HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

USER FACILITIES

Research Field MATTER

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

RESEARCH FIELD *MATTER*

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Participating Helmholtz Centers

DESY Deutsches Elektronen-Synchrotron

FZJ Forschungszentrum Jülich GmbH

GSI Helmholtzzentrum für Schwerionenforschung GmbH

HI Jena Helmholtz-Institut Jena
HIM Helmholtz-Institut Mainz

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

IPP Max-Planck-Institut für Plasmaphysik

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A. *MATTER AND THE UNIVERSE*

The enormous amount of data produced by the experiments within the Program MU are processed in globally networked infrastructures. The Program MU hosts the Tier-1 center GridKa at KIT, which is responsible for the processing, analysis, and archival of data from various particle physics experiments, in particular from the experiments at the Large Hadron Collider (LHC) and its future upgrade, the High-Luminosity LHC (HL-LHC), at CERN. The scope of the Tier-2 center at DESY will be extended. Therefore, the center will be renamed to Interdisciplinary Data and Analysis Facility (IDAF) and moved to the Program MT (see Section B.3)

Within the Program MU, access to accelerators is provided by the GSI LK II facilities. The GSI accelerators deliver beams of stable ions between several MeV and 2 AGeV, as well as proton and secondary radioactive ion and pion beams. The international FAIR Facility for Antiproton and Ion Research is being built next to the GSI campus during the next years. The FAIR accelerator complex will exceed not only the beam energies of GSI by a factor of 10, but also the maximum beam intensities by factors 10 – 1,000, and will offer unique scientific opportunities.

1. GRIDKA

With the launch of the LHC at CERN ten years ago, a new chapter in high-throughput computing was opened: In the Worldwide LHC Computing Grid (WLCG) collaboration, the grid concept has made it possible to successfully process the data stream from the LHC experiments and to fully exploit their physics potential, resulting e.g. in the discovery of the Higgs boson. GridKa has played a central role in this success story. In this section, we describe the planned further development of GridKa to strengthen its leading role within a changing environment in view of the significantly higher computing requirements expected in the coming years.

1.1. Overview

As a WLCG Tier-1 center, GridKa is responsible for the processing, reprocessing, and archival of raw data from the LHC and future HL-LHC experiments. Other WLCG centers, in particular Tier-2 centers, rely on GridKa as their data source and data archive. GridKa is one of only four Tier-1 centers worldwide supporting all four LHC experiments. Besides the LHC experiments, GridKa serves several other particle physics and astroparticle physics experiments with German participation, e.g. the COMPASS experiment at CERN and the Pierre Auger Observatory. GridKa is also foreseen to become one of a few raw-data centers worldwide for the Belle II experiment at KEK in Japan.

As of 2019, GridKa provides a major part of the WLCG Tier-1 resources pledged worldwide: 14,5% of the compute power (CPUs), 14,4% of the online storage (disk), and 13,5% of the tape storage capacity, corresponding to 333 kHS06[1] CPU power, 32 PB usable disk space, and 67 PB usable tape space. For Belle II, GridKa currently provides approx. 6% of the worldwide resources, corresponding to 18 kHS06 and 665 TB disk space. With its excellent wide area network connection of 100 Gb/s to CERN and 2x100 Gb/s to the German research network backbone, GridKa is ready for the upcoming LHC run and its role for Belle II.

As one of the largest and best-performing data centers for particle and astroparticle physics worldwide, GridKa is an indispensable large-scale research infrastructure, enabling the successful participation of German physicists in international particle physics collaborations.

GridKa is hosted and operated by the Steinbuch Centre for Computing (SCC), the scientific computing center of KIT. As a user facility aimed mainly at users outside of the Helmholtz Association, it belongs to the Helmholtz LK II category of activities.

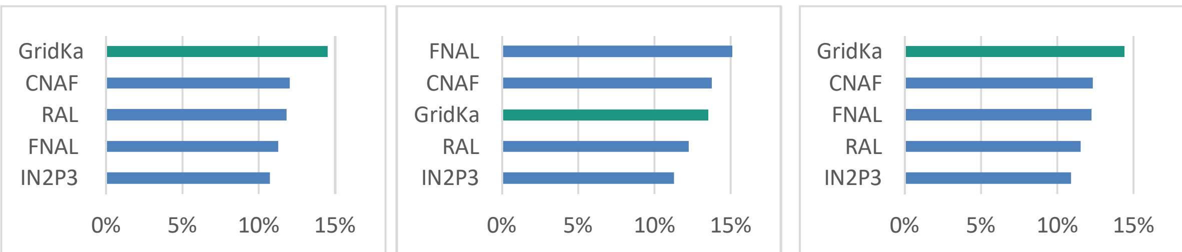

Figure 1: Relative share of pledged CPU (left), disk (center), and tape (right) resources of the largest WLCG Tier-1 centers. Source: REBUS database

1.2. Research Environment and Current Activities

GridKa offers highly reliable high-throughput compute and storage services to its demanding user communities. In order to achieve optimal performance, services and systems are optimized for the individual user groups and their

1 kilo HEP-SPEC06: benchmark for measuring CPU performance: http://w3.hepix.org/benchmarking needs. Close collaborations of GridKa scientists and engineers with computing specialists of the user communities (experiments), with various data centers within the WLCG and elsewhere, and with computer scientists secure the leadership position of GridKa in performance, reliability, innovation, and efficiency.

Within the WLCG, the Grid Deployment Board (GDB), experiment-specific computing boards, WLCG workshops, as well as specific projects and working groups form the basis for the technical collaboration of the WLCG centers and the experiments. GridKa is well represented and active in these boards, working groups, and projects, which are becoming increasingly important as the big-data challenges of the HL-LHC era are coming closer. A current example is the Data Organization Management Access (DOMA) project, which provides a forum for all stakeholders to discuss ideas and which aims to integrate solutions and technologies of national initiatives, (European) projects, and other working groups in order to address the computing challenges of the HL-LHC. The EU-funded project Helix Nebula Science Cloud (HNSciCloud) for example, which was finished in 2019, tested the utilization of commercial cloud resources. GridKa demonstrated the user-transparent and dynamic integration of these resources in its workload management system, a technology that will play an important role in future computing models. Furthermore, cooperative work and joint R&D of data and compute centers for high-energy physics (HEP) are organized on an international level by the HEPiX[2] forum, to which GridKa scientists contribute significantly with studies and results on energy-efficient computing and benchmarking. In addition to the cooperation with other WLCG centers within committees and working groups, there is informal cooperation with various partner centers on specific topics. Especially with CC-IN2P3 in France, there exists a long-standing partnership and frequent information exchange.

On the national level and within KIT, GridKa collaborates with the Helmholtz Program *Supercomputing & Big Data*, which will become part of the future Program *Engineering Digital Futures: Supercomputing, Data Management and Information Security for Knowledge and Action* of the Research Field *Information*. In addition to high-performance computing (HPC), distributed systems, high-throughput computing, data management, and cloud computing are topics that are worked on in this context. Several European projects are carried out within this Program. Examples are the Indigo-DataCloud, AARC, and AARC2 projects, the DEEP Hybrid Data Cloud project, EUDAT, and ELITRANS, as well as several ongoing projects in the context of the development of the European Open Science Cloud (EOSC), in particular EOSCpilot, EOSC-hub, EOSCsecretariat.eu, EOSC-Pillar, and EOSC-synergy. GridKa scientists are cooperating closely with colleagues working on these projects or participating themselves in some of these projects. This benefits the integration of EOSC services and resources with the GridKa infrastructure [milestone GridKa-2].

The collaborative work with the CMS research group at KIT is very successful and produces outstanding results in the fields of data management and in particular workload management systems, aiming to actively shape the HL-LHC computing models. One highlight is the joint development of a specialized high-throughput analysis cluster for the CMS experiment. A special hardware configuration and workload management and caching software enable a performance that is significantly higher than that of common systems[3]. The jointly developed TARDIS[4] and COBalD[5] services allow the efficient usage of opportunistic and long-term available HPC and cloud resources[6]. These services were developed and tested by doctoral students of the Karlsruhe School of Elementary Particle and Astroparticle Physics: Science and Technology (KSETA) graduate school together with GridKa scientists and are in daily operation today.

The Analysis and Data Center for Multi-messenger Astroparticle Physics project, funded by the BMBF Innovation Fund for 2019 and 2020, is the starting point for a closer collaboration with astroparticle physics, with the aim to develop novel data analysis and data management methods and services, taking into account the open data, open access, and FAIR principles[7].

2 High Energy Physics Unix Information Exchange, http://www.hepix.org
3 Heidecker, C. et. al, Provisioning of data locality for HEP analysis workflows,
J. Phys: Conf. Ser./1085 (2018) 032005. doi: 10.1088/1742-6596/1085/032005
4 Transparent Adaptive Resource Dynamic Integration System. doi: 10.5281/zenodo.2240606
5 COBalD – the Opporttunistic Balancing Demon. doi: 10.5281/zenodo.1887873
6 Schnepf, M. et. al, Mastering Opportunistic Computing Resources for HEP,
J. Phys.: Conf. Ser./1085 (2018) 032056. doi: 10.1088/1742-6596/1085/3/032056
7 FAIR principles of data management, see https://www.force11.org/fairprinciples.

In addition to the increased R&D activities towards HL-LHC computing, significant work has recently been invested in improving the technical infrastructure of GridKa. Data center automation techniques allow CPU and storage capacities to be scaled to several times the current level. The space and technical infrastructure of the data center building also allow a massive increase of resources. Since 2018, absorption chillers have been using the waste heat of a power plant on the KIT campus to provide cooling for the GridKa data center. Using this technology, GridKa is competitive to the most modern data centers from an ecological and economical point of view.

1.3. Content and Objectives

In view of the decade from 2021 onwards, with the startup of the HL-LHC and other experiments and their requirements of modern experimentation, the simple scaling of resources no longer seems practicable and affordable. Estimations for the HL-LHC era starting in 2026 predict a further increase of computing requirements by a factor of five to ten. Such an increase would be much higher than that achievable with a flat budget. The experiments need to address this problem by newly developed, domain-specific software and algorithms, following the paradigms of parallel computing, maximum effectiveness and minimization of requirements. Besides the software, the computing models offer potential for improvement. It is becoming apparent that with fewer but larger data centers such as GridKa, more efficient computing models could be implemented. Various accessible computing resources, for example HPC and cloud resources, including temporarily available resources have to be used for appropriate tasks. For certain data intensive computing tasks, however, such as user analysis or stripping and merging of data sets, specialized compute resources at the WLCG centers will still be more cost efficient than generic compute resources. The implementation of more efficient computing models can only be done by the experiments in close collaboration with the data centers and resource providers.

1.3.1. Expected Achievements and Development Potential

The results of both the WLCG community-wide and GridKa's own R&D activities will be used to further develop GridKa in several respects up to the HL-LHC phase: Storage system capacities and throughput capabilities as well as local and remote network connectivity will be scaled up to provide the required storage space and to be able to handle increasing data access also from remote sites and partner centers building a data backbone ("data lake") with GridKa as an integral part [GridKa-4]. The GridKa compute farm will be scaled up [GridKa-1, GridKa-3] and optimized for higher throughput, e.g. by applying the workload management and caching techniques developed for the CMS analysis cluster. Local HPC compute clusters at KIT will be made available for HEP compute tasks. The KIT HPC clusters ForHLR and HoreKa for example provide GPUs that could significantly speed up certain HEP algorithms. Remote resources will be made available through the TARDIS and COBalD services [GridKa-3]. A similar technique could be used to operate some of today's Tier-2 centers as a remote resource.

With its capabilities and capacities for highest throughput as well as its specialized hardware, GridKa will be the optimal place to run all particle physics compute tasks – data-intensive jobs that need high-performance access to the data as well as compute-intensive tasks that can utilize cloud and HPC resources efficiently. GridKa will of course continue to support other, non-LHC particle and astroparticle experiments with similar requirements, which will benefit from these developments. The specialization on these communities allows us to optimize the systems and services for their requirements and guarantees the best possible efficiency for data-intensive computing tasks.

However, many of these technologies will find completely different areas of application. Together with our partners in the WLCG, we will thus push high-throughput computing to extremes over the next decade, with solutions that are not only suitable for the particle physics experiments that profit directly, but that will advance the entire field of extreme high-throughput computing in a general and groundbreaking way. GridKa is in an ideal position and prepared to play a leading role in this development as one of a few major data centers for the HL-LHC and other experiments worldwide. However, this requires substantial investment. Operating costs, including personnel, are covered by the Helmholtz PoF. Investments necessary to maintain and further develop the infrastructure according to the increasing requirements of the particle physics community are currently secured only until 2021. It is planned to apply for the investment funds required in 2022 and 2023 from KIT's internal budget, but funding for the HL-LHC expansion from 2024 is considered a challenge to the entire community – further financing options will have to be explored.

1.3.2. Milestones

The following table shows the milestones for GridKa.

Table 1: Overview of the milestones for GridKa.

	Year	Milestone
GridKa-1	2021	GridKa ready for LHC Run 3, storage and compute capacities in place
GridKa-2	2022	Integration of EOSC services
GridKa-3	2024	Start of resource ramp-up for the HL-LHC, integration of external resources
GridKa-4	2025	Commissioning and testing of storage and network with HL-LHC data rates
GridKa-5	2026	GridKa ready for HL-LHC data taking

1.3.3. Planned Investments/Upgrades of the Facility

GridKa needs to be continuously upgraded to meet the increasing storage capacity and compute power requirements of the particle and astroparticle physics communities, in particular the HL-LHC requirements. In addition, continuous replacements are needed (see Section 1.4). The following table summarizes the estimated investments required for this purpose.

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 2: Estimated investments required for the HL-LHC upgrade.

Year	2021	2022	2023	2024	2025	2026	2027
Investment [TEUR]	3.000	3.000	3.000	4.000*	7.000*	7.000*	6.000*

**funding sources under discussion*

1.4. Life Cycle Analysis

The life cycle of the GridKa facility is fully driven by the large particle and astroparticle physics experiments with German contribution. The lifetime of the LHC experiments and the Belle II experiment reaches well beyond the next 15 years, and data archival and analysis for these experiments will last even longer. Since the typical lifetime of IT resources is about five years and the requirements of the experiments increase annually, continuous replacement and upgrade of resources are necessary, requiring continuous and long-term funds.

1.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to GridKa.

Table 3: Grid Computing Centre Karlsruhe (GridKa) Resources (KIT), planned for 2021. The costs include general and administrative costs, internal services etc.

KIT costs (TEUR)	**7.296,0**
thereof personnel costs (including personnel of infrastructure)	3.322,0
thereof material costs	2.174,0
thereof electricity	1.120,0
thereof other consumables	1.054,0
thereof noncash expenditures	1.800,0
KIT investments	
continuing investments	511,8
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	126,2

Table 4: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

KIT program costs	7.296,0
- noncash expenditures	1.800,0
+ continuing investments	511,8
+ ongoing individual large investments > € 2,5 million	126,2
KIT cash expenditures	**6.134,0**

Table 5: Program personnel capacity by center (FTE), planned for 2021.

KIT part personnel	26
Scientists/Engineers	26
Scientific support personnel	0
for information only: corresponding Helmholtz program (LK I) - KIT contribution	132
Scientists	64
Doctoral students	3
Scientific support personnel	65
for information only: corresponding Helmholtz program (LK I) - total	654
Scientists	360
Doctoral students	170
Scientific support personnel	124

Table 6: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		Third-party funding	
	TEUR	FTE	TEUR	FTE
KIT	2.172,3	26	0,0	0
Scientists/ engineers	2.172,3	26	0,0	0
Scientific support personnel	0,0	0	0,0	0

2. GSI-MU ION FACILITIES

On its campus in Darmstadt, GSI operates a large, worldwide unique heavy-ion accelerator complex. It consists of the UNILAC linear accelerator with a top energy of 11 MeV/u, serving several experimental stations and feeding the low-energy program and the SIS18 synchrotron for further acceleration up to energies of 1 GeV/u, the ESR experimental storage cooler ring with a magnetic rigidity of 10 Tm, capable of storing and cooling ions from 400 MeV/u to 4 MeV/u, and the CRYRING storage ring, installed behind the ESR and providing highly or fully stripped ions at energies of about 10 MeV/u down to 100 keV/u. The two storage rings are part of the LK II facilities of the Program MML. In addition to proton and ion beams, radioactive and pion beams are available. UNILAC and SIS18 will be utilized as pre-accelerators for the FAIR facility, which is currently being built next to the GSI campus.

The facilities serve a broad community and a multitude of scientific topics, including hadron structure and dynamics, the characteristics of compressed strongly interacting matter, nuclear structure and reactions, nuclear astrophysics, as well as materials science, atomic, plasma, and biophysics, engineering, and applied science. In total, more than 1,200 external scientists are using the GSI facilities every year.

2.1. Overview

The UNIversal Linear ACcelerator (UNILAC) accelerates all ion species, from protons to uranium ions, to energies up to 11 MeV/u. Beam time can be shared between several different experimental facilities and injection into SIS18. The major experimental facilities for the Program MU at the UNILAC are:

- SHIP, an electromagnetic separator and velocity filter for (super-)heavy elements (SHE) dedicated to the spectroscopy of neutron-deficient heavy nuclei, nuclear reaction studies, and precision mass measurements;
- TASCA, a gas-filled recoil separator with maximized transmission (efficiency) for transactinides created in hot-fusion reactions of light heavy ions (O to Ca) with actinide targets, used in particular to study the chemical properties of SHE;
- SHIPTRAP, a Penning trap behind SHIP for nuclear structure and atomic physics studies on super-heavy nuclei/atoms;
- Various laser and decay spectroscopy setups as well as chemistry apparatus for physics and chemistry studies of SHE.

The SIS18 is a heavy-ion synchrotron providing high-energy beams to fixed targets or to production targets for the generation of secondary beams. The parameters of the ion beams can be adapted to the requirements of the users in each cycle. Both single-turn fast extraction and slow extraction of the beam up to 20 s are possible. Phase space reduction using powerful electron cooling allows high-efficiency beam transfer to the ESR experimental storage ring as well as stacking by multi-turn injection in order to reach highest-beam-intensity operation. Experimental facilities for the Program MU at SIS18 are:

- FRS, a projectile fragment separator for the production and in-flight separation of exotic nuclei far off stability, with the possibility to install various setups at its focal planes for gamma-ray, decay, and mass spectroscopy;
- R3B, a setup for investigations of reactions with radioactive relativistic beams, allowing kinematically complete reaction studies at relativistic energies up to 1 GeV/u;
- HADES, a high-acceptance di-electron spectrometer for studies of hot and dense strongly interacting matter, with particular emphasis on measuring rare hadronic and leptonic probes;
- mCBM, a test facility for verification and testing of detectors with very high-intensity beams.

