments. Special methods at the particle accelerators apply to both basic and applied research. The live-cell imaging beamline is a unique facility allowing direct visualization of protein recruitment kinetics at sites of DNA double-strand breaks (DSBs) induced by heavy ions at GSI. The study of repair protein kinetics are performed in other laboratories using lasers, but the laser-induced DNA lesions are different from the DSB induced by ionizing radiation or other clastogenic agents. The method allows the identification of the recruitment kinetics of different proteins, their exchange rate at the repair site (using FRAP), the interaction of difference proteins (using FRET and FLIM), and the mobility of the repair sites. Unique infrastructures are available as well for applied nuclear-physics studies. The very high energy of ions as heavy as ^{56}Fe enables a simulation of the energetic cosmic radiation on Earth. The GSI facilities were indeed selected by ESA to carry out ground-based space radiation investigations. The spot scanning delivery, the possibility of accelerating any light ion, the online PET for treatment plan verification, and the capability of handling moving targets make GSI the ideal setup for preclinical studies in heavy-ion therapy. In PoF IV, FAIR will take up operation. The new facility will open up new exciting opportunities not only in hadronic and atomic physics, but also in biomedical applications [8]. In fact, the extremely high energies (up to 10 GeV/u) of FAIR make the accelerator potentially able to simulate the galactic cosmic radiation in a more accurate way than any other ground-based facility worldwide. The high intensity opens up new opportunities for studies in next-generation particle therapy, including grid therapy, flash (ultrahigh dose rate) irradiation, and image-guided therapy with radioactive ion beams (positron emitters such as ^{10}C or ^{11}C that can be visualized by PET). FAIR will therefore be the most advanced new tool for R&D into biomedical applications of heavy ions worldwide. In addition to the GSI accelerators, HZB operates Germany's only proton therapy facility for intra-ocular tumours – one of about a dozen dedicated facilities worldwide. At HZB, more than 3.500 patients have been treated so far.

Objectives and Approach

Molecular movies: The function and behavior of biological molecular systems, complex fluids, and soft matter will be studied using X-ray sources with unprecedented brilliance and peak brightness. These new sources and associated measurement technologies have opened up new application fields by giving the ability to capture structural information through coherent scattering measurements and electronic states through spectroscopy, all with femtosecond shutter speeds to track concerted motions involved in reactions such as binding or fragmentation. Such measurements are often referred to as "molecular movies". Analysis of time-resolved structures of macromolecules at room temperature will be applied to study the influence of water in biochemical reactions, the anomalous properties of water and the role of solvation in biomolecular structures [RT3-5]. These developments will also be used to obtain landscapes of conformations, influenced by factors such as temperature, binding partners, or environment. Big-data measurements allow the discovery of rare events and associations between structures.

Biological processes are driven by interactions between molecules. We aim to elucidate the fundamentals of complex chemical reaction mechanisms in real-time studies of energy conversion and of structural dynamics processes, i.e. in encounter complexes built from amino acids/proteins and small-molecule units, which are selectively triggered or optimized for specific functions [RT3-4]. Such reactions will be followed both in solution and in the gas phase (see below). These studies will contribute to the field of energy conversion (biomolecular electronics), to structural dynamics of peptidomes (the complete set of peptides produced by an organism), and to structural dynamics of small-molecule pharmaceuticals.

During PoF IV, the European XFEL will operate at full capacity, providing experimental data collection rates hundreds of times greater than previously possible. This facility and the associated instruments have a profound impact on our approach and motivate further developments of methods that we pioneered in the PoF III period. We will further develop short-exposure pink-beam serial crystallography at PETRA III (and later PETRA IV) using high-frame-rate detectors at a fully automated experiment end-station [9]. The increased repetition rates extend our studies to the real-time measurement of dynamics of nanoscale materials (rather than the diffusion-controlled time scales between nanoscale entities) and systems characterized by structural heterogeneities and out-of-equilibrium conditions. Likewise, correlation and multidimensional X-ray spectroscopy methods [10] will be extended for research into the real-time dynamics of complex biochemical systems and reactions (Figure 12 left). Earlier "proof-of-concept" diffraction and spectroscopy approaches will now provide high enough statistics and sensitivity for studying the real-time transformations during chemical reactions under meaningful (and transient) conditions. Studies of the structure and nanoscale dynamics of disordered systems (including water, Figure 12 right) will greatly benefit from these improvements, utilizing X-ray photon correlation spectroscopy and X-ray cross-correlation analysis [RT3-3]. The capabilities open up the use of higher-order intensity correlation functions and tailored pulse structures to achieve a more complete understanding of the properties of disordered soft condensed matter model systems. A strong cooperation with MT-DMA will be pursued to devise hardware and software solutions to the "data deluge" and to build the computation into the experiment design. These activities will also be supported within the upcoming Centre for Molecular Water Science (CMWS) in Hamburg (see Infrastructures, below).

Serial crystallography: In addition, the upcoming increased technical capabilities and high data rates will be transferred to improve serial crystallography [RT3-2] in order to measure conformational dynamics of proteins and non-equilibrium dynamics of the interactions of proteins with molecules, connecting to the electronic dynamics that drives the molecular response. As with XFEL measurements, the increase in throughput not only improves the measurement of the response of protein nanocrystals to reactants, but also the extraction of rare events [RT3-4]. Through external collaborations, we will measure the evolution of photosystems and signaling proteins. Together with HZB and partners within the Research Field *Health*, serial crystallography is being further adapted for drug research. This is supported in the framework of the Innovation Pool project SX-FragS. Serial crystallography allows measurements of non-perfect and disordered crystals. We aim to further develop the analysis of the diffraction of imperfect macromolecular crystals to obtain model-free reconstructions of the molecular electron density and to refine ensembles of conformers of structures. This powerful idea of utilizing the imperfections of crystals to gain additional structural and dynamic information will be further pursued by inducing such irregularities (e.g. by strong THz excitation). In order to gain full insights into macromolecular conformational dynamics, we will exploit the full imaging capabilities at X-ray FELs without necessarily requiring crystalline samples. The needed sample preparation and image analysis techniques will be developed in close cooperation with cryo-electron microscopy, by cooperation with the Center for Structural Systems Biology (CSSB) at DESY.

Single-crystal crystallography: Existing capabilities will be extended towards high-throughput single-crystal crystallography with full automation of the respective facilities at BESSY II. With such beamlines becoming operational soon, compound screening by X-ray crystallography will become a new, feasible, and robust (user) experiment. It is envisioned that, within less than one week, several hundred diffraction data sets on macromolecule crystals treated with compounds from a highly diverse chemical library will be collected. This will open avenues towards functional investigations of these macromolecules as well as towards early-stage drug discovery approaches. Given the fact that the current druggable genome is still small and requires the collective efforts of many researchers to be enlarged, this development has the potential for significant scientific and societal impact.

Radiation-induced effects in the gas phase: Mass spectrometry will be combined with ion mobility and can be coupled to synchrotrons, free-electron lasers, and ion beamlines, as shown exemplarily in Figure 15 [11]. We will study radiation effects in biomolecules as a function of ultrahigh dose rates, energy, site-selective absorbers (e.g. radiosensitizers), and secondary electrons. In addition, well-defined water molecules will be attached to the gas-phase systems in order to systematically record the influence of water on radiation damage, e.g. by radicals, structural changes, or increased energy capacity.

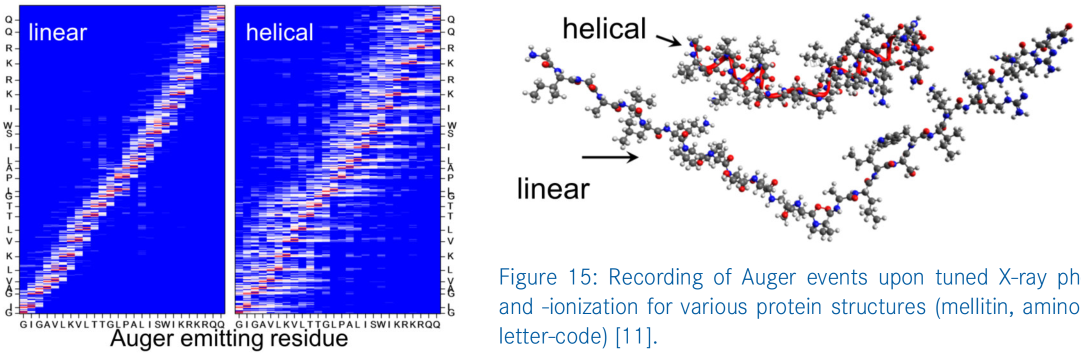


Figure 15: Recording of Auger events upon tuned X-ray photoexcitation and -ionization for various protein structures (mellitin, amino acid in one-letter-code) [11].