For experiments such as HADES, but also ALICE at the LHC, which are producing petabytes of data in experiment campaigns, a strong computing infrastructure is vital for data analysis and detector simulations. The MU research infrastructure at GSI therefore includes the GSI Green IT Cube, the main facility for all computing activities on the campus. Currently, 15,000 physical cores and 20 PB of disk space in addition to a multi-PB tape storage system are offered to the users of the experimental sites.

2.2. Research Environment and Current Activities

The GSI user community of the Program MU is organized along the major subfields *Nuclear Structure, Nuclear Reactions, Properties of Nuclear Matter under Extreme Conditions, Hadron Physics*, and *Applications of Nuclear Science,* with many overlapping research activities. The GSI facilities are fully integrated into the network of European hadron and ion accelerators through EU-financed integrating activities, which have been initiated and are organized by the scientific community.

Accelerator and detector R&D at GSI are embedded into the Program MT. Scientists from the GSI accelerator section are collaborating closely with colleagues from the other participating centers and especially from the neighboring universities. In addition to its participation in MT, GSI collaborates in particular with CERN, ESS Lund, JINR Dubna, GANIL Caen, BINP Novosibirsk, BNL Brookhaven, ELI-NP Măgurele, CEA Saclay, IHEP Protvino, IMP Lanzhou, KVI-CART Groningen, and the MPI für Kernphysik Heidelberg on accelerator and/or detector subjects. Likewise, GSI IT is engaged in the Topic MT-DMA and in the Helmholtz Data Federation (HDF).

The major focus of GSI is the construction and commissioning of accelerator components and detector systems for the FAIR facility. More than 2,500 scientists and engineers from over 50 countries are involved in the preparation of the FAIR experiments, which are organized in four scientific pillars: APPA, CBM, NUSTAR, and PANDA. The latter three experiments contribute directly to the Topic MU-CML. FAIR is scheduled to deliver first beams in 2025.

GSI scientists are involved in all four experimental pillars, building key components of the associated detector systems. In particular, GSI accelerator scientists are in charge of the design and construction of the superconducting SIS100 synchrotron and the Super-FRS of FAIR. In parallel, the existing accelerators UNILAC and SIS18 are undergoing an upgrade program to meet the FAIR requirements regarding intensity and brilliance. Furthermore, GSI serves as the host lab for all the experiments, assuming responsibility for the overall coordination of overarching FAIR activities.

2.3. Content and Objectives

From 2018 until the start of commissioning of the FAIR SIS100 synchrotron, the centerpiece of the FAIR facilities, regular though limited periods of dedicated beamtimes will be offered at GSI. While the construction and commissioning of the FAIR accelerators are ongoing, these beamtime periods of about three months per year will allow extensive testing and early physics experiments with the upgraded GSI accelerators and novel FAIR instrumentation.

More specifically, the major goals for the research infrastructures are:

- Further upgrade measures for the UNILAC and SIS18
- Provision of high-intensity beams of ^{48}Ca and ^{50}Ti at the UNILAC for the SHE physics and chemistry program
- Upgrades of the TASCA and SHIP target areas: higher background suppression to accept higher beam intensities, new focal-plane particle and photon detection systems, and advanced chemistry setups to access shorter-lived elements
- Upgrades of SHIP, SHIPTRAP and its detection setups: installation of a novel setup for high-resolution gas jet laser spectroscopy and of a single-ion mass measurement setup based on electronic detection
- Provision of high-intensity U beams for the production of exotic nuclei at the limit of stability
- Maintaining the FRS fully operational and upgrade of the target region to complete remote control as a test bench for the Super-FRS at FAIR [GSI-MU.3]
- Delivering beams to the ESR/CRYRING facilities (see LK II contribution of GSI to the Program MML)
- Completion and commissioning of the DESPEC detector setup for nuclear spectroscopy and installation in the FRS final focal plane
- Installation and operation of WASA@FRS for pion detection in nuclear reactions [GSI-MU.2]

- Development of new ion-optical modes for FRS/Super-FRS, ensuring higher transmission and yields for all NUSTAR secondary-beam experiments
- Installation and testing of detector components for the Super-FRS and further NUSTAR experiments at the FRS (e.g. Ion Catcher for FAIR Low Energy Branch)
- Operation and stepwise finalization of the R3B setup for FAIR [GSI-MU.5]
- Delivering of high-intensity pion beams for experiments with HADES
- Upgrade of the HADES pion beam tracker and data acquisition system [GSI-MU.1]
- Provision of a high-intensity test site for CBM detector components and for the Distributed Detector Laboratory (DDL) activities

The construction and commissioning of the FAIR accelerators and detectors will be going on in parallel. When the experimental halls of FAIR will be completed, the experimental installations currently located at the GSI accelerators (except the setups for SHE research) will be moved to the respective FAIR sites to profit from the higher beam energies and intensities that will be available at FAIR [GSI-MU.6/7].

2.3.1. Expected Achievements and Development Potential

All activities at the GSI accelerators in the next five years will focus on the requirements of the FAIR experiments regarding intensity and quality of the ion beams. For light intermediate-mass ions, the achieved intensities are sufficient to fill the SIS18 up to its space charge limit. For heavy ions, this limit has not yet been reached, as it is out of the scope of the current UNILAC design. In order to address this issue, an upgrade project for the UNILAC has been initiated to optimize the beam dynamics for high beam brilliance. During PoF IV, the upgraded accelerators and the experimental infrastructure will offer unique opportunities to test the FAIR detectors and perform first scientific experiments with high-intensity beams of radioactive or stable ions.

2.3.2. Milestones

The following table shows the milestones for the GSI-MU Ion Facilities.

Table 7: Overview of the milestones for the GSI-MU Ion Facilities.

	Year	Milestone
GSI-MU.1	2021	Upgrade of pion beam line completed
GSI-MU.2	2021	WASA installation completed
GSI-MU.3	2022	Complete remote control of FRS target region
GSI-MU.4	2022	HADES DAQ upgraded to data rates of 200 kHz
GSI-MU.5	2023	R3B FAIR Phase 1 setup completed
GSI-MU.6	2025	Transfer of NUSTAR detectors to the Super-FRS site completed and first experiments with Super-FRS beam
GSI-MU.7	2025	HADES moved to CBM cave

2.3.3. Planned Investments/Upgrades of the Facilities

During PoF IV, the central goal of the facility-oriented activities of the MU departments at GSI is to support their collaborations in the design, construction, and commissioning of the experimental installations at FAIR (i.e. NUSTAR, CBM, HADES, and PANDA). GSI will also provide substantial support in the execution of experiments utilizing dedicated novel FAIR instrumentation. The accelerators will be further upgraded not only to achieve highest intensities for heavy ions, but also to provide a still higher reliability of operation and to maintain high-duty-factor operation at the UNILAC.

In the context of the HDF, GSI IT will create a National Analysis Facility for the FAIR data in the coming years, modeled along the current ALICE National Analysis Facility at GSI.

2.4. Life Cycle Analysis

The GSI accelerator facilities are continuously maintained and upgraded in order to deliver beams of highest quality and brilliance to the scientific users and to serve as injectors for FAIR in the future. This holds also for the experimental infrastructure. A smooth extension of the research activities at GSI by the new FAIR accelerator and experiment infrastructure is expected during PoF IV, once the experimental infrastructure of GSI has been moved to FAIR.

After the recent upgrades, the lifetimes of the UNILAC and SIS18 accelerators are expected to amount to at least 20 to 30 years. The FRS will continue to be operated for experiments with radioactive beams at the ESR/CRYRING facilities even after the installation of the Super-FRS at FAIR and might be utilized as a test bench for detectors further on.

Once FAIR is operational, the amount of beamtime offered to the user communities will be much larger than during FAIR Phase 0, on the order of nine months per year. The resources that are at the moment allocated to the construction of the FAIR facilities will be shifted to maintenance and operation of the newly built infrastructures.

2.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the GSI-MU Ion Facilities.

Table 8: GSI-MU Ion Facilities Resources (GSI), planned for 2021. The costs include general and administrative costs, internal services etc.

GSI costs (TEUR)	**23.579,0**
thereof personnel costs (including personnel of infrastructure)	11.562,8
thereof material costs	6.016,1
thereof electricity	2.100,0
thereof maintenance costs	3.916,3
thereof noncash expenditures	6.000,0
GSI investments	
continuing investments	3.450,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	

Table 9: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

GSI costs	23.579,0
- noncash expenditures	6.000,0
+ continuing investments	3.450,0
+ ongoing individual large investments > € 2,5 million	0,0
GSI cash expenditures	**21.029,0**

Table 10: Program personnel capacity by center (FTE), planned for 2021.

GSI part personnel	132
Scientists/Engineers	68
Scientific support personnel	64
for information only: corresponding Helmholtz program (LK I) - GSI contribution	138
Scientists	68
Doctoral students	52
Scientific support personnel	18
for information only: corresponding Helmholtz program (LK I) - total	654
Scientists	360
Doctoral students	170
Scientific support personnel	124

GSI does not have any LK II facilities in PoF III, hence, no personnel resources are given for 2019.

B. *MATTER AND TECHNOLOGIES*

In PoF IV *Matter and Technologies* is significantly increasing its activities in the area of scientific computing and big data. The LK II facility Tier-2, formerly attached to *Matter and the Universe*, will be extended and moved to *Matter and Technologies*. The WLCG Tier-1 center GridKa at KIT remains within the Program MU, and is described in Section A.1.

3. IDAF

The enormous amount of data produced by experiments from particle physics, astroparticle physics, research with photons, and by simulations is processed in globally networked infrastructures. The Interdisciplinary Data and Analysis Facility (IDAF), hosted by the Program MT and designed for all the communities of the Research Field *Matter*, encompasses the Worldwide LHC Computing Grid (WLCG) Tier-2 center at DESY, but will cover a large spectrum of applications from all areas of *Matter*. It is described in this section.

3.1. Overview

The current DESY Tier-2 center, which will be at the core of the IDAF, serves high-energy physics (HEP) communities worldwide as an analysis fabric, with access provided through the WLCG (see Volume II B, Section 2.2.3). In terms of the number of successfully handled jobs, it is one of the worldwide leading computer centers for the LHC experiments ATLAS, CMS, and LHCb. In addition to the Tier-2 center, DESY operates a National Analysis Facility for the German HEP users as part of the LK II large-scale facility Tier-2. The resources are currently used by the LHC experiments, the Belle II experiment, the astroparticle experiments, and in studies for future facilities such as FCC or ILC. DESY is committed to continue this engagement, in particular with respect to the upcoming and demanding requests for the HL-LHC.

In PoF IV, the DESY Tier-2 center will grow into the IDAF. Storage and compute resources for additional external and internal scientific users, most significantly from photon science, will need to be prepared and provided. New methods in data analytics, accelerator simulation, the creation of “digital twins”, and theory will need to be supported through the extension of the current high-performance computing (HPC) cluster, which will become a part of the IDAF. In addition, large amounts of accelerator control data will be analyzed at the facility. The IDAF will be integrated into worldwide grid- and cloud-based infrastructures of the experiments and provide an elaborated state-of-the-art set of services for all users. It will include the resources needed for the European XFEL, which is not part of PoF IV and is funded separately through the European XFEL GmbH.

With its expanded scope, the IDAF will serve all the Programs of the Research Field *Matter* – MU, MT, and MML – and maximize the scientific potential of modern experiments and infrastructures. It will provide both interactive and batch-processing capabilities. The facility will be closely connected to the LK I activities in the new Topic MT-DMA. Technology-wise, the IDAF will integrate various types of resources, such as farm computing (HTC), HPC, GPGPUs, and various types of data storage according to the needs of the communities. Since the scientists in *Matter* are part of international communities, standard user services and access methods such as those developed for the European Open Science Cloud (EOSC) will be provided and further elaborated in close cooperation with the domain scientists. A key challenge of the transition of the Tier-2 center to the IDAF will be the integration of these different types and environments of compute resources into one facility and the provision of a well-adapted set of services to the particular user communities.

3.2. Research Environment and Current Activities

The IDAF will provide a full-size computing and data platform for simulation and analysis to a wide variety of communities and scientific users in the Research Field *Matter*.

Providing high-quality service to the HEP communities will continue to be a major challenge and goal for the IDAF. Meeting their demands will require not only investments into the hardware, but also research into new methods and algorithms, which will be done in close coordination with the Topic MT-DMA.

The demands on computing and data resources in photon science have increased dramatically with respect to previous generations of photon sources and detectors. These demands will increase even further with the next generation of facilities. The amount of data is expected to reach 100 PB/year during the PoF IV period, which is comparable to the data sizes expected from the HL-LHC. This necessitates major changes in the computing environment and the user interfaces. In particle physics, the big experiments include up to several thousand collaborators and produce nearly continuous data streams, whereas experiments in photon science are often run for only a few hours or days by a small number of scientists. The data are produced in bursts, which, as a consequence, require major changes to the computing architecture and the set of services provided to the users.

The Tier-2 center at DESY continues to be one of the largest computing centers for the experiments ATLAS, CMS, and Belle II. In Figure 2, the relative share of normalized CPU hours is shown for the largest WLCG sites. The data corresponds to the time frame 2015–2019 (ATLAS/CMS) and 2017 (Belle II).

The amount of computing and storage resources provided by the IDAF to the LHC experiments is in step with DESY's fraction of Germany's pledges to the WLCG. Together with the Tier-1 center GridKa at KIT and the ALICE Tier-2 center at GSI, these three Helmholtz Centers account for about two-thirds of the German LHC computing resources. Universities and the Max Planck Society provide the remaining parts. In addition, the IDAF will become a raw-data center for Belle II.

DESY already operates an HPC cluster primarily used by the photon science community. This cluster will become a part of the IDAF.

With cost efficiency in mind, the storage is organized in a multi-Tier structure. The major mass storage software system used is dCache, developed in a cooperation between Fermilab, the NorduGrid federation and DESY as the leading partner. The dCache development itself is a LK I activity, in future as part of the new Topic MT-DMA. dCache is used to manage large continuous input data for HPC and HTC jobs as well as long-term storage of job output data. It is supplemented by fast, interactive cluster file systems with a high rate for reading and writing of files necessary in HPC and HTC workflows. The current level of CPU and storage resources is given in Table 4.

The demands of users on the IDAF in terms of data handling and storage can only be met with new developments. The IDAF is closely linked to and relies on the LK I activities in MU, MT and MML, with respect to new methods and algorithms. Projects such as the Helmholtz Analytic Framework or AMALEA on AI form some of the close connections between the LK I activities and the LK II facilities.

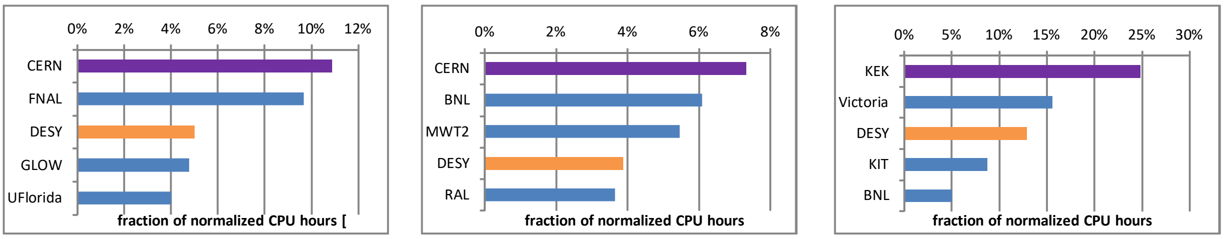

Figure 2: Relative share of normalized CPU hours for the largest WLCG sites for CMS (left), ATLAS (center), and Belle II (right). The Tier-0 centers are colored in purple, DESY in orange. Source: EGI accounting portal.

Table 11: Resources allocated to the HPC and HTC cluster in the IDAF as of April 2019.

Cluster	Number of Cores	Memory [GB]	Interactive Storage [PB]
HPC	26.568	224.871	4,9
HTC	26.728	80.184	18,6

We are very active in computing and big-data projects on the national and European level. We are coordinating proposals from particle physics and from photon science to be launched at the German national research data initiative (NFDI). DESY is a partner in many European projects for the setup of the EOSC and very active in the setup of the computing environment for the HL-LHC and in the context of the League of European Accelerator-based Photon Sources (LEAPS).

3.3. Content and Objectives

Paradigms in science are changing, and the importance of scientific computing in particular is constantly increasing. Access to federated resources across sites and countries is becoming mandatory for scientific research. Driven by user demands, computing and data management need to be provided as an integral part of sites operating large-scale scientific facilities. The IDAF will become an integral and highly relevant part of the experiments and offer a complete analysis environment. The approach outlined in this proposal has been conceived to maximize the scientific harvest of data, adapting to the changing path towards scientific knowledge and discoveries.

The start of the LHC Run 3 in 2022 will result in an increase in computing requirements of about 25% to 40%. Estimations for the following HL-LHC Run 4, which is due to start in 2026, predict a further increase by a factor of 5 to 10 for the computing and storage resources, corresponding to an exabyte per year. As one of the largest Tier-2 centers, the IDAF will continue to be a significant data and analysis hub for the LHC experiments. The photon science facilities PETRA III and European XFEL, which the IDAF will also serve, are expected to collect more than 100 PB/year by 2023.

3.3.1. Expected Achievements and Development Potential

The upcoming PoF IV period will present a series of challenges. The migration of the Tier-2 center to the IDAF by integrating the HPC cluster, new hardware accelerators, and new storage systems demands further improvements to the existing infrastructure. These challenges are driven by requirements from research (e.g. HL-LHC, PETRA III, European XFEL) and accelerator operations. They are impacted by new detectors, higher trigger rates, near-real-time analysis, and the huge number of sensors. New analysis algorithms such as machine learning, new computer hardware such as GPGPUs, FPGAs, and TPUs, as well as new storage systems have to be introduced. New concepts for the provision of resources, in particular regarding their connectivity and federation, have to be developed. This will result in a large set of new services and computing models, which will take open access, open data, and the FAIR principles into account. As a first step, the IDAF will integrate cloud-based services from projects such as the EOSC [IDAF-1].

Cloud technologies allow new concepts to alleviate the scientists' workflows. The IDAF will offer such services to all users independently of their fields of research. These mechanisms are related to the principle of Function as a Service (FaaS). This will allow e.g. scientists at the beamlines to view automatically calibrated and analyzed data using modern tools such as Jupyter notebooks by simply requesting these features at the proposal level [IDAF-2].

The end of the PoF IV period will see the commissioning of the CTA observatory and the HL-LHC, for both of which additional resources and services will need to be provided [IDAF-5, IDAF-6].

3.3.2. Milestones

Table 12: Milestones for the IDAF.

	Year	Milestone
IDAF-1	2022	Integration of EOSC, PANOSC, and EXPANDS services (authentication and authorization infrastructure, data management, catalogs, metadata systems)
IDAF-2	2022	Integration of cloud-based data management services and resources
IDAF-3	2023	Upgrade of the HPC system to $O(100000)$ cores
IDAF-4	2024	Network upgrade to 2x100 Gb/s
IDAF-5	2024	Full integration of CTA into the IDAF
IDAF-6	2026	Full operation of the IDAF for the HL-LHC

3.3.3. Planned Investments/Upgrades of the Facility

The upgrade of the DESY PoF III Tier-2 center into the IDAF requires a major investment of resources at DESY and cannot be achieved with a flat budget. Furthermore, facilities such as the HL-LHC and possibly PETRA IV require additional resources. Advances in technology can reduce, but not solve the problem. Additional sources for investments have to be identified [IDAF-3]. Especially within the context of the HL-LHC, a fast network connection is vital. For this reason, the network bandwidth has to be increased to two times 100 GB/s [IDAF-4].

Finally, upgrades of power and cooling infrastructures are necessary as well.

3.4. Life Cycle Analysis

The research infrastructure of the IDAF is driven by the scientific needs of the Research Field *Matter,* in particular by the LHC and photon science experiments. Plans for all these experiments reach beyond the PoF IV period into the 2030s. In addition, support for new facilities and experiments such as PETRA IV will be added in the future, with computing continuing to play a central role. A continuous replacement policy for the resources is necessary; the lifetime of compute resources is about three to five years, of storage five years, and of network equipment seven to ten years.

3.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to IDAF.

Table 13: IDAF (Successor to Tier-2) Resources (DESY), planned for 2021 (in TEUR). The costs include general and administrative costs, internal services etc.

DESY costs (TEUR)	**6.406,0**
thereof personnel costs (including personnel of infrastructure)	3.066,0
thereof material costs	1.403,0
thereof electricity	1.100,0
thereof maintenance costs	100,0
thereof telephone costs	100,0
thereof noncash expenditures	1.937,0
DESY investments	
continuing investments	2.647,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	

Table 14: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

DESY costs	6.406,0
- noncash expenditures	1.937,0
+ continuing investments	2.647,0
+ ongoing individual large investments > € 2,5 million	0,0
DESY cash expenditures	**7.116,0**

Table 15: Program personnel capacity by center (FTE), planned for 2021.

DESY part personnel	22
Scientists/Engineers	16
Scientific support personnel	6
for information only: corresponding Helmholtz program (LK I) – DESY contribution	154
Scientists	79
Doctoral students	28
Scientific support personnel	47
for information only: corresponding Helmholtz program (LK I) - total	424
Scientists	244
Doctoral students	66
Scientific support personnel	114

Table 16: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
DESY	1.724,9	19	247,5	3
Scientists/Engineers	1.261,8	13	240,3	3
Scientific support personnel	463,1	6	7,2	0

C. *FROM MATTER TO MATERIALS AND LIFE*

The backbone of research within the Program MML is the unique portfolio of complementary large-scale facilities and their development, construction, maintenance, and operation. In the following, the individual facilities are presented along with current development plans, grouped according to infrastructures for photons (I), neutrons (II), ions (III), and high electromagnetic fields (IV).

I. PHOTON FACILITIES

Progress in many scientific fields depends crucially on the availability of sophisticated analytical techniques that are able to reveal the static structure of samples with highest possible resolution and their dynamics at relevant time scales. In this sense, experiments using synchrotron and free-electron laser (FEL) radiation have become indispensable analytical tools for scientists to contribute significantly to solving grand challenges for a wide area of disciplines, such as health, energy, environmental science, information, and mobility-related sciences. The research at photon facilities drives the development of enabling technologies and innovation. The applied photon energies range from THz radiation (≤ 10 meV) over the X-ray regime (several keV) to high-energy X-rays (> 50 keV), allowing for probing the geometric, electronic, and magnetic structure as well as the dynamics and function of matter over a large span of length and time scales. A variety of beam properties can be tuned to the specific requirements of the experiments. Element sensitivity can be achieved by tuning the energy of the incident radiation to specific absorption edges, and polarization control enables the investigation of magnetic properties. Depending on the photon energy and scattering geometry, experiments can be made surface-, interface-, or bulk-sensitive. The coherent fraction of the X-ray beams allows for high-resolution imaging with lenses or techniques such as holography and phase contrast microtomography as well as for studies of the slow dynamics by intensity correlation spectroscopy. Samples that are heterogeneous on the mesoscale or extremely small samples can be studied using extremely focused photon beams with focal spot sizes down to below 10 nm. The penetration power of X-rays allows for a wealth of different sample environments that enable *in-situ* or *operando* investigations under relevant working and processing conditions. The temporal resolution of storage ring sources spans from quasi-static down to tens of picoseconds, while FELs provide a resolution down to the femtosecond time scale.

Within the Program MML, the two storage-ring-based synchrotron radiation sources BESSY II and PETRA III as well as the FEL FLASH are operated as user facilities for a national and international science community. In addition, the Helmholtz Association contributes considerably to the operation of the European XFEL. The characteristics of the individual sources are:

- PETRA III at DESY is one of the most brilliant storage-ring-based X-ray sources for high-energy photons and coherence applications worldwide. It is operated at a particle energy of 6 GeV and is therefore especially suited to produce X-rays at high energies up to 200 keV. The experiments at the currently 21 (27) beamlines with about 40 (50) stations focus on research with hard and high-energy X-rays using nanofocused and well-collimated X-ray radiation (the full capacity will be achieved within PoF IV). In comparison to PETRA III similar sources are the ESRF, APS, and Spring-8. At present PETRA III is the source with the lowest emittance among these competitors. However, PETRA III will fall behind these sources in this respect as soon as the upgrades at ESRF, APS, and SPRING-8 will be concluded. This will be addressed by the proposed upgrade to PETRA IV, which will place PETRA IV at the forefront in terms of emittance a coherent flux.
- BESSY II at HZB is a world-class third-generation synchrotron radiation source optimized for the spectral range from VUV to soft X-rays with currently 27 beamlines and 37 experimental stations in user operation. Based on HZB's long-standing expertise in the development of undulators, precision optics, novel techniques, and instrumentation, high spatial, temporal, and spectral resolution as well as complete polarization control are available for advanced spectroscopy and imaging applications. With its operating particle energy of 1.7 GeV BESSY II is providing complementary radiation properties to most European synchrotron radiation sources that are operating at energies larger than 2.5 – 3 GeV. Therefore, the main application fields of BESSY II concentrate on the soft to tender X-ray regime. Compared to presently operating sources, BESSY II competes very well on an

international level. However, almost all major sources with similar application fields (e.g. ALS, ELETTRA) plan or prepare upgrades for lower emittances. The proposed construction of BESSY III will guarantee worldwide competitive beam parameters in the soft to tender X-ray photon energy regime.

- FLASH at DESY was one of the world's first short-wavelength FEL facilities. Thanks to its superconducting accelerator technology, FLASH is able to deliver up to 8,000 photon pulses per second in bunch trains of 800 µs with 10 Hz repetition rate to experiments. FLASH is operating in the XUV and soft X-ray regime with two FEL lines in parallel with independent photon beam parameters. With its particle energy of 1.25 GeV FLASH concentrates on the XUV and soft X-ray photon energy range. Therefore, it provides complementary radiation to all X-ray FELs and is comparable in terms of photon energy to the soft X-ray FELs such as FERMI or the soft XFEL branches at other FELs for example at SwissFEL or PALFEL. The worldwide unique selling point of FLASH is its high repetition rate that allows for the investigation of extremely dilute samples or experiments with extremely small interaction cross-sections. In this respect only LCLS II in the near future will be able to surpass the FLASH capabilities in its wavelength regime. FLASH is not yet externally seeded for improved spectral and temporal beam parameters as are some other FELs in this energy range. This will be addressed in the FLASH2020+-project.
- The European XFEL X-ray laser in Hamburg and Schenefeld produces X-rays in the range from 0.25 up to 25 keV out of three undulator sections that can be operated simultaneously with up to 27,000 pulses per second. The European XFEL is driven by a 17.5 GeV superconducting linear accelerator, which is operated by DESY. The European XFEL is the most powerful X-ray FEL worldwide in terms of achievable photon energy, photon pulse energy, and presently also in repetition rate. In terms of repetition rate LCLS II will surpass European XFEL in a few years, however, European XFEL will keep its leading position in terms of photon and pulse energy for the foreseeable future.

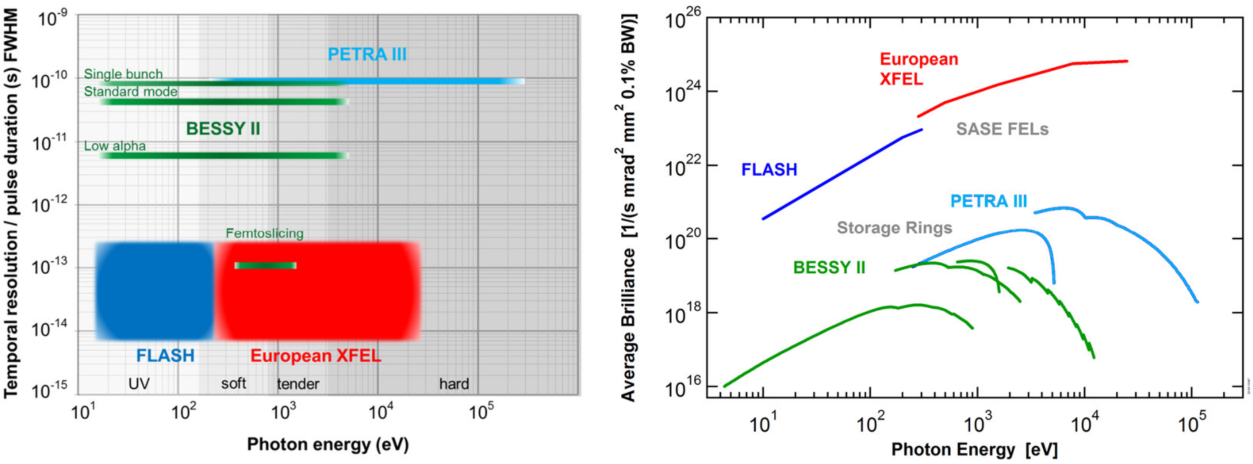

Figure 3: Temporal resolution and average brilliance for the photon energy range covered by the MML large-scale photon facilities. The photon sources cover a broad range of the relevant parameters, thus providing a full set of experimental possibilities to the users. Left: Photon fluxes and repetition rates: PETRA III: ~10^9 ph/pulse at 5.2 MHz, 10^6 ph/pulse at 125 MHz; BESSY II: 10^5 – 10^8 ph/pulse at 1.25/500 MHz, 10^6 ph/pulse at 6 kHz (femtoslicing); FLASH: < 10^{14} ph/pulse at < 8 kHz; European XFEL: < 10^{13} ph/pulse at < 27 kHz.

These MML sources cover the entire photon energy range attainable by storage-ring-based sources and by FELs (see Figure 3). As these photon sources are complementary in photon energy, pulse duration, and brilliance, researchers can address complementary experimental techniques in order to answer their scientific questions.

The MML photon science facilities provide excellent experimental capabilities to about 4,500 scientists every year, giving rise to more than 1,000 scientific publications. Additionally, the German user community has access to the ESRF synchrotron radiation source in Grenoble, France, through the German share in the facility. Funded by the BMBF ErUM framework program (former "Verbundforschung"), German university groups contribute significantly to the instrumentation, method, and technique development at the MML photon sources. On the basis of their unique technical requirements, the MML photon facilities serve to educate and train excellent technicians and engineers for the facilities' own demands and for industry.

Regarding the LK II activities in MML, a number of related cooperative projects are already being pursued and planned to foster the user operation at the MML large-scale facilities. At DESY, together with HZG and the Christian-Albrechts-Universität zu Kiel, a new Centre for X-ray and Nano Science (CXNS) is being built, which will include a nanolaboratory (DESY NanoLab) for the preparation, handling, and pre-characterization of samples on the nanoscale. HZG operates part of its German Engineering Materials Science Centre (GEMS) user facility at DESY. Also at DESY, in collaboration with a number of national and international partners, the new Centre for Structural Systems Biology (CSSB) for macromolecular investigations in the field of infection research provides complementary research possibilities by means of cryo-electron microscopy.

HZB and the Max Planck Society (MPG) are currently setting up the Berlin Joint Lab for Electrochemical Interfaces (BElChem@BESSY II) for detailed investigations of electrochemical processes in complex materials systems under realistic conditions. BElChem complements the unique experimental opportunities provided by the joint HZB/MPG Energy Materials In-Situ Laboratory (EMIL@BESSY II) for *in-situ*, *in-system*, and *operando* investigations of energy materials and processes. HZB and MPG are currently planning to further intensify their strategic partnership in the field of catalysis and energy chemistry.

Of central importance for the competitiveness of the photon facilities is the ongoing development of accelerator technology, detector systems, data analysis and computing, as well as laser systems. This is mirrored in joint projects between the facilities and with groups of the Program MT. Keeping the MML LK II facilities at the forefront of technical and scientific developments is only possible with strong accompanying in-house research activities (LK I) to drive these developments. All photon sources are closely linked to the three MML Topics MML-Matter, MML-Materials, and MML-Life: Research groups of the MML Topics are users of the facilities, and beamline scientists conduct their research within the Research Fields *Matter*, *Energy*, and *Information*.

The field of synchrotron and FEL radiation source development has been processing rapidly, especially during the last years. Using the multibend achromat (MBA) magnet design for storage rings, implemented for the first time at MAX IV in Lund, Sweden, a dramatic reduction in horizontal emittance at storage ring sources can be achieved. After the success of MAX IV, all major synchrotron radiation source operators around the world are planning or carrying out an upgrade of their storage ring to MBA-type lattices. This also holds for the two synchrotron radiation sources within the Program MML. DESY plans to upgrade PETRA III to an ultra-low emittance source in the hard X-ray regime (PETRA IV). Due to its large circumference, PETRA IV is expected to have the lowest emittance of all synchrotron radiation sources worldwide. For this project, a conceptual design report (CDR) will be presented in 2019 and a full technical design report (TDR) by the end of 2021. Construction work is expected to start in 2025 and user operation to begin in 2027. At HZB, the CDR for a novel soft X-ray facility (BESSY III) based on the MBA concept is to be completed by the middle of the PoF IV period at the latest and a corresponding TDR in the second half of the PoF IV period. DESY and HZB have agreed that the existing complementarity in terms of storage ring and main photon energy range between PETRA and BESSY will also be maintained after the respective upgrades. Both upgrades are part of the national photon science roadmap for accelerator-based photon sources.

The technical development of FELs continues to progress rapidly too. For FLASH, DESY has initiated the FLASH2020+ project, which includes the installation of tunable undulators for faster photon energy changes, external seeding for better control of the spectral and temporal properties of the photon pulses, and new lasing schemes targeted at circular polarized light, two-color experiments, and sub-femtosecond pulse duration. These upgrades are planned to be carried out during the first years of PoF IV. Within the Program MML, DESY is operating the superconducting linear accelerator for the European XFEL. As possible upgrade scenarios for this facility, a transition from the current pulsed operation with bunch trains at 10 Hz to a continuous pulse operation as well as a second fan of FEL undulators for an increased number of experiments operated in parallel are under discussion. In this case, however, all possible options still need to be discussed with the European XFEL Council and all member countries. The time frame for the realization of this upgrade will likely be beyond the PoF IV period.

The strategic development of the photon sources within the Program MML will be carried out in close consultations with the other European sources. To this end, the League of European Accelerator-based Photon Sources (LEAPS) was established, which aims at developing joined strategic and technology roadmaps and developments.

4. BESSY II

Figure 4: View of the BESSY II building

4.1. Overview

Within the above-described portfolio of complementary accelerator-based light sources operated by the Research Field *Matter*, BESSY II is Germany's synchrotron radiation facility optimized for experiments in the spectral range of soft to tender X-rays[8]. It provides world-class research opportunities for an ever-growing national and international user community exploiting the unique spectroscopic opportunities available in this spectral range. The operation and development of the BESSY II photon source are explicitly aligned with the needs of its national and international, multidisciplinary user community. The BESSY II facility is recognized worldwide as a leader in high-resolution spectroscopy, flexible pulse patterns for advanced time-resolved experiments, and innovative instrumentation for *in-situ* and *operando* measurements[9].

HZB's strategic objective for BESSY II is to maintain and further develop its unique capabilities, thereby providing the user community with unique experimental opportunities for their research. The specific goals for BESSY II are therefore to:

- Ensure that BESSY II remains a world-leading soft X-ray user facility by continuous modernization of the accelerator, beamlines, end-stations, and supporting infrastructures;
- Develop the variable-pulse-length storage ring (VSR) scheme to enable novel capabilities for time-resolved experiments, and establish novel timing modes;
- Define BESSY III, the successor source of BESSY II, based on scientific and technological needs, and establish the facility project on the relevant roadmaps.

The soft X-ray range is uniquely suited for spectroscopic methods, which are powerful tools for advanced analytics and therefore play a key role for research and development in materials and energy science. The BESSY II source is thus not only pivotal for achieving the goals of the Program MML of the Research Field *Matter*, it also plays a key role for Programs of other Research Fields. Most notably, these are the Program *Natural, Artificial and Cognitive Information Processing* of the Research Field *Information* and the Program *Materials and Technologies for the Energy*

8 From tens of eV to a few keV, referred to in the following as soft X-ray range.
9 More information on BESSY II: www.helmholtz-berlin.de/quellen/bessy/index_en.html

Transition of the Research Field *Energy*. The unique Energy Materials In-Situ Laboratory (EMIL@BESSY II) for *in-situ*, *in-system*, and *operando* investigations of materials and processes is of special relevance in this context. BESSY II is therefore a cornerstone of the Cross-Cutting Activities *Materials Research*, *Quantum Technologies*, and *Structural Biology and Biological Processes* of the Helmholtz Association. The research at BESSY II addresses forefront subjects from physics to chemistry, energy-related research, biology, medical and pharmaceutical research, to materials testing and cultural heritage. Within the approx. 5,600 instrument-days delivered per year, about 800 proposals are granted access to BESSY II: These proposals lead to approximately 3,200 user visits (corresponding to approximately 1,450 individual users) and more than 500 peer-reviewed publications, a clear indication of the quality of the user community and the excellent experimental conditions offered at BESSY II.