In collaboration with the Topic MML-Matter (Sec. 2.2.1), the effects of the extreme intensities of X-ray FEL pulses on matter will continue to be explored in order to understand the limits of biological imaging. Using large-format multilayer Laue lenses, we aim to focus the beam to intensities beyond 10^{22} W/cm^2. While this will increase diffraction signals, the electronic structure will be severely disrupted, even with femtosecond-duration exposures. We will explore whether the ground-state structure can still be recovered from such measurements.

Imaging of cells, tissues, and organisms: On higher hierarchical levels, we will study morphology, morphodynamics, and function of cells [RT3-9], tissues, organs, and complete specimens. We aim to understand the interrelation between morphology and biochemical pathways, the genotype–phenotype correlation, and reactions to biotic and abiotic natural factors. These studies require systematic quantitative image analyses of body, organs, and tissues and their correlation with molecular, genetic, and environmental information. The methodological objectives are dedicated modalities for 2D and 3D digitization of small-animal morphology by synchrotron imaging allowing advanced measurement, visualization, and AI-supported analysis of 3D morphological data sets, e.g. segmentation and morphometrics. These developments require instrumentation, measuring methods, and analysis tools for (a) high-resolution and correlative cell imaging, (b) automated high-throughput full-animal imaging, (c) hierarchical imaging through various levels down to cells, (d) correlative approaches for different contrasts and probes, and (e) *in-situ*, *ex-vivo*, and *in-vivo* radiography, cine-tomography, and time-lapse imaging.

Further challenges are related to dose efficiency, signal-to-noise ratio, flexible field of view, spatiotemporal resolution and automated analysis. For this, we will build on compiling dedicated and complementary approaches, methods, instrumentation, and software developed by the partners and collaborators at BESSY II, GEMS, KARA, and PETRA III, enabling comprehensive data acquisition, handling, and analysis pipelines.

Cell and tissue imaging: Understanding the interaction of macromolecules in the cellular context requires cell imaging at a spatial resolution high enough to identify those molecules, their assemblies, or specific labels of those objects. To complement live-cell fluorescence optical microscopy (which only shows specific components) and cryo-electron tomography (which only allows limited sample thickness), we will develop a new method of low-dose X-ray microscopy based on Compton scattering at 60 keV and multilayer Laue lenses, pushing the resolution to approach 1 nm, which is high enough to identify ribosomes, infectious agents and nanoparticles. Using FIB-SXM microscopy, we will image the 3D cellular ultrastructure of native tissue with natural soft X-ray contrast for all cytoplasmic organelles. To connect the cellular ultrastructure with specific molecular functions, we will combine FIB-SXM at BESSY II with correlative super-resolution fluorescence microscopy [RT3-6]. This will allow the precise localization of important biomolecules in order to understand their role in cellular functions, study nanoparticle uptake by specific tissues in whole animals (Figure 14 E), and correlate this with specific molecular markers that could be altered by the nanoparticles. Hard X-ray studies of 3D scaffold morphology and of the 3D arrangement of single cancer cells in the tissues will enable the 3D visualization of prostate cancer cells cultured in cryogel under treatment with different signaling molecules, such as dihydrotestosterone, which affects the cellular proliferation.

Full animal imaging for studies of phenotype–genotype correlations: We will focus on the vertebrates medaka (*Oryzias latipes*) and South African clawed frog (*Xenopus laevis*), which are important model organisms to study development and disease (in cancer research, toxicology, developmental biology, and genetics) and are essential for preclinical studies and the development of drugs. By correlating morphology/morphometrics to molecular data, e.g. between *different* medaka breeding strains, we can characterize the function of specific *genes* for the development of the respective phenotypes (Figure 14 A, B). In contrast, by comparing the morphology of genetically virtually identical individuals within a *single* breeding strain, we can describe the influence of *external factors*, such as environment, nutrition, and medication on phenotype development. We will learn about the relationship between the genome, its morphological manifestation, and resulting organ function, and finally the effects of genetics and the environment. Finally, we plan 4D *in-vivo* studies of environmental and genetic influences on cell movement and tissue formation in *Xenopus* mutants during various embryonic stages (Figure 14 D).

Full animal imaging for studies of morphology and ecology of arthropods, in particular insects and spiders: With over one million described species, insects are by far the largest group of organisms, which fulfill key functions in our ecosystems. Although insect decline has been apparent for decades, its true extent and the associated consequences of decreasing biodiversity are still unclear. However, the relative wealth of genetic data collected in recent years is hardly matched by comparative 3D morphological information. We will focus on quantitative morphology of highly diverse insect groups such as beetles and parasitoid wasps (Figure 14 C), comprising up to 20% of all insects. As antagonists of a wide variety of arthropods, they have profound ecological and economic impact, and many species are used as important biological pest control agents. Arthropod functional morphology is another important aspect of research. Spiders can walk on glass surfaces upside down thanks to their hierarchical adhesive hair system, which is superior to artificial systems due to its high sustainability and persistence. Its morphology–function relation will be revealed by *in-situ* multiple contrast imaging during mechanical testing [RT3-7].

3D digitization of very large scientific collections: We plan dedicated high-throughput pipelines establishing reliable sample preparation, DAQ, and analysis protocols as a precondition for AI-supported morphological and hierarchical imaging of large sample series (Figure 14) at PETRA III [RT3-8]. In collaboration with Heidelberg University, we will establish the Di-Morph Facility as a smart repository for 3D morphological studies, which will combine AI and human knowledge of the scientific community to evaluate and interpret morphological data in correlation with genetics and the environment and to make results available to the public.

External stressors and translational research: Our basic research on the interaction of radiation with living cells will address the question: What are the molecular mechanisms of DNA damage repair after exposure to densely ionizing heavy ions? Heavy ions produce clustered DNA DSBs, which are generally considered the most important lesions leading to late effects, from cell death to mutation and transformation. Using our unique beamline live-cell imaging facility at GSI, we have already demonstrated that human cells resort to alternative repair pathways, such as resection, to resolve complex DSBs (Figure 16, [12]). Our working hypothesis is that heavy ions elicit different repair pathways than X-rays [RT3-10], and that we will be able to identify potential molecular targets for radiosensitizing tumor cells (in therapy) or protecting normal tissues (in therapy and space) [RT3-10].

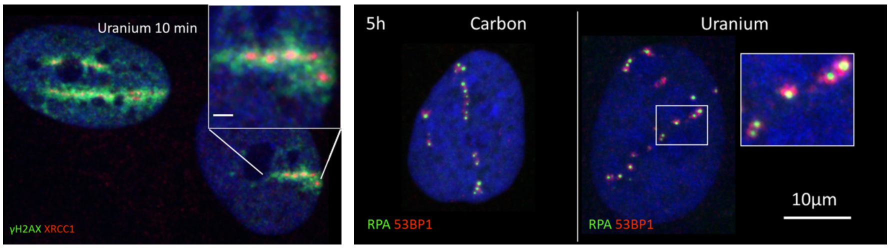


Figure 16: Response of biological systems to external stressors and stimuli and their interaction. Tracks of heavy ions in nuclei of human cells visualized by co-localization of DNA repair enzymes [12].

Heavy-ion-induced effects: The effects of heavy ions at the molecular level have a direct impact on studies at the cellular, tissue, and animal level. Having investigated the cellular effects of heavy ions in the past, in PoF IV we will focus on organoids built from human embryo stem cells. We are now growing brain and heart organoids, which represent highly innovative models for studying the effect of heavy ions on the central nervous system and the cardiovascular system, a subject that is highly relevant for both therapy and space. Organoids are unable to simulate the immune system interaction with the tissue microenvironment, however, and we will thus extend our investigations to mouse models in order to study the immune response to densely ionizing radiation compared to X-rays. This basic radiobiology problem has an enormous impact in translation, considering the many protocols using radiotherapy and immunotherapy employed these days in clinical application, in particular at DKFZ/HIT with heavy ions.

Particle cancer therapy: Radiobiology within MML-Life can be applied into two fields: cancer therapy (in collaboration with DKFZ, HZDR, and HMGU in the Cross-Cutting Activity *Radiation Research*) and space radiation protection (with ESA and DLR). Translational research in cancer therapy involves both radiobiology and medical physics. In radiobiology, the combination of particle therapy with immunotherapy will be tested in pre-clinical mouse models. In close collaboration with DKFZ/HIT, we will extend our previous radiobiology studies with carbon ions to new projectiles that will be used in the Heidelberg clinics in the future: helium, which is ideal for pediatric tumors, and oxygen, which can be used for very radioresistant, hypoxic cancers. We have patented and tested a special cellular phantom that can be used to test treatment planning under normal oxygenation or hypoxia. This phantom will be used to provide the necessary pre-clinical data to Heidelberg Ion Therapy (HIT) center for the implementation of ^{4}He and ^{16}O in cancer patients. The combination of different light/heavy ions (e.g. H+C or He+O) will also be explored, as these techniques can allow both safety for normal tissue and aggressive boosts to radioresistant regions [13]. Research in medical physics will be a further key activity for translational research in particle cancer therapy. Based on our consolidated expertise in the treatment of moving targets with scanned beams, in PoF IV we are planning to establish a 4D treatment planning system in particle therapy. This will allow us to optimize treatment by taking movements of the tumor into account, which will enable treatments of thoracic cancers or of ventricular fibrillation by non-invasive particle therapy (Figure 17 right, [14]). Close cooperation with the Charité – Universitätsmedizin Berlin permits joint interdisciplinary research in proton therapy. We will study material modification of artificial lenses with typical doses used in the proton treatment of uveal melanoma as well as possible side effects of proton therapy using ambulant mouse irradiations, including Class I gene-modified mice [RT3-12]. The experiments will also include the improvement of high-resolution proton dosimetry.

Space radiation protection: The simulation of galactic cosmic radiation for space radiation protection studies will be carried out using high-energy ion beams. So far, tests of shielding materials and radiobiology studies for radiation risk estimation for astronauts have been performed with single high-energy heavy ions (in the USA at Brookhaven National Laboratory and in Europe at GSI (Figure 17 left and middle, [15])). We now propose a hybrid active–passive system, where different energies of a single heavy ion (e.g. ^{56}Fe) are modulated with a 3D-printed ridge filter to produce radiation spectra similar to those found in space (either on a spacecraft or on a planetary base) [RT3-13]. At FAIR, with energies extending to 10 GeV/u, the galactic cosmic-ray simulator will be able to cover the hard part of the energy spectrum, which is of great importance due to its biological effects and its potential damaging impact on microelectronics. In close collaboration with MML-Materials, this facility will make FAIR the best ground-based simulator of galactic cosmic rays worldwide. The simulator will be used to test microelectronics for radiation hardness (especially commercial off-the-shelf components), new shielding materials for protection of crews and instrumentation, and biological targets for risk assessment. The biological systems described above will be exposed at low doses to quantify the risks in long-term interplanetary missions, especially Mars missions. We will focus on non-cancer effects, especially the central nervous system and cardiovascular risks that can be simulated with our organoids. Radiation hardness testing using protons and a ^{60}Co-source are performed at HZB in collaboration with DLR.

Figure 17: Translational research. Radiation shielding for a Moon or Mars base (middle) can be tested at accelerators using high-energy heavy ions (left: Martian regolith [15]). Right: Carbon ion exposure of a swine heart for pre-clincial testing of non-invasive treatment of atrial fibrillation [14].

Expected Results

The sketched work program translates into a number of milestones that are well suited for monitoring the progress of the Topic. These are shown in the following table.

Table 4: Overview of milestones for the Topic.

	Milestone	Year
RT3-1	Concluding first 1,000-compound crystallographic screening experiment	2022
RT3-2	Demonstrating measurement of non-equilibrium protein dynamics via pink-beam serial crystallography	2022
RT3-3	Developing new coherence-sensitive X-ray methods to study the nanoscale dynamics of water and liquids	2024
RT3-4	Studying complex (bio-)chemical and prebiotic reactions in real time	2026
RT3-5	Developing ultrafast high-flux X-ray methods for biochemical reactions in water as life-supporting liquid matrix in (bio-)chemistry	2024
RT3-6	Combining FIB-SXM with correlative super-resolution fluorescence microscopy	2025
RT3-7	Implementing nano-indentation for *in-situ* nanotomography during biomechanical testing	2022
RT3-8	Performing high-throughput and hierarchical small-animal imaging	2024
RT3-9	Demonstrating 3D nanometer-resolution imaging of a cell	2025
RT3-10	Studying DNA repair pathways in the core and penumbra of a heavy-ion track	2022
RT3-11	Determining appropriate materials for artificial lenses in ocular proton therapy	2022
RT3-12	Performing dose studies on radiation retinopathy and combined treatment of radiotherapy and immunotherapy in mice	2023
RT3-13	Building and commissioning a ground-based galactic cosmic ray simulator	2025

Synergies and Collaboration

Serial crystallography and biological imaging are developed in collaboration with European XFEL (primarily with the Serial Femtosecond Crystallography (SFX) user consortium). The development of “molecular-movie” methods for elucidating (bio-)chemical reactions and their driving forces and the investigation of the impact of high X-ray intensities is performed in close collaboration with the Topic MML-Matter (including the international Heisenberg RIXS consortium). Applications of these methods towards biomimetic uses are developed together with the Topic MML-Materials and the Research Field *Energy*. Some cross-topical developments within the Helmholtz Association (between MML and the Research Fields *Energy* and *Health*) and within MML (to the MML topics Matter and Materials) will be pursued within the newly initiated Centre for Molecular Water Science (CMWS) in Hamburg (see Infrastructures, below). The smart repository for 3D morphological studies of organisms at the Di-Morph Facility will be established together with Heidelberg University. The activity on accelerated charged particles is part of the Cross-Cutting Activity *Radiation Research*, which includes eight Helmholtz Centers from the Research Fields *Matter*, *Health*, *Energy*, *Information*, and *Astronautics, Space and Transport*. Formal research collaborations exist between HZB and Charité; and between GSI and DKFZ, HZDR, and DLR. Serial-crystallography and imaging activities will be part of the Cross-Cutting Activity *Structural Biology and Biological Processes*, in cooperation with HZB and MDC from the Research Field *Health*.

Infrastructures

The photon sources PETRA III, BESSY II, and European XFEL provide X-ray beams of highest brilliance, peak brightness, and coherence. They are crucial to MML-Life for developing methods for soft-condensed-matter, water, (bio-) chemical, and structural-biology research, such as X-ray spectroscopy and X-ray-based biological imaging. In the field of structural biology, the existing beamlines provide automated high-throughput crystallography, and a new serial-crystallography end-station is being planned for PETRA III. In the field of time-resolved X-ray research, three beamlines are dedicated to the needs of soft-matter, chemical, and water research in MML-Life. We will build the HIKA experimental station, thereby transferring high-throughput and hierarchical imaging technology from KARA to PETRA III. For nanoscale 3D imaging, a new FIB-SXM microscope will be established at BESSY II. Research into the properties of water and its role in macromolecular function will be supported by the CMWS, which was recently founded at DESY. The radiation research activity is world-leading thanks to the outstanding accelerator infrastructures available, in particular UNILAC and SIS18 at GSI, the proton accelerator used for therapy at HZB, and, towards the end of PoF IV, SIS100 at FAIR.