4.2. Research Environment and Current Activities

HZB is a cornerstone of the vibrant Berlin–Brandenburg science area. The Physikalisch-Technische Bundesanstalt (PTB) and the Max Planck Society (MPG) are quintessential strategic partners of HZB. PTB uses BESSY II as the European radiation standard and operates a dedicated metrology laboratory at BESSY II that frequently attracts industrial users. The MPG has built and operates a suite of beamlines at BESSY II and collaborates with HZB in energy research through EMIL@BESSY II, the Joint Lab for Electrochemical Interfaces (BEIChem), and a joint research group. The partnership with MPG is being further intensified in the field of catalysis and energy chemistry research using BESSY II.

HZB has longstanding collaborations with the Berlin–Brandenburg universities and universities of applied science. BESSY II is of strategic relevance to the Berlin University Alliance, the framework within which Freie Universität Berlin, Humboldt-Universität zu Berlin, Technische Universität Berlin, and Charité – Universitätsmedizin Berlin received the University of Excellence status of the German government's Excellence Initiative. Several universities and non-university research centers operate experimental stations at BESSY II and participate in state-of-the-art instrumentation development through joint laboratories or collaborative research. For example, the Berlin universities, Max Delbrück Center, Leibniz-Forschungsinstitut für Molekulare Pharmakologie, and Charité collaborate with HZB within the Joint Berlin MX-Laboratory on structural biology research projects as well as on continuously improving the capabilities of the HZB-MX beamlines. Next-generation photoelectron spectroscopy techniques, which utilize pulse-picking methods to enable time-of-flight measurements in regular user operation modes, are developed within the Uppsala-Berlin Joint Lab (UBjL).

As part of the continuous modernization of BESSY II, the increasing demands of the user community in terms of reliability, stability, and flexibility have been addressed over the past years by a series of accelerator hardware upgrades (e.g. new HOM-damped cavities, high-power solid-state amplifiers). These resulted in a noticeable increase in storage ring stability and reliability, as quantified e.g. by the achieved availability and mean time between failures (MTBF) values. New undulators and X-ray optics have been developed, exploiting HZB's long-standing expertise in these fields, to improve the facility's capabilities in the tender X-ray range relevant for the *in-situ* and *operando* characterization of energy materials and processes as well as for structural studies in the life science. New beamlines and end-stations taking full advantage of the source improvement have been put into operation. Among these are the EMIL@BESSY II infrastructure, the VEKMAG end-station for element-specific and time-resolved scattering and ferromagnetic/paramagnetic resonance spectroscopy, the upgrade of the X-ray transmission microscope (XM) beamline, and the novel resonant inelastic X-ray scattering end-station PEAXIS for energy materials research on solid samples, solutions, and liquid–solid interfaces. Several measures have been implemented to further improve the user service at BESSY II: A stringent and regular training program for beamline scientists has been launched; periodic beamline reviews are performed under the auspices of the HZB Scientific Advisory Council (SAC); a dedicated sample environment group has been established at BESSY II to develop novel capabilities and support users in their exploitation. An ISO 9001 certified quality management system for user beamtime projects has been implemented to ensure that the defined highest-quality standards for the user service are maintained. In view of the increasing relevance of data management and analysis tools, HZB has defined an implementation plan for data management and archiving as well as an open data access policy. An ongoing series of foresight workshops explores the future needs of established and emergent user communities, addressing short-term needs at BESSY II, plans for time-resolved experiments at BESSY VSR, and long-term visions for the next-generation light source at HZB.

4.3. Content and Objectives

4.3.1. Expected Achievements and Development Potential

With BESSY II entering its third decade of operation, the modernization of key components will play a crucial role over the coming years (see planned investments below). This offers the opportunity to provide the user community with novel experimental capabilities and to develop technologies on which the future source BESSY III will be based. New unique end-stations will be installed, among them as a first milestone [BES.1] the METRIXS station, which is optimized for RIXS measurements at resonances of transition metals, carbon, oxygen, and nitrogen. METRIXS is complementary to the hRIXS end-station that is being realized at the European XFEL within the Helmholtz International Beamline (HIB). Optimized access to the tender X-ray range with full polarization control will be enabled by the realization of an in-vacuum helical undulator (IVUE-32) and multilayer-coated grating technology [BES.3]. Ever more stringent requirements on beam quality lead to increased complexity of the beamlines and the need for advanced diagnostics. Novel control system concepts for the storage ring and the beamlines are therefore necessary for the optimization and daily supervision of these installations. The framework of the novel control system is currently being defined in view of BESSY III, and the foundations will be laid within the Topic MT-DMA. Once developed, the system will be implemented in a new undulator beamline, which will serve as a test bed prior to the role-out of the system as a new beamline diagnostics, control, and data acquisition standard [BES.4]. The BESSY VSR project capitalizes on HZB’s scientific and technological expertise in accelerator research and development (Topic MT-ARD) as well as its expertise in developing, operating, and realizing time-resolved experiments down to the femtosecond time scale. The ability to produce short pulses in a superconducting radio frequency (RF) cavity in a storage ring will be demonstrated with the preparatory phase module [BES.5]. This is an important step to enable the realization of the full VSR scheme, to generate simultaneously long and short photon pulses in a storage ring.

4.3.2. Milestones

Table 17: Milestones for BESSY II.

	Year	Milestone
BES.1	2021	User operation of the Momentum Transfer Resonant Inelastic X-ray Scattering (METRIXS) beamline
BES.2	2022	BESSY III CDR
BES.3	2023	User operation of a short-period in-vacuum elliptical undulator at a beamline with multilayer-coated blazed grating enabling X-ray microscopy in the tender X-ray range
BES.4	2023	Implementation of a novel beamline diagnostics and control system at a reference beamline at BESSY II/BESSY VSR
BES.5	2024	First operation with the BESSY VSR preparatory phase module
BES.6	2025	BESSY III TDR

4.3.3. Planned Investments/Upgrades of the Facility

A number of investments are planned within the PoF IV funding period for the continuous modernization of BESSY II (18 M€) as well as the realization of the BESSY VSR project and the preparation of the BESSY II beamlines and end-stations for their scientific exploitation (10 M€). In addition, the setup of a flexible infrastructure to implement the HZB strategy for data management, archiving, and open access to data requires investments in both hard- and software (3 M€).

4.4. Life Cycle Analysis

BESSY II has been in operation since 1998. With the decision of the Helmholtz Association in June 2017 to fund the development of the variable-pulse-length storage ring (VSR) scheme and to implement it in BESSY II, a commitment was made to extend the lifespan of the facility over the coming decade. However, only by developing a novel source – BESSY III – can international competitiveness be preserved. Smart optimization and specialization of this facility and its associated infrastructure will yield worldwide unique experimental capabilities, matching the need of HZB's research and attracting the brightest minds from all over the world. Complementarity with other national (DALI, PETRA IV, FLASH) and European photon sources will be a key aspect for the development of BESSY III. This is also ensured by HZB's active participation in LEAPS and the related roadmap process. A key aspect of the novel BESSY III facility will be highest stability, enabling nanometer spatially resolved experiments with unprecedented spectral resolution. The combination of a diffraction-limited storage ring with the VSR concept would allow the implementation of longitudinal bunch shaping in addition to transversal bunch shaping. This would provide stable, diffraction-limited beams in the soft X-ray region together with flexibility for time-resolved experiments, thus opening up new scientific opportunities. The BESSY III project has recently been implemented, and the conceptual design phase has started. HZB's strategic partners, especially the PTB and MPG, are closely involved in the process. The finalization of the CDR is planned for 2022 [BES.2]. This will be followed by the technical design phase, with the concluding TDR foreseen for 2025 [BES.6]. The integration of BESSY III into the research infrastructure strategy of the Helmholtz Association will be part of this process, as will be the application for inclusion in the national roadmap for large-scale research infrastructures (BMBF).

4.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 18: BESSY II Resources (HZB), planned for 2021. The costs include general and administrative costs, internal services etc.

HZB costs (TEUR)	**48.718,1**
thereof personnel costs (including personnel of infrastructure)	29.328,6
thereof material costs	11.125,9
thereof electricity	5.984,0
thereof noncash expenditures	8.263,6
HZB investments	
continuing investments	7.500,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	649,0

Table 19: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

HZB costs	48.718,1
- noncash expenditures	8.263,6
+ continuing investments	7.500,0
+ ongoing individual large investments > € 2,5 million	649,0
HZB cash expenditures	**48.603,5**

Table 20: Program personnel capacity by center (FTE), planned for 2021.

HZB part personnel	216
Scientists/Engineers	152
Scientific support personnel	64
for information only: corresponding LK I contribution HZB	36
Scientists	23
Doctoral students	11
Scientific support personnel	2
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 21: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
HZB	16.031,0	216	459,3	7
Scientists/Engineers	12.191,0	152	417,50	6
Scientific support personnel	3.840,0	64	41,80	1

5. FLASH

5.1. Overview

FLASH is the world's first short-wavelength FEL facility. It started user operation in 2005. Based on the superconducting accelerator technology developed within the TESLA Technology Collaboration at DESY, it can presently provide up to 5,000 pulses per second to users for experiments in diverse fields. With its wavelength range, FLASH is fully complementary to the only other running high-repetition-rate FEL, the European XFEL in Hamburg and Schenefeld. FLASH is currently – and will likely be in the future – the world's only high-repetition-rate FEL in the XUV/soft X-ray regime[10]. In the coming years, the ambitious upgrade plans FLASH2020+ will develop the potential of the FLASH user facility even further.

Several hallmark experiments have been carried out at FLASH that demonstrate the unique capabilities of short-wavelength FELs as well as key developments in photon diagnostics and beamline instrumentation that are now used at many FEL facilities around the world.

Figure 5: The FLASH facility with its two FEL lines and experimental halls.

Since 2016, FLASH has been providing users with pulses from the second FEL line FLASH2 in parallel to the operation of FLASH1 (see Figure 5). FLASH2 improves the performance for users with variable-gap undulators that enable easy wavelength tuning and novel FEL lasing schemes. The progress in creating and measuring ultrashort, fully coherent single-spike self-amplified spontaneous emission (SASE) pulses as well as the new state-of-the-art suite of dedicated end-stations (operated by DESY and its partners) ensure the continuing attractiveness of FLASH for users.

With its current parameter range and performance and even more so with the planned upgrade, FLASH brings unique opportunities to the Research Field *Matter* and plays an important role for the Topics MML-Matter and MML-Materials, as acknowledged in the recent Helmholtz center review report.

The facility also contributes actively to the Topics MT-ARD, MT-DTS, and MT-DMA.

5.2. Research Environment and Current Activities

FLASH has been the initial spark of a worldwide unique hub for FEL science in Hamburg, which includes the Center for Free-Electron Laser Science (CFEL) and the European XFEL. The facility is embedded in an excellent environment for photon science on the DESY campus with PETRA III, the DESY NanoLab – a laboratory for preparing and characterizing nanometer-sized samples –, the new Center for Structural Systems Biology (CSSB), the European Molecular Biology Laboratory (EMBL) outstation, several institutes of the Universität Hamburg, and the new Max Planck Institute for the Structure and Dynamics of Matter (MPSD).

10 More information on FLASH: http://photon-science.desy.de/facilities/flash/index_eng.html

On the national level, FLASH greatly benefits from funding by the BMBF for collaborative research with German universities (ErUM framework program). Science at FLASH also receives substantial support by the Universität Hamburg cluster of excellence *Advanced Imaging of Matter* (AIM).

A number of collaborations on technological and methodological developments as well as science applications with short-wavelength FELs exist with other FEL facilities, e.g. FERMI in Trieste, SwissFEL at PSI, LCLS at SLAC, and the European XFEL. FLASH is also a strong partner in activities on the European level, such as EUCALL, CALIPSOplus, FELs of Europe, and in particular the LEAPS consortium. The scientific activities at FLASH currently cover the research areas atomic, molecular, and optical (AMO) physics, chemistry and energy science, condensed matter science, life sciences, nanoscience, warm dense matter research (WDM), and method and instrumentation development (M&I), as shown in Figure 6. FLASH serves approximately 350 individual users per year (corresponding to 500 user visits).

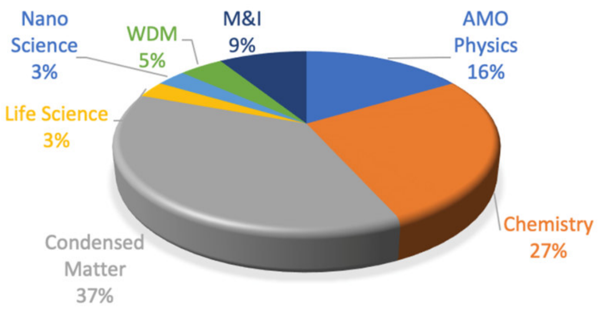

Figure 6: Research areas covered by the scientific activities at FLASH.

The outstanding opportunities for time-resolved studies at FLASH, which are based on exquisite pump–probe instrumentations including fully synchronized optical lasers, a variety of X-ray split-and-delay units, a THz source that is phase-stable with respect to the FEL pulses, and sophisticated diagnostics for pulse arrival time and duration, have led to close to 90% of current experiments performed at FLASH targeting ultrafast processes in the sub-picosecond range.

5.3. Content and Objectives

DESY's intention for PoF IV is to continue the operation of FLASH as a worldwide unique user facility. Therefore, the future goal for FLASH is an upgraded high-repetition-rate XUV and soft X-ray FEL facility, which ensures that FLASH stays at the forefront of FEL science and technology for the next decade. The resulting strategy FLASH2020+ is based on an ambitious development program for the two FEL lines and the FLASH accelerator, which focuses on maintaining operation of two independent FEL lines (FLASH1 and FLASH2) for users.

5.3.1. Expected Achievements and Development Potential

Within FLASH2020+, both FEL lines will be equipped with fully tunable undulators and be able to deliver photon pulses with variable polarization. Up to now, this capacity is limited due to the fixed-gap undulators at FLASH1, which imply that the wavelength requested for experiments at this FEL line determines the beam energy of the linear accelerator. Tunable undulators at FLASH1 [milestone FLA.2] will allow fully parallel operation of the two FEL lines. This will increase the available time for user experiments by almost 50%. Furthermore, with the new undulator configuration, it will be possible to run the accelerator with typically only two working points in terms of beam energy, which will significantly reduce tuning time overhead and increase stability, again increasing the attractiveness and available beamtime for users. Along with the undulators, the FLASH1 photon diagnostics will be upgraded to FLASH2 standards [FLA.3], since some of the basic diagnostic components at FLASH1 are already 15 years old.

In addition to the improvement based on the evolution of the current working conditions, the FLASH2020+ project will also add new qualities to the provided beams that are strongly requested across the user community.

One of the two FEL lines will be fully externally seeded [FLA.4] at the full repetition rate that FLASH can provide in burst mode. The other line will exploit novel FEL lasing concepts based on variable undulator configurations [FLA.5]. Together with a small increase in electron beam energy to 1.35 GeV [FLA.1], this will extend the wavelength reach of the fundamental harmonics to the oxygen K-edge, in order to cover the important elemental resonances for energy research and the entire water window for biological questions, while still staying complementary to the European XFEL.

With close to 90% of the experiments at FLASH being time-resolved and carried out in some kind of pump–probe scheme, an important user request is pump pulses with a large flexibility in wavelength range. While the condensed-matter community requires THz and mid-IR pump pulses, experiments targeting molecular reactions need tunable pump sources from the visible to the UV and even VUV range. To meet these requirements and enable seeding at high repetition rate, the FLASH2020+ concept includes further efforts in the development of high-average-power short-pulse lasers.

Users at FLASH but also at other facilities worldwide strongly push towards ever shorter pulses even down to the attosecond regime. Single-spike SASE FEL pulses have been recently realized at FLASH, pushing the limits in time resolution towards the few-femtosecond and sub-femtosecond regime. Here, synchronization and timing stabilization of the FEL lines with respect to external lasers will be of key importance for experiments and are constantly being improved at FLASH. However, reaching few hundred attosecond photon pulses requires – in particular in the XUV and soft X-ray regime – the realization of new concepts based on laser manipulation of the electron bunches. From simulations for FLASH2, it was deduced that attoFLASH would be very competitive below 10 nm in comparison to lab-based laser sources, which rely on high-harmonic generation and have certain limits in average power. FLASH2020+ includes a dedicated R&D program towards this goal.

The upgraded FLASH facility will combine the established, unique characteristics of FLASH (short and intense XUV to soft X-ray pulses at high repetition rate) with some essential new features that are very beneficial for scientific studies:

- Improved wavelength tunability of FLASH1 [FLA.2] together with the smaller seeded bandwidth will optimize the FLASH1 radiation for high-throughput time-resolved spectroscopy.
- Seeding at FLASH1 [FLA.4] will yield fully coherent pulses with completely new scientific applications, e.g. for phase control, interferometric experiments, and novel coherent methods.
- Full polarization control at FLASH1 and FLASH2 allows for selectivity to sample symmetries, such as orientations of orbitals, chirality, or magnetic properties.
- Few- to sub-femtosecond tunable two-color pulses at FLASH2 [FLA.5] provide unique access to sub-femtosecond dynamics with high resonant element selectivity and sufficient intensity, not achievable with alternative sources.
- The extended wavelength range [FLA.1] provides spectroscopic access to the full water window, the chemically most relevant C, N, and O K-edges, and the L-edges of all 3d transition metals with highest information content.
- Novel opportunities for time-resolved experiments will allow tailored trigger pulses to initiate non-equilibrium dynamics.
- Pulses with a duration down to below 100 as and with nJ pulse energies below 10 nm will open up new opportunities for attosecond science.