Opportunities and Risks

The Topic MML-Life strongly benefits from and depends on the reliable operation of the involved large-scale facilities and instruments. Obviously, malfunctions or delays in the completion of the main infrastructures may affect the outcome of our research program. Significant new opportunities will arise with the upcoming startup of FAIR and the planned PETRA IV source, which, together with the European XFEL and the other involved sources, will strengthen Germany’s world-leading position in large-scale-facility-based life science experiments.

The efficiency of data acquisition, transfer, handling, and analysis (e.g. segmentation) is presently the bottleneck for the processing of large sample series. We will address this challenge by developing automated, AI-based high-throughput imaging, crystallography, and spectroscopy strategies for measurements and data analysis, which will enable the digitization and interpretation of huge biological sample series with tremendous increase in efficiency, accuracy, and reliability. Smart repositories linking large-scale facilities with data centers and the science communities will additionally enhance the impact of the life sciences within MML.

3. PROGRAM ORGANIZATION

3.1. Strategic Partners and Cooperation

The Program MML utilizes a broad portfolio of instruments to establish new forms of partnerships and deepen cooperation with already existing partners. Universities are the main cooperation partners from academia within MML, in particular for the (joint) education of Ph.D. students and junior scientists through the establishment of joint professorships and research groups, e.g. at the universities HU Berlin, TU Chemnitz, TU Clausthal, TU Cottbus-Senftenberg, Freiburg im Breisgau, Leoben (Austria), Lübeck, Marburg, MEPhI Moscow (Russia), Potsdam, and KTH Stockholm (Sweden). The strategic university partners provide essential contributions for the Program to fulfill its mission (see Table 5). The scientists from MML cooperate closely with their university colleagues in the framework of collaborative research centers (SFBs and Transregio) and of clusters of excellence in the German Excellence Initiative. In addition, they may organize and operate common research institutes and laboratories as well as networks of joint research and education projects.

A dedicated funding scheme from the BMBF ErUM framework program enables university partners to develop and perform innovative experiments at the MML large-scale facilities (currently about 150 funded projects). Several Helmholtz Young Investigator Groups, Helmholtz Graduate Schools, and other projects for networking with national and international partners have been acquired from the Helmholtz Initiative and Networking Fund in the context of the Program MML, crosslinking the research foci of several Helmholtz Centers, universities, and third parties.

Table 5: Strategic university partners of MML listed in alphabetical order.

University	Topics/Facilities	Activities
RWTH Aachen	MML-Materials, Photons, Neutrons	Jülich Aachen Research Alliance JARA; common operation Heidi, POLI at MLZ, construction of POWTEX at MLZ, JARA-SOFT, JARA-FIT, SFB 917 *Nanoswitche*s, SFB 985 *Functional microgels*
Berlin University Alliance (FU, HU, TU, Charité)	MML-Materials, MML-Life, Photons	Joint professorships, joint research groups, Joint MX Laboratory, CRC/Transregio 227 *Ultrafast Spin Dynamics,* joint research for proton therapy
Bayreuth	MML-Materials	Research Training Group 1640, SFB 840 *From particle nanosystems to meso-technology*, SFB/Transregio 225 Biofab
TU Darmstadt	MML-Matter, MML-Materials, MML-Life, Ions	Joint professorships, Extreme Matter Institute, Helmholtz Graduate School HGS-HIRe, Helmholtz International Center for FAIR
TU Dresden	MML-Matter, MML-Materials, Neutrons, Highest Fields	Joint professorships, joint research groups, DRESDEN concept, SPP 1681 *Field controlled particle matrix interaction*, MoU Moderator development, clusters of excellence *Quantum Matter* and *Physics of Life*, SFB 1143 *Correlated Magnetism*, joint laboratory Felsenkeller
Frankfurt	MML-Matter, Neutrons	Joint professorships, Extreme Matter Institute, Helmholtz Graduate School HGS-HIRe, Helmholtz International Center for FAIR, MoU Accelerator development HBS

Gießen	MML-Matter, Ions	Helmholtz Graduate School HGS-HIRe, Helmholtz International Center for FAIR
Göttingen	MML-Life	Joint professorships, joint research groups, SFB 1073 *Atomic scale control of energy conversion,* SFB 755 *Nanoscale Photonic Imaging*
Hamburg	MML-Matter, MML-Materials, MML-Life, Photons	Joint professorships, joint research groups, Partnership for Innovation, Education and Research (PIER), Center for Free-Electron Laser Science, PIER Helmholtz Graduate School, Graduate School of the Hamburg Centre for Ultrafast Imaging, cluster of excellence *Advanced Imaging of Matter*, Data Science in Hamburg – Helmholtz Graduate School for the Structure of Matter, SFB 986 *Tailor Made Multi-Scale Materials Systems*, SFB 925 *Light induced dynamics and control of correlated quantum systems*, Centre for Structural Systems Biology, Klinikum Hamburg-Eppendorf (UKE)
TU Hamburg-Harburg	MML-Materials	Joint professorships, joint research groups, Centre for Advanced Materials (ZHM), ZHM Graduate School for Materials Science, SFB 986 *Tailor Made Multi-Scale Materials Syste*ms
Heidelberg	MML-Matter, MML-Materials, MML-Life	Joint professorships, joint research groups, Helmholtz Graduate School HGS-HIRe, Di-Morph Facility, HiKA collaboration
Jena	MML-Matter	Helmholtz Institute Jena, joint professorships, joint research groups, cluster of excellence *Balance of the Microverse,* Helmholtz Graduate School HGS-HIRe, Research School of Advanced Photon Science
Kiel	MML-Matter, MML-Materials, Photons, Neutrons	Joint professorships, joint research groups, GEMS, Center for X-ray and Nano Science, Ruprecht Haensel Laboratory
TU München	MML-Materials, MML-Life, Neutrons	Heinz Maier-Leibnitz Zentrum (MLZ)
Potsdam	MML-Matter, MML-Materials, Photons	Joint professorships, joint research group
Nevada Las Vegas, USA	MML-Materials	Joint professorships, cooperation on soft X-ray spectroscopy
Uppsala, Sweden	MML-Materials, Photons	Uppsala–Berlin joint Laboratory to develop and use X-ray-based methodology

The main non-university strategic partners of MML are the Max Planck Society (MPG) and the Physikalisch-Technische Bundesanstalt (PTB), the German national metrology institute. These partners have established research groups at various MML facilities, operating several beamlines and end-stations as well as common institutes. For an overview of existing collaborations with strategic non-university partners, see Table 6.

Thanks to the long-standing networks and the exchange of expertise among the large-scale research facilities worldwide, the Program MML is well positioned in the international context, as highlighted for instance by its leading involvement in the international projects European XFEL, ESS, and FAIR. Furthermore, with regard to the future development of photon sources, a common national and coordinated strategy roadmap process has been initiated at the European level within the framework of the League of European Accelerator-based Photon Sources (LEAPS), which comprises 18 partner institutions. For neutrons, the League of advanced European Neutron Sources (LENS) was founded to integrate the neutron community, in which MML plays an active role. Moreover, a number of binational cooperations have been established.

Table 6: Strategic non-university partners of MML listed in alphabetical order.

Partner	Topics/Facilities	Activity
CEA, ILL Grenoble, France	MML-Materials, MML-Life, Neutrons	German shareholder of ILL (33%); operation of three neutron instruments; joint research programs
EMBL	MML-Life, Photons	Contributions to beamlines at PETRA III, outstation at DESY
EMFL	Highest Fields	Distributed research infrastructure (ESFRI landmark; four large-scale high-magnetic-field user laboratories in Europe: HLD, LNCMI Toulouse, LNCMI Grenoble, HFML)
ESA	MML-Materials, MML-Life, Ions	ESA test laboratory for cosmic radiation with high-energy ions
ESS	MML-Materials, Neutrons	Construction of instruments: T-REX, DREAM, SKADI, MAGIC, contribution to target station
ESRF	MML-Matter, MML-Materials, MML-Life, Highest Fields	Collaboration in High Power Laser Facility project, KIT Laminostation
FAIR	MML-Matter, MML-Materials, MML-Life, Ions	Construction and operation of APPA experimental areas for MML research and APPA collaboration
IFW (Dresden)	MML-Materials, Highest Fields	Collaboration at HLD, Cluster of excellence *Complexity and Topology in Quantum Matter*, SFB 1143 *Correlated Magnetism*
JNCASR, India	Photons	Contributions to beamlines at PETRA III
MPG	MML-Matter, MML-Materials, MML-Life, Photons, Highest Fields	Close collaboration to study the electronic structure of liquid water and aqueous solutions, theory support in the field of frustrated magnetism, collaboration at HLD, contributions to beamlines at PETRA III and BESSY II, Research Training Group (GRK 1631), SFB 1143 Correlated Magnetism, Center for Free-Electron Laser Science, Excellence Cluster *Advanced Imaging of Matter*; Excellence Cluster *Complexity and Topology in Quantum Matter*
ORNL, USA	MML-Materials, Neutrons	Neutron science, advanced materials (energy), supercomputing
PNPI, Russia	Neutrons	Instrumentation at new neutron source (PIK reactor)
PTB	MML-Matter, MML-Materials, Photons	European metrology standards for VUV and EUV radiation, close cooperation on metrology and on the development of BESSY II source and instrumentation
RIKEN, Japan	Neutrons	Compact accelerator-based neutron sources
Russian-German Laboratory	Photons	Contributions to beamlines at BESSY II
Swedish Research Council	Ions, MML-Matter, Photons	CRYRING at GSI and contributions to beamlines at PETRA III
European XFEL	MML-Matter, MML-Materials, MML-Life, Photons, Highest Fields	Helmholtz International Beamline: SFX, HIBEF, hRIXS; HIBEF user consortium

3.2. Infrastructures

For our MML research based on large-scale infrastructures, we currently exploit the following facilities:

Table 7: Existing large-scale research infrastructures (> 2.5 million euros) listed in alphabetical order. Facilities indicated with an asterisk (*) have relevant contributions also in other programs of the Research Field Matter and will therefore also be listed there.

Facility	Center(s)	Description (year of first operation in brackets)
BESSY II* VSR	HZB	Germany's synchrotron radiation facility optimized for experiments in the spectral range of soft to tender X-rays (1999)
Cyclotron HZB	HZB	Accelerator serving as a source for proton therapy and radiation research (1998)
DRESDYN	HZDR	DREsden Sodium facility for DYNamo and thermohydraulic studies (2020)
ELBE*	HZDR	Superconducting CW accelerator serving as a driver for multiple secondary beams (MeV photons, IR, THz, positrons, neutrons) and high-power laser systems (1 PW) DRACO and PENELOPE (2004/2008)
ESR Complex	GSI	Central ion storage ring ESR (1990) with its extensions, the trapping facility HITRAP (2013) and the low-energy ring CRYRING (2019)
FLASH*	DESY	Free-electron laser (FEL) operating in the VUV and soft X-ray regime with two FEL lines in parallel with independent photon beam parameters (2005)
Helmholtz International Beamline (HIB)	DESY, HZDR	Instrumentation and contribution to the user consortia SFX (Serial Femtosecond Crystallography), HIBEF (Helmholtz International Beamline for Extreme Fields) and hRIXS at the European XFEL (approx. 2019)
HLD	HZDR	High-magnetic-field facility generating highest possible non-destructive pulsed magnetic fields (2007)
IBC	HZDR	Ion beam facility for materials and interdisciplinary research (1992)
JCNS	FZJ	Jülich Centre for Neutron Science with outstations and instrumentation at MLZ, ILL, and SNS (2006)
Karlsruhe Research Accelerator KARA*	KIT	Synchrotron radiation delivery to beamlines for experiments with radiation ranging from IR to intermediate-energy X-rays (2015, ANKA since 2000)
Laser platform	DESY	Development of high-repetition-rate, high-power short-pulse lasers. Includes laser systems for attosecond science and for pump–probe experiments at FLASH (2016)
MML@GSI	GSI	Various MML ion beam (single-pass) experimental areas at UNILAC (1975); SIS18 (1990) and PW-class high-power laser system PHELIX at UNILAC (2008)
DESY NanoLab instrumentation	DESY	DESY NanoLab provides methods complementary to photon facilities; new instrumentation within the Centre for X-ray and Nano Science (approx. 2020)
PETRA III	DESY, HZG	Third-generation synchrotron radiation source with high brilliance, mainly for experiments in the hard and high-energy X-ray range (2010)
High Power Laser Systems*	HI Jena	High-power laser systems (JETI200 and POLARIS) with dedicated experiment infrastructure and metrology (2010 and 2015)
Soft X-ray laser facility HZB	HZB	Ultrashort-pulse laser-driven soft X-ray facility to selectively probe molecular dynamics on chemically relevant time scales (under commissioning, 2021)

A particular challenge is to pursue upgrade plans for our large-scale facilities in order to maintain and enhance the world-leading capabilities and to stay at the forefront of science. Currently, the following upgrade plans of the large-scale research infrastructures are under discussion, planned, or under construction (see tables 8 and 9). For details, we refer to volume III, section C "*From Matter to Materials and Life*". The investment numbers are current estimations. Note, in general projects with investments below 15 million € (table 8) are financed via the base budget of the centers whereas larger investment projects require consent of the Helmholtz General Assembly. Under 'Helmholtz Investment' all Helmholtz project contributions including investment contributions from the base funding of the centers are summarized.

Table 8: Planned large-scale research infrastructures (2.5 – 15 million €) listed in descending order of investments. In the column "Description", the numbers in the brackets refer to the anticipated construction and implementation period. Column "Planned Start of Operation" refers to the full implementation and full operation of the specific infrastructure. Facilities indicated with an asterisk (*) have relevant contributions also in other programs of the Research Field Matter and will therefore also be listed there. Please note the used notation which applies to the entire proposal: Costs are given in thousand euros, and for all numbers the thousands separator is a dot, and the decimal separator is a comma.

Name	Contributing Centers	Helmholtz Investment (Total Project) in TEUR	Planned Start of Operation	Project Status	Description
BESSY II Modernization (accelerator, beamlines, infrastructures)*	HZB	18.000 (18.000)	2026	Advanced planning, ready to start *(fund.)*	Modernization (accelerator, beamlines, infrastructures). (2021-2026)
Beamline & end station upgrades for VSR	HZB	10.000 (10.000)	2027	Advanced planning (*fund.*)	Adaption and upgrades a necessary to make full use of BESSY VSR. (2021-2027)
Engineering Materials Science Centre (EMSC)	HZG	4.700 (4.700)	2021	Under construction (*fund.*)	HZG-part of the Center for X-ray and Nanoscience (CXNS) building at DESY. (2018-2021)
DREAMS extension at IBC	HZDR	3.500 (3.500)	2022	Proposal submitted (*prop.*)	Increases of competences and corresponding capabilities of the IBC in the field of AMS. (2021-2022)
***In situ*- und in *operando* sample environment (INSO)**	HZG	3.125 (3.125)	2022	Preparation phase (*fund.*)	*In situ*- and in *operando* sample environment. (2020-2022)
IT Infrastructure (e.g. implementation Open Access to Data)	HZB	3.000 (3.000)	2025	Advanced planning (*fund.*)	Investments in IT-infrastructure are required to cope with the rising needs in open data and open science. (2021-2025)
Pilot projects water research including instrumentation	DESY	2.700 (2.700)	2026	Advanced planning (fund.)	Instrumentation for pilot projects in the frame of the Centre for Molecular Water Science (CMWS). (2020-2026)

** Continuous allocation of in-house investment funds; no participation in competitive call at the level of the Helmholtz Association.*

Table 9: Planned large-scale research infrastructures (> 15 million €) listed in descending order of investments. In column "Description", the numbers in brackets refer to the anticipated construction and implementation period. Column "Planned Start of Operation" refers to the full implementation and full operation of the specific infrastructure. Facilities indicated with an asterisk (*) have relevant contributions also in other programs of the Research Field Matter and will therefore also be listed there.