The upgraded FLASH facility will ensure that national and international users will find unique research opportunities at FLASH also in PoF IV. FLASH2020+ will provide excellent conditions for continued research in AMO science and astrochemistry, quantum materials and magnetism, chemistry and energy science. Furthermore, FLASH2020+ will create new opportunities for the life sciences and imaging as well as non-linear X-ray and attosecond science.

As a result, FLASH will continue to play a prominent role in the Research Field *Matter* with a strong emphasis on contributions to the Topics MML-Matter and MML-Materials.

5.3.2. Milestones

Table 22: Milestones for FLASH.

	Year	Milestone
FLA.1	2021	Upgrade of the linear accelerator: increase in energy, change of the FLASH compression scheme, implementation of a transverse deflecting structure (TDS) and afterburner undulator at FLASH2
FLA.2	2021/2022	Installation of new undulators with variable gap for FLASH1
FLA.3	2021/2022	Upgrade of the FLASH1 photon diagnostics to FLASH2 standards
FLA.4	2022/2023	Seeding with high repetition rate (range of 100 kHz)
FLA.5	2024/2025	New configuration of magnet structures at FLASH2 for novel lasing concepts

5.3.3. Planned Investments/Upgrades of the Facility

The upgrade of FLASH within the FLASH2020+ - project will require investments in new variable-gap undulators for the FLASH1 line [FLA.2], in high-repetition-rate seeding lasers at FLASH1 [FLA.4], in flexible pump–probe laser schemes, and finally in new undulator magnet structures for advanced lasing options and for the generation of few-femtosecond down to attosecond pulses at FLASH2 [FLA.5]. It is planned to fund this project from DESY's major investment corridor.

5.4. Life Cycle Analysis

FLASH2020+ will fulfill almost all of the user requirements for a future high-repetition-rate FEL facility in the XUV/soft X-ray regime, with great potential for scientific breakthrough results for the next decade. The only exception is that user wishes for operation in a quasi-continuous pulse mode with a variable repetition rate up to 100 kHz (similar to plans at SLAC with LCLS II and in Shanghai with the SHINE project) will not be realized within FLASH 2020+.

Therefore, the DESY strategy beyond 2030 includes a possible, proposed scenario where, after the European XFEL is turned into a quasi-continuous-wave (CW) FEL and a second fan of FEL lines is added – which implies major investments and approval by the European XFEL management and Council – DESY explores the option to offer the user community the operation of an independent "FLASH-like" user facility at a lower-electron-energy branch as part of an upgraded European XFEL. Further details of such an activity need to be worked out as soon as boundary conditions from the European XFEL side have been clarified.

5.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 23: FLASH Resources (DESY), planned for 2021. The costs include general and administrative costs, internal services etc.

DESY costs (TEUR)	**44.365,0**
thereof personnel costs (including personnel of infrastructure)	24.843,0
thereof material costs	12.463,0
thereof electricity	5.600,0
thereof operation cryo plant	711,0
thereof gases	300,0
thereof noncash expenditures	7.059,0
DESY investments	
continuing investments	6.096,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	10.000,0

Table 24: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

DESY costs	44.365,0
- noncash expenditures	7.059,0
+ continuing investments	6.096,0
+ ongoing individual large investments > € 2,5 million	10.000,0
DESY cash expenditures	**53.402,0**

Table 25: Program personnel capacity by center (FTE), planned for 2021.

DESY part personnel	181
Scientists/Engineers	125
Scientific support personnel	56
for information only: corresponding LK I contribution DESY	197
Scientists	109
Doctoral students	57
Scientific support personnel	31
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 26: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
DESY	14.626,9	177	0,0	0
Scientists/Engineers	10.942,5	119	0,0	0
Scientific support personnel	**3.684,4**	**58**	**0,0**	**0**

6. PETRA III

6.1. Overview

The third-generation synchrotron radiation source PETRA III delivers bright beams mainly in the hard and high-energy X-ray range, enabling users to exploit the high brightness and coherence for *in-situ* and *operando* X-ray experiments. PETRA III is the central facility for experiments with high photon energies for the Program MML. With its unique experimental capabilities, it serves users from a wide spectrum of research fields[11].

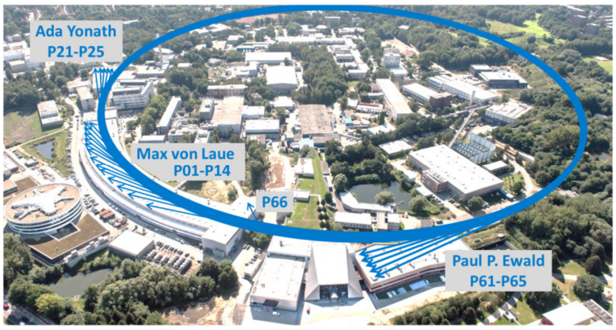

Figure 7: View of the PETRA III storage ring (blue ellipse) with the three experimental halls. Beamlines are sketched as blue arrows.

As of 2019, PETRA III is the brightest storage-ring-based X-ray sources for high-energy photons worldwide. It operates at a particle energy of 6 GeV and a beam current of 100 mA in top-up mode both with a continuous bunch filling and in a timing mode of operation. During about 5,000 hours per year, PETRA III serves experiments with photon energies between 150 eV and 200 keV. A maximum spectral brightness of 10^{21} photons/(s·mm^2·mrad^2·1% BW) is achieved thanks to the low horizontal and vertical emittances of 1.2 nm rad and 0.01 nm rad, respectively, outperforming any other current high-energy (6 GeV and higher) storage ring in the world by at least a factor of 2. This makes PETRA III an exceptional synchrotron radiation light source with unique applications in physics, chemistry, and biology, materials, biomedical, and nanoscience, as well as cultural heritage. Many experiments are carried out under *in-situ* or *operando* conditions, making use of the superior coherence and focusing properties of the X-rays. For user experiments, 21 insertion device beamlines distributed over three experimental halls are in operation with more than 40 different experimental stations (see Figure 7).

The major goals for the PoF IV period are: 1) completion of the beamlines of the ongoing PETRA III extension project, 2) upgrade to the ultralow-emittance light source PETRA IV, and 3) implementation of the full scope of computational user support.

6.2. Research Environment and Current Activities

PETRA III is an important part of the local, national, and international photon science communities and serves specialized experiments to satisfy the strategic needs of cooperation partners and user communities.

Three different and complementary X-ray sources are operated on the science campus in Hamburg-Bahrenfeld: PETRA III, the VUV and soft X-ray free-electron laser FLASH, and the European XFEL hard X-ray laser. At DESY, several research groups and infrastructures are strongly linked to PETRA III: The X-ray detector development group at DESY, which is part of the Program MT, designs, develops, and builds X-ray pixel detectors for high-end applications at the PETRA III beamlines. Research groups within MML and beyond are connected to PETRA III, for example through interdisciplinary science centers on the campus. The Center for Free Electron Laser Science (CFEL) and the Center for Structural Systems Biology (CSSB) strongly rely on the experimental capabilities at PETRA III, in particular in macromolecular crystallography. The Center for X-ray and Nano Science (CXNS), which is currently being built in

11 More information on PETRA III: http://photon-science.desy.de/facilities/petra_iii/index_eng.html cooperation with the Christian-Albrechts-Universität zu Kiel and HZG, hosts the DESY NanoLab, which complements experiments at PETRA III with various nanoscience methods for research within MML and in terms of user support. In the future, the Center for Molecular Water Science (CMWS) will be strongly be connected to the PETRA III beamlines for studying various aspects of water science, such as water dynamics and water under extreme conditions. Of particular relevance will be the link with the future Center for Data and Computing Sciences (CDCS), which is planned to bundle expertise in research from the Hamburg universities and DESY regarding data analysis and computer science in Hamburg.

The PETRA III experiments are operated in collaboration with Helmholtz partner institutes: HZG is responsible for the beamlines P07 and P05, which are dedicated to materials science and complement the neutron experiments at the MLZ in Garching and at the future neutron source ESS in Lund, Sweden. Helmholtz Centers from the Research Field *Health* are shareholder of the bioimaging and diffraction beamline P11. With its specialization on coherence and nanometer focus applications, the soft to tender X-ray beamline P04 complements experimental capabilities at BESSY II. Max Planck Institutes hold significant shares of the Dynamics Beamline P01 and the chemical crystallography beamline P24. The priority access beamtime provided at these beamlines is of high significance for the strategic goal of these institutions to understand complex materials. All these partner institutions cover at least parts of the investments and operation costs of the beamlines and bring in their expertise to extend the experimental possibilities at PETRA III.

A unique instrument for cooperation is the BMBF ErUM framework program, which provides federal grants with three-year duration to university groups collaborating with large-scale facilities. Since 2010, grants with direct PETRA III context and total budgets of more than 5 million euros per year have been awarded, proving the eminent impact of PETRA III on the German science landscape.

On the European level, PETRA III is part of the League of European Accelerator-based Photon Sources (LEAPS) and leads the LEAPS activity for developing a standardized timing system with sub-nanosecond accuracy. The European Molecular Biology Laboratory (EMBL) operates three beamlines with the strategic goal of solving the structure of biological matter to reveal its function. Swedish institutes have identified PETRA III as an ideal complement to the Swedish medium-energy X-ray source MAX IV and fund the Swedish materials science beamline P21 at PETRA III for experiments using high-energy photons.

Internationally, the Republic of India has declared the beamlines and experiments at PETRA III strategically important for Indian scientists and provides funds amounting to an equivalent of 1,3 beamlines to guarantee Indian users access to PETRA III through a separate peer-review process.

In the recent years, with an average 18 beamlines in operation, PETRA III served approximately 2,700 individual academic and industrial users per year (corresponding to 4,600 user visits), of whom about one third have international affiliations. Among the German users, 21% are from Helmholtz Centers. The number of users will increase in the next few years as another five beamlines will become operational.

In conjunction with PETRA III beamtimes, users can apply for access to the DESY NanoLab, which offers full support for certain nanocharacterization and -preparation methods, such as atomic-force microscopy (AFM), scanning electron microscopy (SEM), focused ion beam (FIB), ultrahigh-vacuum surface analytics, and dedicated sample environments for *in-situ* and *operando* experiments.

With increasing complexity of experiments at PETRA III, a growing computational effort for interpreting the experimental data is required, and users need more advanced support for data handling and evaluation. In many cases, the amount of data is too large to be transferred to and handled at the users' home institute. Therefore, PETRA III aims for a completely new user support concept: Users will be offered the full pathway from data collection over visualization, near-real-time analysis, and data management to full analysis including simulation and modeling. To this end, the DESY strategy comprises a significant upgrade of the data evaluation and scientific computing infrastructure. The realization of this concept is closely connected to the MT facility IDAF and reaches out to research groups at DESY and at the local universities in the frame of the CDCS.

The storage ring PETRA has a particularly large circumference (2,304 m) and thus offers the unique opportunity to push the generation of synchrotron radiation to its physical limits. DESY plans a major upgrade of PETRA III to the ultralow-emittance source PETRA IV. With a horizontal and vertical emittance in the range of 10–20 pm rad, PETRA IV would reach the diffraction limit for hard X-rays of up to about 10 keV in both planes. In this way, PETRA IV would become the ultimate X-ray microscope, enabling users to follow chemical and physical processes in complex and materials *in-situ* and on all length and time scales from atomic dimensions to millimeters and nanoseconds to hours, respectively[12].

6.3. Content and Objectives

6.3.1. Expected Achievements and Development Potential

The remaining three open beamlines at PETRA III are planned to be completed by 2021: The beamline P66 will be dedicated to inelastic scattering of fluorescent materials. Beamline P25 will focus on X-ray imaging techniques specifically emphasizing bio- and medical imaging (possible partner: Otto-von-Guericke-Universität Magdeburg). Beamline P63 is foreseen as an in-situ catalysis beamline in cooperation with the Fritz Haber Institute [milestone PE.1].

Until 2025, new support structures for data handling through the IDAF will be established [PE.5]. This activity is critical for the future success of PETRA III and IV, since the majority of users will no longer be able to handle the ever-growing amount and complexity of data generated in the PETRA III and IV experiments. To realize this new computer-science-related user support, dedicated additional computing personnel will be required.

In the PoF IV period, each PETRA III beamline will be evaluated on its science case and future perspectives for the international user community, in the context of the LEAPS facilities, and in particular with respect to PETRA IV. Beamlines with clear visions towards PETRA IV will be upgraded in terms of soft- and hardware towards operation at PETRA IV [PE.3].

The PETRA IV upgrade project is currently in the conceptual design phase, which will be completed in 2019 with a CDR. A detailed technical design of the new ultralow-emittance source will be completed by the end of 2021 [PE.2]. The Helmholtz FIS roadmap process was started for the category B facility PETRA IV and is expected to be finalized in 2020, followed by the submission of the project to the German national roadmap of large-scale facilities (BMBF). After approval of funding, new accelerator and beamline components for the PETRA IV upgrade will be prepared until 2025. During this period, user operation at PETRA III will be fully maintained.

Beginning with the shutdown of PETRA III in 2025, the upgrade to PETRA IV will take about two years, starting with civil construction in 2025 [PE.5], followed by installation of new beamlines and refurbishment of existing beamlines until 2027. The start of PETRA IV commissioning and operation is expected by the end of 2027 [PE.6].

6.3.2. Milestones

Table 27: Milestones for PETRA III and IV.

	Year	Milestone
PE.1	2021	PETRA III in full operation: all beamlines including P25, P63, and P66 operational or in commissioning
PE.2	2021	Completion of the PETRA IV TDR
PE.3	2023	Completion of the PETRA III beamline evaluation
PE.4	2025	Start of the PETRA IV construction phase
PE.5	2025	Scientific computing installed as new user support structure
PE.6	2027	Start of PETRA IV commissioning/operation

12 C. G. Schroer, et al., J. Synchrotron Rad. 25, 1277 (2018).

6.3.3. Planned Investments/Upgrades of the Facility

For the full user operation of PETRA III, an extension of personnel and ongoing investments in the existing beamlines and the accelerator are planned to ensure the necessary personnel at each beamline and keep the facility up-to-date. In order to establish scientific computing service as a new DESY user support structure, corresponding personnel will be hired. The computing experts will collaborate closely with the beamline scientists. The major investment for PETRA within the PoF IV period will be the upgrade of the facility to PETRA IV. This includes the upgrade of the accelerator and storage ring to reach ultralow emittance, the construction of an additional experimental hall, and the upgrade and construction of optimized beamlines to take full advantage of this worldwide unique photon source. After approval, funding for the PETRA IV project phase needs to start from 2021/2022 in order to keep the presented schedule. A possible funding scenario includes funds from DESY's core budget, the Helmholtz strategic investment corridor, PETRA IV partner institutions, and projects funds from BMBF and the city of Hamburg.

6.4. Life Cycle Analysis

With the resources described below, PETRA III can be kept state-of-the-art until the planned shutdown for the start of the upgrade to PETRA IV in 2025. A particular risk is a failure of parts of the PETRA III injectors, which would imply a major shutdown of the facility and multimillion-euro additional costs. With the upgrade to PETRA IV, the relevant infrastructure will be refurbished to extend the lifetime of the facility well beyond 2040. During the planned operation break between 2025 and 2027, 26 beamlines overall will be missing in the European synchrotron radiation landscape. In order to reduce the effect of the various upgrade shutdowns, the European facilities within LEAPS will try to avoid overlapping shutdowns. In addition, all possible measures will be taken to keep the PETRA shutdown period as short as possible. With the startup of PETRA IV, the users will strongly request the extraordinary new beam conditions. The number of users of PETRA IV will therefore quickly ramp up in after restart and will likely grow compared to the one of PETRA III.

6.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 28: PETRA III Resources (DESY), planned for 2021. The costs include general and administrative costs, internal services etc.

DESY costs (TEUR)	**63.981,0**
thereof personnel costs (including personnel of infrastructure)	36.173,0
thereof material costs	15.371,0
thereof electricity	10.762,0
thereof operation cryo plant	672,0
thereof gases (Helium and other gases)	404,0
thereof noncash expenditures	12.437,0
DESY investments	
continuing investments	8.097,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	

Table 29: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

DESY costs	63.981,0
- noncash expenditures	12.437,0
+ continuing investments	8.097,0
+ ongoing individual large investments > € 2,5 million	0,0
DESY cash expenditures	**59.641,0**

Table 30: Program personnel capacity by center (FTE), planned for 2021.

DESY part personnel	263
Scientists/Engineers	186
Scientific support personnel	77
for information only: corresponding LK I contribution DESY	197
Scientists	109
Doctoral students	57
Scientific support personnel	31
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 31: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
DESY	21.725,7	263	3,8	267
Scientists/Engineers	17.227,0	193	1,0	96
Scientific support personnel	4.498,7	70	2,8	171

7. GEMS

The large-scale HZG research infrastructure German Engineering Materials Science Centre (GEMS) is a user facility with an instrumentation that is unique on an international scale in its concentration on engineering materials research with both photons and neutrons. Within GEMS, photons are provided at the GEMS Hamburg branch at the PETRA III synchrotron radiation facility at DESY, and neutrons are provided at the GEMS Garching branch at the FRM II research reactor of the Heinz Maier-Leibnitz Zentrum (MLZ)[13].

GEMS will be introduced in Section C.II.9 below.

13 More information on GEMS: http://gems.hzg.de

8. ACCELERATOR OF THE EUROPEAN XFEL

8.1. Overview

The European X-ray Free-Electron Laser Facility (European XFEL) is a worldwide unique international research infrastructure, constructed and operated by 12 nations. The responsibility for the facility's overall operation and development is with the European XFEL GmbH, the operation and development of the accelerator are mandated to DESY. These two institutions form a close strategic partnership, and the day-to-day operation of the facility is highly integrated. Specific accelerator R&D is financed through a dedicated R&D budget, subject to approval by the European XFEL Council[14].

The European XFEL is the first hard X-ray FEL based on a high-electron-energy superconducting linear accelerator. The superconducting technology allows for the acceleration of many electron bunches within one radio frequency (RF) pulse of the accelerating voltage and, in turn, for the generation of a large number of hard X-ray pulses. A sophisticated electron bunch distribution system enables the simultaneous operation of several experiments. The high repetition rate and the high particle energy of European XFEL provide unique conditions for experiments that require a large number of exposures, like for serial crystallography or for the investigation of highly dilute or weakly interacting samples at high photon energies for both high atomic temporal and spatial resolution.