Name	Contributing Centers	Helmholtz Investment (Total Project) in TEUR	Planned Start of Operation	Project Status	Description
PETRA IV	DESY, HZG	100.000 (552.000)	2027	Preparation: TDR/feasibility study (*prep.*)	Upgrade of PETRA III into an ultra-low emittance source in the harder X-ray regime. (2021-2027)
BESSY III	HZB	50.000-60.000 (490.000)	2030	CDR in preparation (*prep.*)	Next generation soft and tender X-ray light source. (2027-2030)
DALI*, the Dresden Advanced Light Infrastructure	HZDR	tbd (180.000)	2030 (commissioning 2029)	Preparation phase (*prep.*)	Conception of a follow-up of the ELBE facility (pulsed IR to THz source, VUV option under discussion). (2023-2028)
HBS Prototype	FZJ HZG	45.000 (50.000)	2028	Preparation: CDR, TDR (*prep.*)	Prototype for a High Brilliance neutron Source. (2021-2028)
ESS Instrumentation	FZJ HZG	32.900[1] (32.900)	2024	(Preparation for) construction phase *(fund.)*	Instrumentation FZJ: DREAM, MAGIC, SKADI, T-Rex (25,8 Mio €); Instrumentation HZG: BEER (7,1 Mio €). (2020-2024)
MLZ2030 Upgrades of instrument suite at FRM II	FZJ HZG	30.000[2] (30.000)	2030	Positively evaluated; pending on MLZ contract prolongation *(prop.)*	Upgrade, renewal and extension of instrument suite at MLZ. (2021-2030)
PIK User Platform	FZJ HZG	up to 30.000 (30.000)	2029	German-Russian Roadmap (*disc.*)	German contribution to PIK international user center according to German-Russian Roadmap. (2020-2029)
InnoMatSy*	HZG	tbd	2026	Draft application available (*prep.*)	*In-situ*-Innovation platform for multifunctional material systems. financial scope and participating centers currently being planned (2022-2026)

---

[1] "Sondermittel" financed via the German In-kind contribution to the ESS

[2] "Sondermittel" financed via MLZ Kooperationsvertrag

FLASH 2020+	DESY	18.000 (18.000)	First beam operation 2023	Preparation: TDR/feasibility study (*prep.*)	Upgrade of FLASH facility including gap-tunable undulators, external seeding schemes, and capabilities for new FEL schemes. (2021-2027)

Explanation of the project status:

- In discussion *(disc.)*
- Preparation: TDR/feasibility study *(prep.)*
- Proposal submitted *(prop.)*
- Funding commitment: > 50% of the estimated project costs *(fund.)*

The funding decisions for the large-scale infrastructures are part of the German BMBF roadmap process. In particular, a photon science roadmap process has been initiated for the proposed new or upgraded photon sources DALI, BESSY III, and PETRA IV to provide input for the BMBF roadmap process.

3.3. Management

Our governing body is the MML Program board, which consists of the spokespersons of the Program, the three Topics, and the four Facility Topics as well as representatives of the involved centers. The MML Program board, headed by the Program spokesperson, decides on all important issues concerning the Program in close interaction with the directors of the contributing Helmholtz Centers and the Research Field coordinator. It meets at least twice a year, complemented by frequent phone conferences.

The Topics and Facility Topics are the responsible units for achieving the objectives as described in the current proposal. Each Topic combines experts and infrastructures in a specialized scientific area and interacts with the corresponding international scientific community on a highly competitive level. Meetings on the Topic level are held twice per year and, in the case of the Facility Topics, often in combination with meetings of the MML Program board. The three Topics require an especially high degree of internal coordination based on the scientific cooperation across the centers. Therefore, as in the current funding period, regular scientific workshops are organized by the spokespersons of the Topics (see section on the Topics). Regular Program workshops are organized in addition, dedicated to the discussion of forefront science done at our large-scale facilities, with the aim to strengthen or establish cooperation between research groups at the participating centers and to discuss subjects overarching the complementary possibilities offered by our various probes. The spokespersons on all levels are responsible for the identification of synergies within and among the Topics and research facilities as well as their translation into scientific collaborations and results. The Program is organized in such a way that the majority of synergies will be covered within the Topics. Here, the engagement of MML in the various Cross-Cutting Activities is also addressed.

3.3.1. Talent Management

The Program MML is committed to bringing young scientists and academics closer to research at large-scale facilities, to supporting and training young scientists, and to continuously reinforcing gender equality. Therefore, the centers participating in the Program MML have a broad portfolio of instruments to address these issues, which cover the whole career path from high-school students to senior scientists.

Talent management starts at high-school level, aiming to inspire young people for science. Here, the centers of the Program help to organize on-site visits for interested high-school students, run school labs, and participate in the Germany-wide Girls’ Day initiative or in “Jugend Forscht” projects. MML scientists are involved in the education of undergraduate students at universities (teaching activities) and offer dedicated workshops, summer schools, and courses for national and international students, such as the DESY, GSI, HZB, and HZDR Summer Student Programs, the JCNS Neutron Lab Course, the HZG Matrac School, and the HZB Photon School. For structured Ph.D. studies, a number of graduate schools have been established at DESY, GSI, HZG, and HZDR (see Table 5 "Strategic university partners"). Beyond the Ph.D. level, the talent management programs at the centers also address postdocs, providing them with extensive support in defining their career aims and individual career steps. Furthermore, the centers strongly support young talents with their applications for all instruments provided by the Helmholtz Initiative and Networking Fund. Concerning the lead scientists, the centers contributing to the Program MML have been successful in the Helmholtz recruiting initiative, which aims at winning the best scientists for the German scientific community in order to reverse the so-called brain drain. Within the last years, four top scientists (three female, one male) from abroad could be recruited as senior lead scientists (full professors) for the Program MML. Moreover, at all centers involved in MML, particular emphasis is devoted to training and educating the technical personnel and engineers in handling the most advanced research infrastructures and instrumentation in order to allow for a most efficient use of beam times and user service.

The Program MML and its participating centers are strongly committed to gender equality and specifically see the need to support women pursuing an academic/scientific career at all career levels. All centers participating in MML have established corresponding programs, comprising support with child day care, flexible working time and part-time models, as well as relocation services, dual-career opportunities, and other measures. Moreover, there are various mentoring programs especially for women to support them in their career or in the pursuit of executive positions, as well as programs of the Helmholtz Association for recruiting female scientists as professors (first-time appointments of excellent female scientists (associate professors/full professors), Helmholtz Distinguished Professorship for female scientists (full professors)).

3.3.2. Transfer of Knowledge and Technology

At all involved centers, **Technology Transfer** is responsible for accompanying the transfer of research results. Technology Transfer handles administrative and financial processes as well as the contract management of publicly funded research projects and contract research with academic and industrial partners. Further support instruments applied by Technology Transfer are entrepreneurial qualification (mainly for doctoral candidates and postdocs), business coaching, access to external experts and service providers, opportunity recognition, and business model design workshops. Innovation workshops and expert platforms foster exchange with industry. This is also done via participation in international trade fairs and conventions. Technology Transfer advises scientists on transfer-oriented projects and the foundation of spin-offs. The centers have implemented their own funding programs (e.g. the FZJ incentive program InnovationPlus or the HZDR Innovation Fund), take advantage of a number of external funding programs (e.g. EU), and maintain close contacts with private investors (business angels, venture capital companies) to support the initial phase of spin-off companies. One example is the company Class 5 Photonics on the DESY campus in Hamburg, which was founded in 2014 as a spin-off company of DESY and HI Jena with focus on powerful femtosecond lasers. First related products were launched with support of Helmholtz Enterprise funding.

In addition, the MML large-scale facilities are open to industrial use, which is encouraged by the respective institutions. An example is the HZDR Innovation GmbH, a subsidiary of the center set up in 2012, that has been established primarily to manage the commercial access to and use of the research infrastructures of HZDR, in particular of the Ion Beam Center. Moreover, it provides a portfolio of technology transfer services (e.g. production, marketing or support for spin-offs). As a further example, DESY introduced among other measures an industrial liaison officer at PETRA III, who supports the professional and fast handling of industrial requests for beam time and the user service at the beamlines.

Besides cooperation with peers in academia, research, and industry, the strategies of the centers also include **knowledge transfer** into society, in the form of information services for experts or the public, consultancy for society or politics, participation in the social discourse, honest brokership in platforms, networks, and stakeholder processes, educational activities such as school labs, trainings for teachers or experts, as well as citizen science.