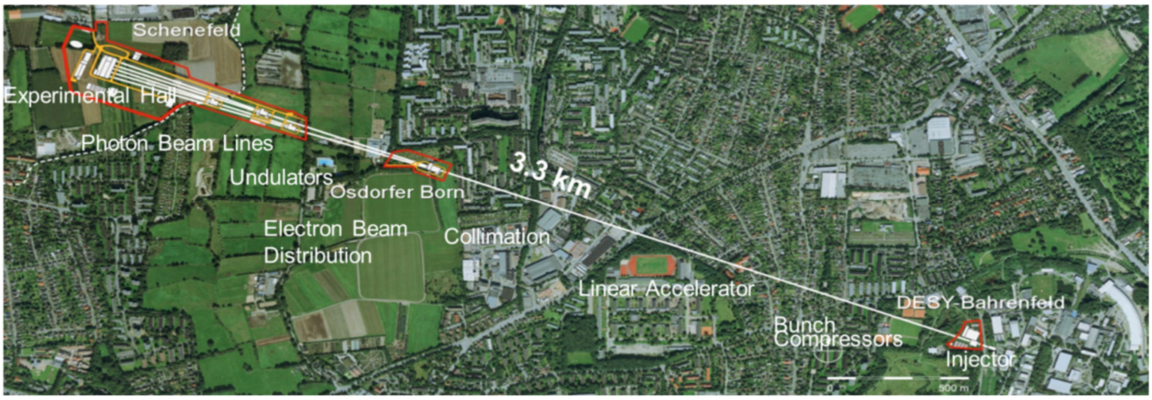

Figure 8: Layout of the European XFEL: Starting from the injector on the DESY campus, electrons are accelerated to up to 17,5 GeV and then distributed in two electron beamlines providing space for up to five FEL undulators (three presently installed), each pointing into a separate tunnel so that a fan of five almost parallel tunnels enters the experimental hall 3,3 km away from the electron source.

8.2. Research Environment and Current Activities

The European XFEL is an international research facility serving a diverse worldwide user community. Research groups of all three Topics within the Program MML use the European XFEL and contribute to experimental developments mainly through the user consortia of the Helmholtz International Beamline (HIB) and several smaller ones. Within the Research Field *Matter*, access to the experiments at European XFEL is complementary to FLASH with respect to the available photon energy range. At FLASH, mainly time-resolved spectroscopy experiments in the VUV and soft X-ray range are carried out, aiming at the dynamics of the electronic structure of the valence levels, and the core levels of lighter elements. At European XFEL - due to its shorter wavelength - the atomic structure, as well as spectroscopy at the core level also of heavier elements are accessible. While the synchrotron radiation

14 More information on the accelerator of the European XFEL: http://xfel.desy.de/

sources BESSY II and PETRA III (and their possible upgrades) will mainly target the static and slow dynamics of matter down to the nanosecond range, the FELs are ideally suited for ultra-fast dynamics down to the femtosecond regime or for experiments that require ultra-high pulse intensities, e.g. to exploit of non-linear effects.

The European XFEL accelerator has been constructed within a consortium of leading European accelerator technology institutes. The superconducting accelerator is the first large-scale installation of the TESLA-type accelerator technology, and other projects (LCLS II, SHINE, PolFEL) interact with DESY within the TESLA Technology Collaboration and in bilateral relations in view of implementing this technology. The operation and development of the worldwide FEL user facilities would be impossible without a vivid exchange of personnel, ideas, and hardware among facilities. The specific R&D for the European XFEL is performed in close collaboration with the Topic MT-ARD in the Subtopics ST1 (superconducting technology) and ST3 (picosecond and femtosecond electron and photon beams). The usage of novel acceleration techniques (ST4) to alter and tailor electron beam properties is a new research field that will draw more attention in the upcoming PoF IV funding period.

8.3. Content and Objectives

8.3.1. Expected Achievements and Development Potential

User operation at the European XFEL started in 2017. The consolidation of the X-ray program will extend well into 2021. Continuous improvement will be needed to increase the operation efficiency, and developments in machine learning and big-data analysis are expected to support these efforts.

Further development and improvement of the radiation characteristics will be vigorously pursued, benefitting from both the unique properties of the superconducting accelerator and the long undulators. This includes short wavelengths, high average brightness, and high-peak-brightness operation.

Specific attention will be given to the generation of short (sub-femtosecond) photon pulses, for which moderate upgrades are already being pursued [milestone XFEL.1].

8.3.2. Milestones[15]

Table 32: Milestones for the accelerator of the European XFEL.

	Year	Milestone
XFEL.1	2021	Circular polarization in undulator beamline SASE3; sub-femtosecond photon pulses
XFEL.2	2022	TDR for CW accelerator module and CW electron gun
XFEL.3	2024	Installation of new undulator beamlines SASE4/SASE5
XFEL.4	2026	CDR for CW extension and beamline extension (second tunnel fan)

8.3.3. Planned Investments/Upgrades of the Facility

The present layout of the European XFEL includes free tunnels for two additional FEL undulators. Plans are presently being developed to fill these tunnels in the coming years [XFEL.3].

A major upgrade would be the extension of the European XFEL capabilities by a continuous-wave (CW) operation mode. This requires substantial prior R&D to verify the viability of the superconducting RF and electron source solutions [XFEL.2]. A CDR could be ready towards the end of PoF IV, complemented by a proposal to about double the facility's experimental capacity through the addition of about five more undulator tunnels and an associated experimental hall [XFEL.4].

15 The details of the strategy presented here are under discussion with the European XFEL management and subject to approval by the European XFEL Council.

8.4. Life Cycle Analysis

As a new facility, the European XFEL accelerator has a basic lifetime of at least 20 years. This can only be achieved through an extensive maintenance and refurbishment program, as foreseen in the operation budget.

The accelerator and its infrastructure can serve as the backbone for this unique scientific instrument well beyond the basic lifetime.

8.5. Resources

The responsibility for the facility's overall operation and development is with the European XFEL GmbH, the operation and development of the accelerator are mandated to DESY. The total Helmholtz contribution including DESY to the operation costs of European XFEL are exempt from the PoF evaluation process.

II. NEUTRON FACILITIES

Neutron probes provide unique information on condensed matter over many orders of magnitude in space and time, and are among the primary analytical tools applied to solve the grand challenges of modern societies. Thus, they are fundamental for research in the Program MML. Two LK II facilities contribute to the Facility Topic *Neutrons Facilities*: FZJ operates the Jülich Centre for Neutron Science (JCNS) and HZG the German Engineering Materials Science Centre (GEMS). Due to their different scientific foci, the two facilities are largely complementary. Research at JCNS has three major thrusts: (i) soft matter and life science, (ii) quantum materials and collective phenomena, and (iii) neutron analytics for energy research. GEMS provides complementary research with photons and neutrons in the field of engineering materials science. In their respective fields of research, both facilities are key drivers of innovative method and instrument development. Moreover, their close cooperation includes the development of sample environment, instrument control, and analysis tools. Together, they enable forefront research in an ever-increasing number of disciplines. National and international users get access to these facilities through a proposal-based peer-review access scheme. The user community includes the about 1,950 registered primary neutron users in Germany, which come from all sectors of the German science system (universities, Max Planck Society, Helmholtz Association, Leibniz Association, and industry).

Together, JCNS and GEMS are engaged at major neutron sources and/or source projects:

- Within the Heinz Maier-Leibnitz Zentrum (MLZ)[16], JCNS and GEMS join forces with the Technische Universität München for the scientific exploitation of the FRM II research neutron source. The MLZ is the national neutron infrastructure and one of the leading facilities worldwide. It brings together the main players in research with neutrons in Germany and offers outstanding instrumentation, education, and professional user service, as confirmed by a recent evaluation in November 2018. Reacting to the shutdown of the BER II reactor in Berlin, MLZ aims at expanding its capabilities. For the new MLZ cooperation contract, to be concluded for the period 2021–2030, a sophisticated upgrade program called Vision MLZ2030 has been developed. It includes the transfer of instruments from BER II to MLZ after 2020.
- The European Spallation Source (ESS) project[17] in Lund, Sweden, aims to become the world-leading neutron research infrastructure. Together with international partners, JCNS and GEMS are building five instruments and contribute to several work packages in instrumentation, sample environment, and scientific computing. Moreover, FZJ will deliver the moderator–reflector assembly.
- The future PIK high-flux research reactor[18] in Gatchina near St. Petersburg, Russia, will complement research opportunities in Europe in the medium to long term. Germany considers becoming involved in the construction of instruments and components, in their scientific use, and in the establishment of an international user center.
- Compact accelerator-driven neutron sources (CANS) have the potential to add substantial value to the network of neutron facilities and to provide a basis for the efficient use of top Tier sources such as ILL and ESS. CANS are scalable (also in investment and operational costs), do not need nuclear licensing, and are inherently safe. Through additional funding from BMBF (Helmholtz Innovation Pool), FZJ (JCNS and IKP) and HZG work together with GSI to further develop the High Brilliance Neutron Source (HBS) project[19], which aims at a full-fledged medium-size facility designed to maximize beam brilliance. It answers the increased demand for experiments on small samples, such as systems of biological macromolecules or nanostructured quantum materials. HBS-type

16 https://www.mlz-garching.de/
17 https://europeanspallationsource.se/
18 http://www.pnpi.spb.ru/en/facilities/reactor-pik
19 https://www.fz-juelich.de/jcns/jcns-2/EN/Forschung/High-Brilliance-Neutron-Source/_node.html

sources have the potential to fill the gap in instrument days anticipated with the ongoing closure of older neutron sources.

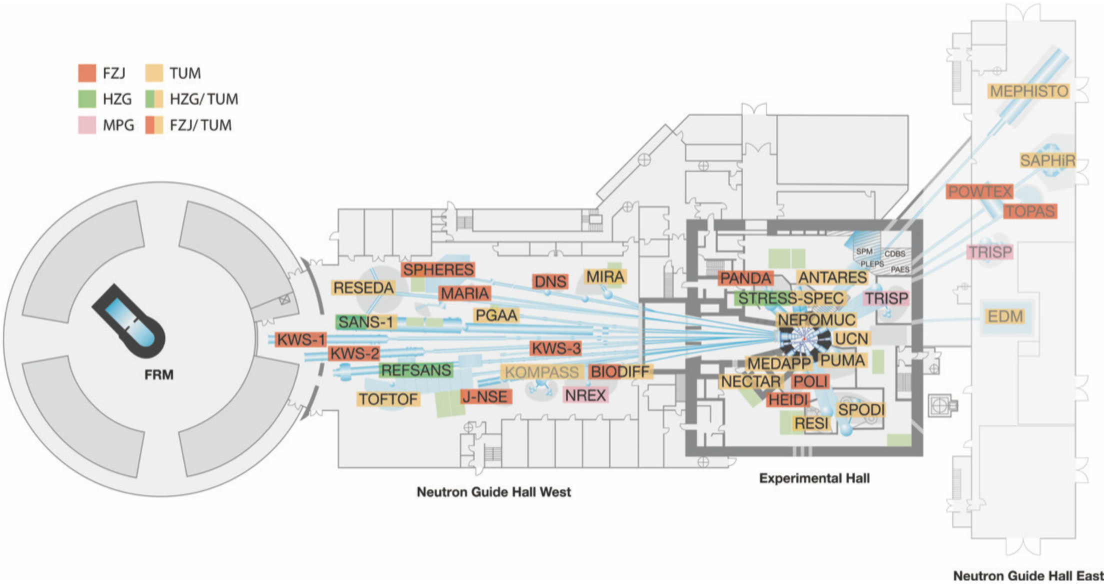

Figure 9: MLZ instrument suite showing the assignment of instruments to the MLZ partners, also demonstrating their close cooperation in instrument operation.

Besides the cooperation between GEMS and JCNS on the neutron infrastructures mentioned above, the two Helmholtz LK II facilities have independent further engagements. For complementary research with photons, GEMS operates a branch at DESY at the PETRA III synchrotron radiation source. FZJ is the German associate of the Institute Laue-Langevin (ILL) in Grenoble, France. JCNS operates outstations at this European flagship and at the megawatt spallation source SNS in Oak Ridge, USA.

The topics mentioned above are elements of the German neutron strategy[20], agreed upon between the facilities and supported by the KFN, the German Committee for Research with Neutrons, representing the neutron user community[21]. Coordination on a European scale between European-level neutron infrastructure providers happens within the League of advanced European Neutron Sources (LENS), in which MLZ and FZJ are members[22].

20 S. Schmidt et al; (2018) "Strategy Paper on Neutron Research in Germany: 2015–2045."
21 https://www.sni-portal.de/de/nutzervertretungen/komitee-forschung-mit-neutronen/dokumente
22 https://www.lens-initiative.org/

9. GEMS

9.1. Overview

Within the large-scale research infrastructure and user facility German Engineering Materials Science Centre (GEMS), photons are provided at the PETRA III synchrotron radiation facility of DESY and neutrons at the FRM II research reactor of the MLZ. Thus, GEMS enables the full exploitation of the complementarities of the two different probes at Germany's most recent and highest-flux sources. GEMS has a clear focus on engineering materials research, making it unique in the German large-scale facility landscape. Engineering materials research includes a high variety of industrial production processes and of materials with a specific functionality. For studying these processes, complex *in-situ* and *operando* experiments are developed at the GEMS beamlines and instruments – often in cooperation with user groups – and constructed in the HZG central technical department. Furthermore, users have access to engineering-specific user support facilities (laboratories, workshops) for preparation and pre-characterization of samples near the GEMS beamlines and instruments.[23]

Beamtime at the GEMS instruments for both probes is awarded according to the scientific excellence of the proposals by panels of international experts in the field of materials research. HZG coordinates the materials science committees of the review panels at DESY and MLZ.

HZG collaborates with industry, authorities, and other institutions based on cooperating contracts or just on orders, using the unique capabilities of synchrotron radiation and neutrons to solve materials problems with cutting-edge research in order to take advantage of the latest developments in engineering materials science.

The GEMS strategy is to provide beamlines and sample environments optimized for engineering materials research at the best photon and neutron sources in Europe. The expertise for such experiments is gained by cooperation with strong HZG in-house groups as well as with strategic university partners.

9.2. Research Environment and Current Activities

Photon facilities

At the world's most brilliant synchrotron radiation source PETRA III at DESY, GEMS runs two beamlines and operates one experimental station at a further beamline. In addition, a new beamline for white-beam experiments is currently being built together with DESY. All beamlines meet the research requirements of engineering materials science over a wide range of X-ray energies and spatial resolution and provide the necessary means to perform *in-situ* experiments. The new GEMS outstation within the CXNS building at DESY (EMSC; milestone GEMS-1) will provide urgently needed additional GEMS laboratory and office space as well as improved infrastructure for sample preparation, characterization, and data analysis close to the beamlines.

The GEMS activities at DESY are divided into diffraction and imaging. The focus of the diffraction group is on measuring industrially relevant processes *in-situ*, particularly in the field of engineering materials research, using diffraction and small-angle scattering techniques. The imaging department maintains a complementary suite of high-resolution imaging techniques: microtomography, nanotomography, and scanning nanodiffraction. These highly flexible instruments combine detectors optimized for high dynamic range, high resolution, and continuously high scan rates with different contrast modes (absorption, phase, and diffraction contrast) and *in-situ* sample

23 More information on GEMS: http://gems.hzg.de environments to take full benefit of synchrotron-based imaging. This combination is unique worldwide and particularly valued by users from materials-science- and life-science-related research.

Neutron facilities

The GEMS photon beamlines are complemented by neutron instruments at the MLZ and in future also by an engineering materials diffractometer at the ESS. With this instrumental suite, non-destructive structural characterization of materials is possible over a broad range of length scales both for interfaces and for bulk materials. Given the high penetration of neutrons in matter and the different interactions of neutrons and X-rays with matter, neutron scattering methods are complementary to the X-ray methods and instruments operated at DESY.

The Materials Science Laboratory at MLZ, jointly operated by GEMS and TUM, combines sample preparation and state-of-the-art analytical equipment. The lab also develops specific sample environments for *in-situ* and *operando* studies.

At the ESS, HZG and the Nuclear Physics Institute (NPI) from the Czech Republic are jointly building a new neutron time-of-flight engineering materials diffractometer, the Beamline for European Materials Engineering Research (BEER)[24]. The design of the instrument takes advantage of the long pulses of the ESS and will offer the users a higher flux at the sample position than any other engineering instrument in the world. Another project in the construction phase of the ESS is the development of ^{3}He-free neutron detectors based on $^{10}B_4C$ converter plates and a demonstrator detector suitable for use at BEER[25].

In the framework of the High Brilliance Neutron Source (HBS) project led by FZF, HZG is involved in the design of neutron instrumentation focused on materials science for a compact accelerator-driven neutron source.

In the framework of a German–Russian collaboration at the PIK high-flux research reactor of the Petersburg Nuclear Physics Institute (PNPI), HZG offers to upgrade some of the neutron instruments transferred to the PNPI from the former Geesthacht research reactor FRG-1.

9.3. Content and Objectives

9.3.1. Expected Achievements and Development Potential

Photon facilities

New sample environments are currently being developed, covering topics at different research frontiers. The initiative for new projects is usually based on requests from external and internal cooperation partners, and the science case is defined together with these partners. Since 2018, activities of the diffraction group have focused on additive manufacturing techniques, especially selective laser melting (SLM). Other *in-situ* sample environments are an experiment for studying the twin roller casting process of Mg alloys (FlexiRoll) and the grinding process (FlexiGrind). The new white-beam beamline P61A [GEMS-2] will be one of the very few of this kind in Europe. It has the potential to fill the gap opened by the shutdown of the EDDI beamline at BESSY II. Thus, a large user demand is expected for the beamline for depth-resolved phase and residual stress analysis. Its development potential is in sophisticated *in-situ* sample environments and novel energy-dispersive area detectors.

The main objectives of the imaging activities are to further increase the speed of high-resolution data acquisition and processing, to improve throughput and time resolution, and to enhance the data quality from challenging high-attenuation/high-density samples by providing phase contrast at all stations. High-resolution, fast detector systems and the growing scientific demand for *in-situ* tomography and high-throughput studies have led to very high data rates that challenge data storage and processing. A new, more performant IT infrastructure as well as novel

24 J. Fenske et al., J. Phys.: Conf. Ser. 746 (2016) 012009
25 G. Nowak et al., J. Appl. Phys. 117 (2015) 034901

machine-learning concepts will be used to further improve the performance of the imaging data analysis pipelines [GEMS-3]. These plans are in accordance with the research goals pursued in the Topic MT-DMA and with the strategy for data analysis at PETRA III.