4. RESOURCES

In this section, we present different aspects of the planned and current resources, in terms of costs and personnel, for the Program MML.

Please note the used notation which applies to the entire proposal: Costs are given in thousand euros (TEUR), and for all resource numbers the thousands separator is a dot, and the decimal separator is a comma.

Table 10: Costs and personnel resources of the Program and its Topics, planned for 2021. The costs include general and administrative costs, internal services etc.

Program costs (TEUR)	**96.885**
Matter - Dynamics, Mechanism and Control	32.010
Materials - Quantum, Complex and Functional	48.055
Life - Building Blocks of Life	16.820
Program personnel (FTE)	**634**
Matter - Dynamics, Mechanism and Control	**234**
Scientists	105
Doctoral students	92
Scientific support personnel	37
Materials - Quantum, Complex and Functional	**296**
Scientists	179
Doctoral students	58
Scientific support personnel	59
Life - Building Blocks of Life	**105**
Scientists	62
Doctoral students	19
Scientific support personnel	24

Table 11: Program resources by center (in TEUR), planned for 2021. The costs include general and administrative costs, internal services etc.

Proposed program costs	**96.885**
DESY part costs	**27.742**
thereof personnel costs (including personnel of infrastructure)	17.364
FZJ part costs	**13.281**
thereof personnel costs	9.633
GSI part costs	**14.169**
thereof personnel costs (including personnel of infrastructure)	7.503
HZB part costs	**7.356**
thereof personnel costs (including personnel of infrastructure)	5.867
HZDR part costs	**23.343**
thereof personnel costs (including personnel of infrastructure)	16.354
HZG part costs	**2.285**
thereof personnel costs (including personnel of infrastructure)	1.387
KIT part costs	**8.709**
thereof personnel costs (including personnel of infrastructure)	5.767

DESY part investments	
continuing investments	4.460
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	2.000
FZJ part investments	
continuing investments	1.741
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0
GSI part investments	
continuing investments	2.009
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0
HZB part investments	
continuing investments	1.348
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0
HZDR part investments	
continuing investments	2.236
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0
HZG part investments	
continuing investments	391
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	1.500
KIT part investments	
continuing investments	773
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	191

Table 12: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

DESY program costs	**27.742**
- noncash expenditures[1)]	5.161
+ continuing investments	4.460
+ ongoing individual large investments > € 2,5 million	2.000
DESY cash expenditures	**29.041**
FZJ program costs	13.281
- noncash expenditures[1)]	1.815
+ continuing investments	1.741
+ ongoing individual large investments > € 2,5 million	0
FZJ cash expenditures	**13.207**
GSI program costs	14.169
- noncash expenditures[1)]	3.039
+ continuing investments	2.009
+ ongoing individual large investments > € 2,5 million	0
GSI cash expenditures	**13.139**
HZB program costs	7.356
- noncash expenditures[1)]	1.194
+ continuing investments	1.348
+ ongoing individual large investments > € 2,5 million	0

HZB cash expenditures	**7.510**
HZDR program costs	23.343
- noncash expenditures[1)]	5.915
+ continuing investments	2.236
+ ongoing individual large investments > € 2,5 million	0
HZDR cash expenditures	**19.664**
HZG program costs	2.285
- noncash expenditures[1)]	554
+ continuing investments	391
+ ongoing individual large investments > € 2,5 million	1.500
HZG cash expenditures	**3.622**
KIT program costs	8.709
- noncash expenditures[1)]	1.091
+ continuing investments	773
+ ongoing individual large investments > € 2,5 million	191
KIT cash expenditures	**8.582**

1) depreciation, reserves, variations in receivables and liabilities.

Table 13: Program personnel capacity by center (FTE), planned for 2021.

DESY part personnel	**197**
Scientists	109
Doctoral students	57
Scientific support personnel	31
FZJ part personnel	**92**
Scientists	61
Doctoral students	8
Scientific support personnel	23
GSI part personnel	**127**
Scientists	50
Doctoral students	56
Scientific support personnel	21
HZB part personnel	**36**
Scientists	23
Doctoral students	11
Scientific support personnel	2
HZDR part personnel	**122**
Scientists	65
Doctoral students	28
Scientific support personnel	29
HZG part personnel	**17**
Scientists	7
Doctoral students	9
Scientific support personnel	1
KIT part personnel	**44**
Scientists	32
Doctoral students	0
Scientific support personnel	12

Current resources

The current personnel resources are listed in the proposed PoF IV structure and are thus not directly comparable to the Program resources for PoF III.

Table 14: Current personnel resources projected to the PoF IV structure, preliminary resources for 2019.

	Helmholtz program		third-party funding	
	TEUR	FTE	TEUR	FTE
DESY	**13.955**	**209**	**3.486**	**70**
Scientists	8.888	100	2.322	28
Doctoral students	2.422	68	969	28
Scientific support personnel	2.645	41	195	14
FZJ	**7.327**	**92**	**587**	**10**
Scientists	5.480	61	327	4
Doctoral students	345	8	252	6
Scientific support personnel	1.502	23	8	0
GSI	**5.411**	**113**	**2.067**	**43**
Scientists	3.773	50	1.050	14
Doctoral students	891	46	792	24
Scientific support personnel	747	17	225	5
HZB	**2.462**	**36**	**166**	**3**
Scientists	1.879	23	80	1
Doctoral students	429	11	24	1
Scientific support personnel	154	2	62	1
HZDR	**8.068**	**111**	**2.620**	**44**
Scientists	5.193	60	1.593	21
Doctoral students	1.241	23	898	21
Scientific support personnel	1.634	28	129	2
HZG	**959**	**14**	**100**	**2**
Scientists	519	6	100	2
Doctoral students	300	7	0	0
Scientific support personnel	140	1	0	0
KIT	**3.663**	**44**	**1.910**	**30**
Scientists	3.060	33	1.262	18
Doctoral students	56	1	593	11
Scientific support personnel	547	10	55	1

5. LIST OF PUBLICATIONS RELATED TO THE PROGRAM PROPOSAL

The following publications have been referenced in the text.

References MML-Matter

[1] J. Ullmann et al., High precision hyperfine measurements in Bismuth challenge bound-state strong-field QED, Nature Commun. 8, 15484 (2017). doi: 10.1038/ncomms15484

[2] L. Deák et al., Realizing total reciprocity violation in the phase for photon scattering, Sci. Rep. 7, 43114 1-8 (2017), doi: 10.1038/srep43114

[3] A. Rudenko et al., Femtosecond response of small polyatomic molecules to ultra-intense hard X-rays, Nature 546, 129 (2017). doi: 10.1038/nature22373

[4] R. Schneider et al., Quantum imaging with incoherently scattered light from a free-electron laser, Nature Phys. 14, 126 (2018). doi:10.1038/nphys4301

[5] H. Hafez et al., Extremely efficient terahertz high-harmonic generation in graphene by hot Dirac fermions, Nature 561, 507–511 (2018). doi: 10.1038/s41586-018-0508-1

[6] S. C. Meier et al., Access to the bis-benzene cobalt(I) sandwich cation and its derivatives: synthons for a “naked” cobalt(I) source?, Angew. Chem. Int. Ed. 57, 9310 (2018). doi: 10.1002/anie.201803108

[7] M. N. Pohl et al., Do water's electrons care about electrolytes?, Chem. Sci. 10, 848 (2019). doi: 10.1039/C8SC03381A

[8] D. Zhang et al., Segmented terahertz electron accelerator and manipulator (STEAM), Nature Photon. 12, 336 (2018). doi: 10.1038/s41566-018-0138-z

[9] O. Pedatzur et al., Double-blind holography of attosecond pulses, Nature Photon. 13, 91 (2019). doi: 10.1038/s41566-018-0308-z

[10] W. Cayzac et al., Experimental discrimination of ion stopping models near the Bragg peak in highly ionized matter, Nature Commun. 8, 15693 (2017). doi: 10.1038/ncomms15693