With the increased data rate resulting from improvements of sources and detectors, there will be a growing need for new, equally performant software for diffraction and imaging analysis in the next years. New *in-situ* experiments will rely on online data reduction and analysis, as timely analyses are essential to adjust experiment parameters. While cooperative efforts of several facilities solve one part of this problem, GEMS staff will work on adapting software solutions to experiment environments, on contributing to new software based on GEMS experience, and on training users in the use of software packages.

Neutron facilities

According to the objective of GEMS to offer the best instruments at the best sources, HZG is involved in the upgrade of existing instruments at the MLZ, the construction of a new neutron instrument at the ESS, the instrumentation of the upcoming PIK research reactor, and the HBS project.

At the MLZ, the partners TUM, FZJ, and HZG are working on Vision MLZ2030, the basis of a prolonged cooperation agreement for the next decade. A stronger involvement of GEMS in neutron imaging would yield synergies with the imaging activities at PETRA III. Of particular importance to GEMS are ambitious upgrades of existing instruments, tailored materials-science-related sample environments, an increased use of robotics for optimal use of beamtime, and novel methods of data reduction and analysis. While the data rates are by far not as high as at X-ray sources, most of the other challenges regarding the obtained data are valid for neutron and X-ray scattering and imaging alike and will be tackled together.

The focus at the ESS lies on the engineering diffractometer BEER. The high flux of the instrument will cover the continuously growing demand of the users for *in-situ* and *operando* characterization of materials and their microstructure under industrial processing conditions. The capabilities of BEER will therefore strengthen the complementary use of neutrons and X-ray photons, in particular for *in-situ* and *operando* investigations [GEMS-4].

At the PIK reactor, HZG will contribute to the instrumentation for an international user center at PIK through upgrades of former Geesthacht instruments transferred from the FRG-1 reactor to PIK after the FRG-1 shutdown in 2010 [GEMS-5].

Industrial relations

In order to enable industry to make better use of the GEMS instrumentation, GEMS participates in different networks and projects that aim at improving the service to industry at synchrotron and neutron facilities as well as raising the awareness about the possibilities for industry at these unique facilities. In the EU Interreg project CAROTS, GEMS is currently working on establishing a network between already existing service providers (or commercial analytical research organizations, CAROs) and on the evaluation, in which regions and industry sectors new CAROs could be successfully established. Within the frame of CAROTS, GEMS will evaluate the possibility to outsource parts of the industry service to such a company.

While GEMS has successfully implemented the concept of an industry liaison officer (ILO) in the last years, it is now time to further develop industry cooperation by hiring an industry project officer (IPO) working together with the ILO. The IPO must be a materials scientist capable of solving a company’s problems using not only beamtime at GEMS but also additional techniques, such as mechanical testing and microscopy, that are available at a university. The IPO will be hired jointly with a partner university. The new ILO/IPO concept will make GEMS a true partner for companies, able to understand their problems and develop solutions involving all necessary materials science methods.

9.3.2. Milestones

Table 33: Milestones for GEMS.

	Year	Milestone
GEMS-1	2021	Completion of the new GEMS outstation in the CXNS building at DESY
GEMS-2	2021	Beamline P61A at PETRA III in full user operation
GEMS-3	2022	Demonstration of machine-learning-assisted imaging data processing
GEMS-4	2024	First experiments at BEER at the ESS
GEMS-5	2023	First experiments at former HZG instruments at PIK
GEMS-6	2025	Finalized definitions and designs for the GEMS beamlines at PETRA IV
GEMS-7	2027	Commissioning of the GEMS beamlines at PETRA IV

9.3.3. Planned Investments/Upgrades of the Facility

Photon facilities

A major effort is foreseen for the development of new in-situ experiments together with internal and external Helmholtz partners (strategic investment InnoMatSy). The planned upgrade of PETRA III to PETRA IV will most likely lead to a shift of the positions of all GEMS beamlines along the storage ring and, consequently, will effectively require a new construction of all GEMS beamlines. The required significant budget is far beyond the budget available for running the beamlines [GEMS-6 & GEMS-7]. In addition, custom-developed X-ray optics will be needed to make efficient use of the improved beam characteristics and to provide a useful field of view in tomography despite the reduced horizontal divergence.

Neutron facilities

The GEMS instruments and sample environments at the MLZ will be constantly upgraded. While most upgrades are incremental, some plans such as new neutron delivery systems exceed the budget for normal instrument operation by far. One of the instruments with GEMS involvement will pioneer the further use of robotics for sample handling at the MLZ.

Sample environments will be required for the new engineering diffractometer BEER at the ESS.

9.4. Life Cycle Analysis

Photon facilities

HZG will continue to run beamlines at the DESY synchrotron sources with a clear focus on engineering materials research. Experiments at the European XFEL are planned as well. The use of these new hard X-ray sources, which are world-leading in terms of emittance and photon flux, form an excellent basis for the successful operation of the photon part of GEMS for the next decades. The upgrade of PETRA III to PETRA IV with the corresponding reconstruction of the beamlines will secure the excellence and competitiveness of the GEMS beamlines for the coming decades.

Neutron facilities

GEMS will continue its involvements in the MLZ and the ESS. Assuming a typical lifetime of neutron sources of 40 to 50 years, these new sources should offer a sound foundation for the successful continuation of the neutron part of GEMS for the decades to come. The GEMS neutron activities will be supported by a share of beamtime at the new

PIK reactor. The high flux of the PIK reactor will enable experiments that need more flux than available at the MLZ. The involvement of GEMS in the HBS project offers the opportunity for an even longer-term perspective.

9.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 34: LK II GEMS Resources (HZG), planned for 2021. The costs include general and administrative costs, internal services etc.

HZG costs (TEUR)	**6.219,0**
thereof personnel costs (including personnel of infrastructure)	3.954,5
thereof material costs	467,5
thereof electricity	73,5
thereof other consumables	394,0
thereof noncash expenditures	1.797,0
HZG investments	
continuing investments	473,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	2.730,0

Table 35: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

HZG costs	6.219,0
- noncash expenditures	1.797,0
+ continuing investments	473,0
+ ongoing individual large investments > € 2,5 million	2.730,0
HZG cash expenditures	**7.625,0**

Table 36: Program personnel capacity by center (FTE), planned for 2021.

HZG part personnel	25
Scientists/Engineers	19
Scientific support personnel	6
for information only: corresponding LK I contribution HZG	17
Scientists	7
Doctoral students	9
Scientific support personnel	1
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 37: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		Third-party funding	
	TEUR	FTE	TEUR	FTE
HZG	2.320,0	26	431,0	6
Scientists/Engineers	1.843,0	19	431,0	6
Scientific support personnel	477,0	7	0,0	0

10. JCNS

10.1. Overview

The Jülich Centre for Neutron Science (JCNS)[26] at FZJ uses neutrons as microscopic probe to conduct research on condensed matter and life science systems. For this purpose, JCNS develops and builds neutron scattering instruments at leading national and international sources. On the one hand, it operates these instruments for its own research, mainly within the Topic MML-Materials. On the other hand, following the central Helmholtz mission, JCNS offers its instruments as an LK II user facility to a broad national and international user community. Driven by the scientific foci of JCNS, a unique suite of neutron instruments spanning wide length and time scales has been created. At present, JCNS offers beamtime to users at 17 instruments at the MLZ, ILL, and SNS. Two further instrument projects at the MLZ are awaiting completion. Key elements of the JCNS instrument suite are polarized neutron techniques, high-resolution spectroscopy, and scattering under grazing incidence – all of them internationally recognized hallmarks of JCNS.

For the design, construction, and further advancement of instruments, JCNS relies heavily on the exceptional expertise of the Jülich Central Institute of Engineering, Electronics and Analytics (ZEA)[27]. Its unique know-how in state-of-the art engineering is an essential advantage and enables Jülich to develop, operate, and maintain world-leading neutron instruments at some of the world-leading neutron sources – the central mission statement of JCNS.

All JCNS instruments are made available to external users through a proposal system based purely on scientific merit. This is ensured by peer review by independent international experts. JCNS thus offers its users access to state-of-the-art neutron scattering instruments under uniform conditions at the neutron source best suited for the respective experiments. Through its instrument scientists, JCNS offers expert support at world-class instruments, including specialized sample environment and ancillary laboratory access for external users from science and industry.

The strategy of JCNS is well aligned with the national neutron roadmap (see overview on Neutron Facilities, Section C.II) and answers the challenges raised by the ESFRI neutron landscape working group[28]. As a neutron facility active at the best national and international sources, JCNS is a main driver of the international neutron research strategy (see Section 10.2). It is an active partner in various European projects to develop and improve access and service for neutrons in Europe, such as the consortia BrightnESS2, SINE2020, NFFA, EU-SMI, and LENS. Through collaboration with German universities, the instrumentation of JCNS profits from the BMBF ErUM framework program, which is intended to enable universities to contribute to the further development of large-scale facilities.

10.2. Research Environment and Current Activities

National research environment with neutrons

JCNS is a major player at the MLZ[29], exploiting the FRM II reactor together with its partners HZG and TUM. In order to involve the broader German neutron community, several instruments are being operated in close cooperation with nine German universities and the Max Planck Society. The JCNS presence at the MLZ amounts to a total of about

26 https://www.fz-juelich.de/jcns/EN
27 https://www.fz-juelich.de/zea/zea-1/EN
28 "European Landscape of Research Infrastructures: Neutron scattering facilities in Europe – Present status and future perspectives" (2016), Eds: Colin Carlile and Caterina Petrillo.
29 https://www.mlz-garching.de/

80 scientific and technical staff members, postdocs, doctoral, master, and bachelor students and guests. Currently, JCNS operates 11 user instruments at the MLZ and is realizing two further instruments in the new guide hall east. JCNS's scientific computing group develops software solutions for acquisition, analysis, and modeling of neutron scattering data and participates in the Topic MT-DMA.

As recommended by the Helmholtz Senate, the integration of JCNS at the MLZ has been strengthened through shared leadership, common and new instrument projects, a common proposal system and user office, and common science and service groups. Further integration will be achieved with the new science buildings [milestone JCNS-1], which will bring together all instrument scientists and host user and service group laboratories, a workshop, seminar and conference rooms, as well as kitchenettes and common rooms, which will promote brainstorming in a relaxed atmosphere. The integration is further strengthened by the foundation of the new JCNS department for neutron methods (called JCNS-4) at the MLZ.

Based on a strategic analysis of research with neutrons in Germany and Europe and as part of the strategy of the Research Field *Matter*, the need for a novel type of scalable, compact accelerator-driven High Brilliance Neutron Source (HBS) has been realized. Together with its strategic partners IKP and ZEA at FZJ, JCNS has taken up this challenge by establishing a corresponding research network, demonstrating the technical readiness of the concept at the JULIC cyclotron of IKP, and developing a technical design report for such future sources. On the one hand, their scalability will allow major universities to operate their own neutron source as a central facility. On the other hand, pushing the concept to the limits will enable the realization of neutron facilities competitive to today's medium-flux sources, supporting the European flagship project ESS.

International research environment with neutrons

FZJ acts as the German associate of the ILL[30] and is thus a key driver of the institute's strategic development. Through JCNS, FZJ is also involved in instrument operation and construction. The Collaborative Research Group (CRG) consortium of JCNS and the French Alternative Energies and Atomic Energy Commission (CEA) operates three user instruments. Moreover, JCNS participates in the operation of the high-resolution spin echo spectrometer and the construction of the wide-angle spin echo spectrometer.

At the SNS[31], JCNS is strongly committed to the operation of its own spin echo instrument and the provision of access to two additional instruments for the German user community.

At the ESS[32], JCNS plays the leading role in the German involvement in instrument construction. Seven out of initially 15 instruments for the ESS are being realized by the MLZ partners JCNS, GEMS, and TUM together with further international partners. Four of these seven instruments are being realized by or with JCNS. Construction is enabled through close collaboration with the FZJ institute ZEA, which is also responsible for the realization of the moderator–reflector assembly of the ESS.

Further activities to develop and improve the neutron landscape include the collaboration with the Kurchatov Institute in Russia, the Chinese Academy of Sciences, and the HBS project. The future PIK reactor[33] has the potential to offer a neutron flux comparable or even higher than that of ILL. Together with Russian and German partners, JCNS explores the possibility to establish an international center for neutron research at PIK, thus ensuring the availability of a high-flux continuous neutron source for Europe for the coming decades. At the CARR facility[34] in Beijing, China, three instruments of the former DIDO reactor of FZJ are in operation.

30 *https://www.ill.eu/*
31 *https://neutrons.ornl.gov/sns*
32 *https://europeanspallationsource.se/*
33 *http://www.pnpi.spb.ru/en/facilities/reactor-pik*
34 *http://www.ciae.ac.cn/eng/carr/*

JCNS user community

JCNS offers beamtime free of charge (and even covers travel expenses for some user groups) to national and international users (about 1,000 annually at the MLZ, thereof about half at JCNS-owned instruments) based purely on scientific merit under the condition that the research results are being published. Proprietary research by industry that will not be published is subject to payment. The majority of users come from the focal areas of research of JCNS – soft matter, magnetism, and energy materials – where the center offers highly performing instruments, specialized sample environment, ancillary laboratory infrastructure, and last but not least expert support by JCNS instrument scientists. As proven by a recent literature survey, the European and therein the German neutron user communities (about 1,950 registered German users in the KFN[35] database) are particularly productive[36].

10.3. Content and Objectives

10.3.1. Expected Achievements and Development Potential

Vision MLZ2030: Negotiations are underway to prolong the cooperation agreement between TUM, FZJ, and HZG for the period 2021 to 2030, during which the FRM II reactor at the MLZ will remain the only national neutron source. A development plan for the facility has been worked out. It contains the following major elements, which are strongly supported by the review of the MLZ at the end of 2018: (i) an upgrade program for the instrument suite in three steps: start of operation of instruments in the guide hall east, transfer of instruments from the BER II reactor to the MLZ, as well as renewal of ageing instruments and construction of new instruments particularly at the hot source; (ii) support of user experiments by synergetic sample environment and additional laboratories for materials preparation and characterization [JCNS-1]; (iii) support of user data reduction, analysis, modeling, simulation, and visualization (see Topic MT-DMA), and (iv) engagement in automation and robotics.

ESS: Together with its European partners, FZJ will complete and deliver the instruments DREAM (powder diffractometer), SKADI (small-angle diffractometer), T-REX (bispectral chopper spectrometer), and MAGIC (magnetism single-crystal diffractometer) to the ESS. According to the ESS project planning, DREAM is expected to be among the first three instruments to take up user operation [JCNS-2].

PIK: Negotiations are underway to establish an international neutron user center at this future high-flux neutron reactor. At present, the instrument suite is being agreed upon between the Russian and German partners. Germany will likely provide three to four instruments to the PIK in this initial phase [JCNS-3]. The engagement is entirely embedded in the German–Russian roadmap.

HBS*:* The TDR for this novel type of neutron facility (see Figure 10) will be completed in the beginning of the PoF IV period [JCNS-4]. Subsequently, FZJ aims at constructing a prototype facility to verify the expected performance, optimize the design of the components through experimental evidence [JCNS-5], and prepare for the construction of a full-fledged HBS, which should become operational around 2030.

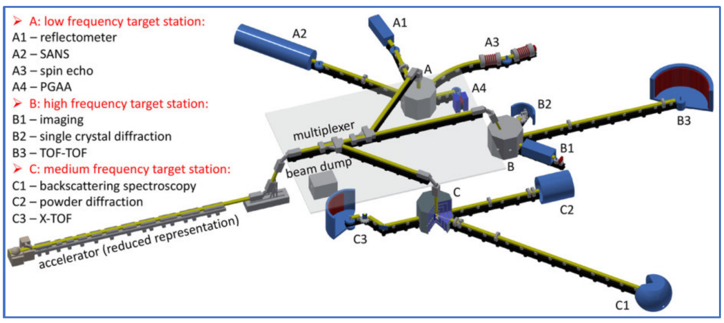

Figure 10: Possible layout of an HBS-type facility with a representative instrument suite.

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35 https://www.sni-portal.de/en/user-committees/committee-research-with-neutrons
36 T. Gutberlet, et al., Do neutrons publish? A neutron publication survey; Neutron News 29, 18 (2018)

10.3.2. Milestones

Table 38: Milestones for JCNS.

	Year	Milestone
JCNS-1	2021	New science buildings at MLZ operational with additional user laboratories
JCNS-2	2024	Start of user operation of the DREAM instrument at ESS
JCNS-3	2026	JCNS instruments at PIK operational
JCNS-4	2022	TDR for HBS completed
JCNS-5	2027	HBS prototype demonstrates the potential of this new type of facility

10.3.3. Planned Investments/Upgrades of the Facility

All of the development plans described in Section 10.3.1. will need major investment. For Vision MLZ2030, this is expected to be provided through the renewed collaboration contract. Instruments for the ESS are provided as a German contribution, instruments for the PIK as an element of the Russian–German research roadmap. The realization of the HBS prototype is planned to be financed through a proposal for major strategic investment from the Helmholtz Association.

10.4. Life Cycle Analysis

The presence of JCNS at several major sources provides stability for JCNS as a neutron user facility. The FRM II research reactor at the MLZ is the backbone of research with neutrons in Germany, with large international impact. It started operation in 2004 and is expected to operate smoothly for the upcoming decades. The scientific user operation at the FRM II is secured by the cooperation agreement between TUM, FZJ, and HZG with financial support from the BMBF within the framework of the MLZ. At the SNS in Oak Ridge, JCNS will continue to operate the spin echo instrument until the end of the contract in 2020 and the planned transfer of the instrument ownership to the SNS for long-term usage. The ESS will become operational after 2020, and PIK, where an international user center with involvement of FZJ is being considered, will follow around 2025. The ILL, where FZJ is the German stakeholder and operates instruments, is expected to remain in operation at least within the next decade. Finally, in an effort to offer a versatile alternative for the provision of neutrons for science and industry in the medium and long term and to compensate in time for the loss of reactor-based neutron sources, JCNS is pushing the development of accelerator-driven HBS, which is a strategic goal in the Research Field *Matter* and a priority in the research-political objectives for PoF IV.

10.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 39: FZJ JCNS Resources (FZJ), planned for 2021. The costs include general and administrative costs, internal services etc.