[11] C. Gaida et al., Watt-scale super-octave mid-infrared intrapulse difference frequency generation, Light Sci. Appl. 7, 94 (2018). doi: 10.1038/s41377-018-0099-5

[12] D. Kraus et al., Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions, Nature Astron. 1, 606-611 (2017). doi: 10.1038/s41550-017-0219-9

[13] T. Kluge et al., Observation of Ultrafast Solid-Density Plasma Dynamics Using Femtosecond X-Ray Pulses from a Free-Electron Laser, Phys. Rev. X 8, 031068 (2018). doi: 10.1103/PhysRevX.8.031068

[14] F. Stefani et al., The DRESDYN project: liquid metal experiments on dynamo action and magnetorotational instability, Geophys. Astrophys. Fluid Dyn. 113, 51-70 (2019). doi: 10.1080/03091929.2018.1501481

[15] J. Hofbrucker, A. V. Volotka, and S. Fritzsche, Maximum Elliptical Dichroism in Atomic Two-Photon Ionization, Phys. Rev. Lett. 121, 053401 (2018). doi: 10.1103/PhysRevLett.121.053401

References MML-Materials

[1] Schroth, P. et al., Radial Growth of Self-Catalyzed GaAs Nanowires and the Evolution of the Liquid Ga-Droplet Studied by Time-Resolved *in Situ* X-ray Diffraction, Nano Lett. 18, 101 (2018). doi: 10.1021/acs.nanolett.7b03486

[2] Schwartzkopf, M. et al., Role of Sputter Deposition Rate in Tailoring Nanogranular Gold Structures on Polymer Surfaces, ACS Appl. Mater. Interfaces 9, 5629 (2017). doi: 10.1021/acsami.6b15172

[3] Movsesyan, L. et al., ZnO Nanowire Networks as Photoanode Model Systems for Photoelectrochemical Applications, Nanomaterials 8, 693 (2018). doi: 10.3390/nano8090693

[4] dos Santos Rolo, T. et al., A Shack-Hartmann Sensor for Single-Shot Multi-Contrast Imaging with Hard X-rays , Appl. Sci. 8, 737 (2018). doi: 10.3390/app8050737

[5] Chen, B. et al., All-oxide–based synthetic antiferromagnets exhibiting layer-resolved magnetization reversal, Science 357, 191 (2017). doi: 10.1126/science.aak9717

[6] Biniskos, N. et al., Spin Fluctuations Drive the Inverse Magnetocaloric Effect in Mn_5Si_3, Phys. Rev. Lett. 120, 257205 (2018). doi: 10.1103/PhysRevLett.120.257205

[7] Sluka, V. et al., Emission and propagation of 1D and 2D spin waves with nanoscale wavelengths in anisotropic spin textures, Nature Nanotechnology 14, 328 (2019). doi: 10.1038/s41565-019-0383-4

[8] Wang, Z. et al., Experimental observation of Bethe strings, Nature 554, 219 (2018). doi: 10.1038/nature25466

[9] Gorbunov, D. I. et al., Microscopic Nature of the First-Order Field-Induced Phase Transition in the Strongly Anisotropic Ferrimagnet $HoFe_5Al_7$, Phys. Rev. Lett. 122, 127205 (2019). doi: 10.1103/PhysRevLett.122.127205

[10] Thielemann-Kühn, N. et al., Ultrafast and Energy-Efficient Quenching of Spin Order: Antiferromagnetism Beats Ferromagnetism, Phys. Rev. Lett. 119, 197202 (2017). doi: 10.1103/PhysRevLett.119.197202

[11] Yuan, Y. et al., Interplay between localization and magnetism in (Ga,Mn)As and (In,Mn)As, Phys. Rev. Materials 1, 054401 (2017). doi: 10.1103/PhysRevMaterials.1.054401

[12] König-Otto, J. C. et al., Four-Wave Mixing in Landau-Quantized Graphene, Nano. Lett. 17, 2184 (2017). doi: 10.1021/acs.nanolett.6b04665

[13] dos Santos, J. F. et al., Understanding precipitate evolution during friction stir welding of Al-Zn-Mg-Cu alloy through *in-situ* measurement coupled with simulation, Acta Materialia 148, 163 (2018). doi: 10.1016/j.actamat.2018.01.020

[14] Hejral, U. et al., Identification of a Catalytically Highly Active Surface Phase for CO Oxidation over PtRh Nanoparticles under *Operando* Reaction Conditions, Phys. Rev. Lett. 120, 126101 (2018). doi: 10.1103/PhysRevLett.120.126101

[15] König, N. et al., Cooperativity during Melting and Molecular Exchange in Micelles with Crystalline Cores, Phys. Rev. Lett. 122, 078001 (2019). doi: 10.1103/PhysRevLett.122.078001

[16] Mercurio, G. et al., Surface structure determination by x-ray standing waves at a free-electron laser, New J. Phys. 21, 033031 (2019). doi: 10.1088/1367-2630/aafa47

[17] Bajt, S. et al., X-ray focusing with efficient high-NA multilayer Laue lenses, Light: Science & Applications 7, 17162 (2018). doi:10.1038/lsa.2017.162

References MML-Life

[1] Raiser, D., et al., Evolution of hot polaron states with a nanosecond lifetime in a manganite perovskite, Advanced Energy Materials, 7(12): 1602174 (2017). doi:10.1002/aenm.201602174.

[2] Perakis, F. et al., Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics, Nat. Commun. 9, 1917 (2018). doi: 10.1038/s41467-018-04330-5

[3] Wiedorn, M. O. et al., Megahertz serial crystallography, Nat. Commun. 9, 4025 (2018). doi: 10.1038/s41467-018-06156-7

[4] Seuring, S. et al., Femtosecond X-ray coherent diffraction of aligned amyloid fibrils on low background graphene, Nat. Commun. 9, 1836 (2018). doi: 10.1038/s41467-018-04116-9

[5] Müller, M. et al., Myoanatomy of the velvet worm leg revealed by laboratory-based nanofocus X-ray source tomography, Proc. Natl. Acad. Sci. USA 114, 12378 (2017). doi: 10.1073/pnas.1710742114

[6] van de Kamp, T. et al., Parasitoid biology preserved in mineralized fossils, Nat. Commun. 9, 3325 (2018). doi: 10.1038/s41467-018-05654-y

[7] Weinhardt, V. et al., Quantitative morphometric analysis of adult teleost fish by X-ray computed tomography, Sci. Rep. 8, 16531 (2018), doi: 10.1038/s41598-018-34848-z

[8] Durante, M. et al., Applied nuclear physics at the new high-energy particle accelerator facilities, Phys. Rep. 800, 1(2019). doi: 10.1016/j.physrep.2019.01.004

[9] Meents, A. et al., Pink-beam serial crystallography, Nature Comm. 8, 1281 (2017),. doi: 10.1038/s41467-017-01417-3

[10] Z. Yin et al., Cationic and Anionic Impact on the Electronic Structure of Liquid Water, J. Phys. Chem. Lett. 8, (2017) 3759., doi: 10.1021/acs.jpclett.7b01392

[11] Bari, S. et al., Soft X-ray Spectroscopy as a Probe for Gas-Phase Protein Structure: Electron Impact Ionization from Within, Chem: Eur. J. 24, 7631 (2018). doi: 10.1002/chem.201801440

[12] Natale, F. et al., Identification of the elementary structural units of the DNA damage response, Nat. Commun. 8, 15760 (2017). doi:10.1038/ncomms15760

[13] Sokol, O. et al., Kill painting of hypoxic tumors with multiple ion beams, Phys. Med. Biol. 64, 045008 (2019). doi: 10.1088/1361-6560/aafe40

[14] Rapp, F. et al., Biological Cardiac Tissue Effects of High-Energy Heavy Ions – Investigation for Myocardial Ablation, Sci. Rep. 9, 5000 (2019). doi: 10.1038/s41598-019-41314-x

[15] Giraudo, M., et al., Accelerator-Based Tests of Shielding Effectiveness of Different Materials and Multilayers using High-Energy Light and Heavy Ions. Radiation Research, 190(5), 526-537 (2018). doi:10.1667/RR15111.1