FZJ costs (TEUR)	20.000,0
thereof personnel costs (including personnel of infrastructure)	12.181,4
thereof material costs	5.805,9
thereof electricity	45,0
thereof noncash expenditures	2.012,7
FZJ investments	
continuing investments	3.694,8
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0,0

Table 40: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

FZJ costs	20.000,0
- noncash expenditures	2.012,7
+ continuing investments	3.694,8
+ ongoing individual large investments > € 2,5 million	0,0
FZJ cash expenditures	**21.682,1**

Table 41: Program personnel capacity by center (FTE), planned for 2021.

FZJ part personnel	93
Scientists/Engineers	93
Scientific support personnel	0
for information only: corresponding LK I contribution FZJ	92
Scientists	61
Doctoral students	8
Scientific support personnel	23
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 42: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
FZJ	7.342,2	93	0,0	0
Scientists/Engineers	7.342,2	93	0,0	0
Scientific support personnel	0,0	0	0,0	0

III. ION FACILITIES

Ion beams provide unique experimental capabilities for research in the realm of atomic physics, plasma physics, materials science, and biophysics. Within the Helmholtz Association, they are accessible at two facilities: the HZDR Ion Beam Center (IBC) and GSI. The two facilities are complementary with respect to instrumentation and ion energies, going far beyond the accelerators and implanters available at universities and in the semiconductor industry. Together, they cover an extremely broad ion energy range from sub-keV up to hundreds of GeV (see Figure 11). They deliver a large variety of beams, including all stable ions from protons up to uranium as well as secondary beams of exotic nuclei. This worldwide broadest user platform for research and applications with ion beams offers unique experimental opportunities for the national and international scientific communities, and in particular for the Program MML. MML-related scientific subjects to be pursued with ion beams during PoF IV include: matter and materials under extreme electromagnetic fields, pressures, densities, and temperatures, materials for nanotechnology, energy applications, and quantum information technology, as well as interdisciplinary projects in geology, biophysics, space research, and astrophysics.

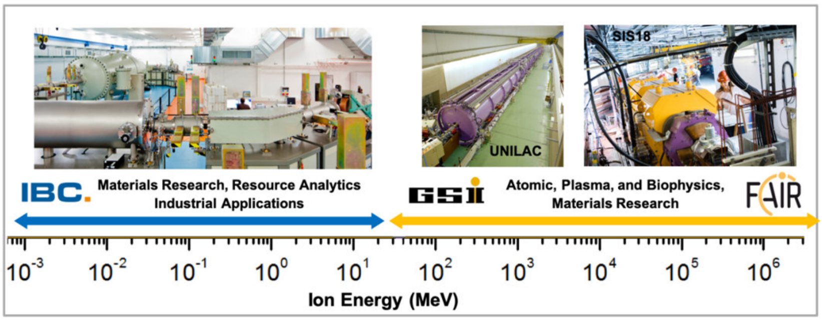

Figure 11: The HZDR (IBC) and GSI facilities are complementary. Together, they provide ion beams within an energy range of more than 10 orders of magnitude, including highly charged and fully stripped stable and radioactive ions.

The IBC operates several accelerators for ions in the sub-keV to MeV energy range and is internationally highly competitive in the application of ion beams in materials research. New application areas, e.g. resource technology, geology, and life sciences, are addressed with improved ion beam analysis and with unprecedented lateral resolution, chemical sensitivity, and high throughput. The energy range will be extended towards 10 eV for new users in the field of two-dimensional materials and molecular layers. In addition, the IBC facilities and services are available for industry projects in close collaboration with the spin-off company HZDR Innovation GmbH.

The GSI accelerators provide ions of all species with energies up to several hundred GeV. During PoF IV, key efforts will be devoted to the installation of the infrastructure and novel equipment for the FAIR experiments. FAIR will further boost ion beam intensities and increase the ion energy by one order of magnitude. GSI is unparalleled worldwide regarding the combination of ion species, energies, intensities, and ion storage and cooling facilities, as well as the broad range of interdisciplinary MML research.

Both Helmholtz facilities provide regular beam access for national and international users (in total approx. 1,000 users per year), foster strategic international cooperation with other ion beam laboratories, and strongly promote new scientific directions in physics and materials research with ion beams. In addition, the MML activities are well embedded into various Helmholtz programs and closely connected to the national research and university landscape.

11. GSI-MML ION FACILITIES

11.1. Overview

GSI operates a worldwide unique, versatile ion facility for interdisciplinary research related to matter, materials, and life, where all ion species in virtually all charge states can be delivered at specific energies (energy per atomic mass unit u) ranging from 1 MeV/u up to more than 1 GeV/u for heavy ions. Figure 12 shows the schematics of GSI and the future FAIR facilities along with the location of the experimental stations devoted to the Program MML. The experimental areas and storage rings dedicated to MML research are located at the two central ion accelerators: the linear accelerator UNILAC (beam energies up to 11 MeV/u) and the synchrotron SIS18 (beam energies up to 1 GeV/u) (both facilities are described in the LK II section of the Program MU).

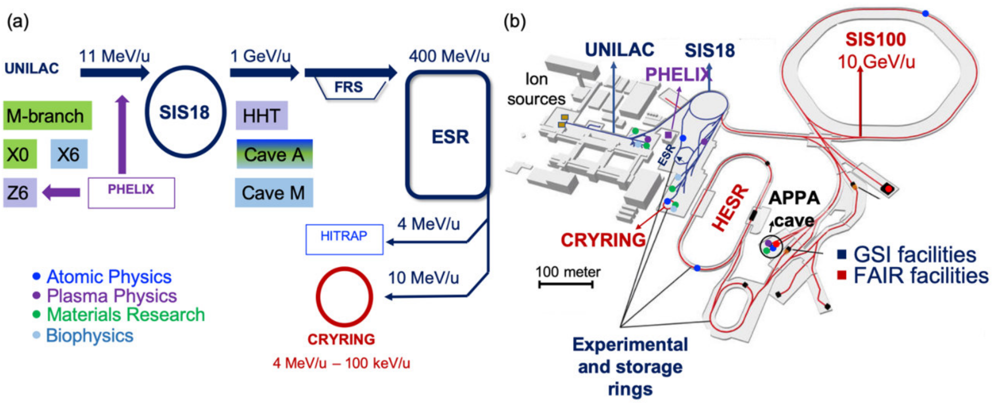

Figure 12: (a) Schematics of current MML-related experimental stations and corresponding typical ion energies. (b) Overview of the ion accelerator facilities and MML-related experimental stations at GSI (blue) and FAIR (red). (Th. Stöhlker et al., Nucl. Instr. Meth. B 365, 680 (2015)).

- **MML areas at UNILAC (11 MeV/u)**: Four experimental stations are available: (i) the M-branch, designed for *in-situ* and online analysis of beam-induced effects and defects in materials by means of numerous spectroscopic and microscopic techniques, (ii) the beamline X0 for high throughput irradiations, including sample exposures to single ions for nanoscience and the heavy-ion microprobe for targeting with individual ions (precision below 1 µm) and testing the radiation hardness of electronic devices and biological cells, (iii) the beamline X6, where biological samples can be automatically positioned and irradiated on Petri dishes using the BIBA facility (Biologische Bestrahlungs-Anlage), and (iv) the beamline Z6, which includes a laser-driven proton beamline (LIGHT) and a laser–ion pump–probe setup, combining the ion beam with the PHELIX laser and with the nanosecond nhelix laser. The PHELIX laser is an integral part of the MML ion facilities and not a separate LK II user facility.
- **MML areas at SIS18 (80 MeV/u – 1 GeV/u):** Three experimental stations are in operation. Due to the high ion energies, the ions have ranges in condensed matter up to several centimeters. The irradiation station in Cave M houses experiments related to new approaches within carbon cancer therapy. In Cave A, automated and remote-controlled systems such as a robotic arm and a conveyor belt provide efficient positioning of solid state and biological samples. At the High energy, High Temperature (HHT) station, the highest ion beam intensities can be exploited to reach warm dense states of matter. In addition, a proton microscope setup (PRIOR), currently being commissioned, enables high-spatial-resolution dynamic measurements of thick materials.
- **ESR storage ring complex**: The ESR offers electron-cooled ion beams in a well-defined charge state between 3 MeV/u and 400 MeV/u. The ring is equipped with a broad variety of dedicated instrumentation. It also serves as a decelerator and injector providing ions for the trapping facility HITRAP (designed for further deceleration,

capturing, and cooling of highly charged ions at rest) and for the CRYRING, a dedicated FAIR low-energy storage ring. Experiments on the structure and dynamics of high-*Z* ions as well as studies at the interface to nuclear astrophysics are conducted in both CRYRING and HITRAP by colliding the stored or trapped ions with photons, electrons, or atoms and enabling e.g. high-precision *g*-factor experiments for single ions.

- **MML at FAIR (10 GeV/u):** During PoF IV, two new experimental areas will be developed: The multipurpose APPA cave will be equipped with two dedicated beamlines, one for plasma physics and one with setups dedicated to atomic physics, materials research, and biophysics. Intense beams of ions at medium and highest charge states (e.g. U^{92+}) and specific energies of up to 10 GeV/u will become available. In addition, the High-Energy Storage Ring (HESR) will be available for atomic physics experiments with high-energy, heavy-ion beams. The HESR will store cooled beams at relativistic energies (γ values: 2–6) and enable worldwide unique experiments, such as Doppler tuning of a dedicated XUV laser into the X-ray regime for pump–probe experiments in the sub-femtosecond regime. Dedicated instrumentation for these new MML-FAIR areas will be designed and installed during PoF IV.

11.2. Research Environment and Current Activities

The GSI/FAIR large-scale facilities described above serve and support the research of four large user communities related to all three Topics in the Program MML, MML-Matter, MML-Materials, and MML-Life:

Atomic physics researchers exploit the unique beams of cooled, highly charged heavy ions and exotic nuclei with excellent momentum definition provided by the unique portfolio of storage rings and traps (HITRAP, CRYRING, ESR). Their research focuses on studies of atomic matter subject to extreme electromagnetic fields as well as on investigations of atomic processes mediated by ultrafast electromagnetic interactions. In addition, the intersection of atomic and nuclear physics is explored by studying e.g. the influence of electrons on nuclear properties.

For plasma physicists, GSI provides a worldwide unique combination of a high-energy (kJ) PW-class laser with intense high-energy heavy-ion bunches. The PHELIX laser can generate secondary sources of photon, electron, and ion beams for diagnostic purposes. Intense ion beams from SIS18 can heat macroscopic volumes of condensed matter uniformly, generating high-density and high-entropy states that are difficult to access by other means. For novel diagnostics, a unique 4.5 GeV proton microscope (PRIOR) for proton radiography is being commissioned.

Materials researchers, active in condensed-matter physics, geosciences, mineralogy, space science, nanoscience, and biochemistry, use the UNILAC and SIS18 beams to study a large variety of subjects, including radiation hardness of materials in extreme environments, radiation of electronic devices for space applications, ion–solid surface and bulk interaction, and novel ion-induced phase transitions by irradiation under high pressure. Using ion track nanotechnology, nanochannels and nanowires are developed for sensorics, catalysis, and energy applications.

Biophysicists concentrate on space radiation protection and cancer therapy. Most users currently exploit the SIS18 accelerator with 400 MeV/u C ions (therapy) or 1 GeV/u Fe ions. The cancer therapy activities focus on the treatment of moving targets (e.g. lung) with scanned ion beams and the combination of ions with systemic cancer drugs, especially immunotherapy. Space radiation protection is supported by the European Space Agency (ESA) to study biological risk in space and develop effective shielding. Research on DNA damage is carried out at the UNILAC.

To jointly coordinate the common experimental installations at FAIR and exploit synergies in selected research projects, these four GSI research divisions along with HI Jena and their scientific communities are embedded in the MML-related international FAIR collaborations SPARC (atomic physics), HED@FAIR (plasma physics), BIO (biophysics), and MAT (materials research). Together, they form the Atomic Physics, Plasma and Applied sciences (APPA) umbrella organization. In total, the APPA pillar represents a steadily growing group of more than 700 scientists from over 30 countries. The four MML-related research divisions at GSI also play an important role by covering the host laboratory tasks and facilitating the MML research program at the existing and future infrastructures. Access to beamtime is granted upon proposal approval and recommendation by the corresponding program advisory committees. Until the start of FAIR commissioning in 2025, regular periods of beamtimes (~3 months/year) will be offered.

At the national level, over 30 user groups are involved in MML-related projects. With the support of the GSI research divisions and HI Jena, instrumentation is developed and installed at various experimental MML areas by the GSI strategic partner universities in Heidelberg, Gießen, Mainz, Darmstadt, Frankfurt, and Jena, and German university groups supported by the BMBF ErUM framework program. Within the Helmholtz Association, GSI participates in all the Topics of the Program MT, and the GSI/FAIR bioactivities collaborate with the Research Field *Health*. At the European level, GSI is involved in various programs such as the Horizon 2020 Infrastructure Program INSPIRE, a network of all the European accelerators involved in particle therapy research, the Horizon 2020 Integrating Activity project ARIES, which aims to develop European particle accelerator infrastructures and offers access to 14 European testing facilities, and various Marie Skłodowska-Curie actions. Users from European countries are supported by the EU large research infrastructures access program ENSAR2.

11.3. Content and Objectives

11.3.1. Expected Achievements and Development Potential

During PoF IV, the MML-relevant new FAIR experimental stations and the required novel instrumentation will be developed. Setups, detectors, and diagnostic tools will be tested at the current operative facilities and transferred to the APPA cave, CRYRING, and HESR for commissioning and FAIR operation. In PoF IV, the GSI-MML activities will concentrate on the following:

For atomic physics, the main objectives are precision experiments exploiting the portfolio of storage rings and traps as well as the preparation and commissioning of first experiments at the APPA cave and HESR [milestone GSI-MML.7]. All the planned experimental activities will require the steady development of dedicated state-of-the-art equipment, such as high-resolution µ-calorimeter for X-ray spectroscopy (also embedded into the DDL of the Program MT), in-ring lepton spectrometer, highly sensitive beam diagnostics (cryogenic Schottky and current comparators), windowless coupling of high-repetition XUV lasers (secondary light sources) to the ring vacuum ($\sim 10^{-11}$ mbar), and in-ring internal jet targets.

Plasma physicists will exploit the ion beam properties to probe exotic states of matter at high energies (PRIOR) [GSI-MML.1] and low energies (stopping-power experiments at Z6), created by external drivers such as lasers. Laser-accelerated ions will be injected into the accelerator beamline at the Z6 target area. Alternatively, heavy ions will be employed to generate long-time-scale mesoscopic samples of matter at extreme temperatures and pressures, diagnosed using laser-generated secondary sources of photons or particles. Two main objectives are maintenance of the existing unique laser–ion experimental capabilities and development of new volumetric X-ray-based plasma characterization methods [GSI-MML.4].

Materials researchers will design and test specific equipment at the existing beamlines (X0, M-branch, and Cave A) and subsequently transfer it to the APPA cave to access the higher ion intensities and energies available at FAIR. This equipment includes a fully automatized irradiation setup with beam monitoring, laser heating, and sample analysis for materials in high-pressure cells, online tools to study the radiation hardness of nuclear and accelerator materials, and a platform to test electronic devices for space applications [GSI-MML.6]. In addition, a new ultrahigh-vacuum (UHV) station will be installed at a CRYRING extraction beamline for irradiation and analysis of materials with highly charged (up to fully stripped) heavy ions of various kinetic and potential energies [GSI-MML.2]. This station will also be used to produce nanostructures in 2D and 3D materials.

Biophysicists will deal with basic and applied research in radiobiology, cancer therapy, and space radiation protection. The high intensities provided by FAIR will allow tests for a radiotherapy that uses very high dose rates ("flash radiotherapy"), where treatments are delivered in less than 1 s; minibeam therapy, where the beam is spatially fractionated (spacing between 0.1 and 1 mm) to spare the normal tissue; and radioactive ion beams, e.g. positron-emitting beams such as ^{11}C [GSI-MML.5]. The high energies at FAIR will provide the most complete cosmic-ray simulator worldwide [GSI-MML.6] and allow particle radiography, using the beam for therapy and target imaging (theranostics).

The recently installed storage ring CRYRING will start regular user operation in 2021, offering slow and highly charged ions for in-ring experiments, such as precision recombination studies with unparalleled ultracold electrons only available at the CRYRING cooler. Additionally, extraction of ions from the ring will enable novel materials research opportunities with slow and highly charged ions [GSI-MML.2]. The installation of the FISIC setup at CRYRING will allow ion–ion collisions to be addressed in the unexplored regime between slow (keV/u) and fast (MeV/u) ions for the first time [GSI-MML.3]. The sophisticated reaction setup will enable unparalleled opportunities for precision collision studies for atomic and astrophysics. Also starting in 2021, first experiments at HITRAP with heavy one- and few-electron ions confined in a Penning trap are envisioned.

11.3.2. Milestones

Table 43: Milestones for the GSI-MML ion facilities.

GSI-MML.1	2022	Commissioning and first dynamic experiments of PRIOR at SIS18
GSI-MML.2	2022	Installation of UHV setup for materials research at CRYRING
GSI-MML.3	2023	Integration and commissioning of FISIC setup at CRYRING for SPARC
GSI-MML.4	2023	Commissioning of X-ray backlight of ion-beam-heated targets at SIS18
GSI-MML.5	2024	Commissioning of gamma-PET detectors for visualizing exotic ion beams for BIO
GSI-MML.6	2025	Commissioning of experiment stations in the APPA cave including high-pressure irradiation setup for MAT and BIO target handling system
GSI-MML.7	2026	Commissioning of HESR and first SPARC experiments

11.3.3. Planned Investments/Upgrades of the Facilities

During PoF IV, the GSI divisions and their collaborations will design and construct the MML/APPA experimental installations at FAIR (e.g. in the APPA cave and at the HESR). For PoF IV, no additional investments beyond the ones required for the FAIR experiments and an upgrade of the current PHELIX laser are foreseen.

11.4. Life Cycle Analysis

The life time of all relevant structures amounts to at least 20 to 30 years. In view of FAIR, the ion facilities have recently been upgraded and restarted. The MML-related experimental sites at the UNILAC and SIS18 have been continuously upgraded and maintained, and they are planned to run throughout PoF IV and beyond, as foreseen in the operation budget.

11.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 44: MML Ion facilities Resources (GSI), planned for 2021. The costs include general and administrative costs, internal services etc.

GSI costs (TEUR)	**8.789,0**
thereof personnel costs (including personnel of infrastructure)	3.986,5
thereof material costs	2.203,5
thereof electricity	450,0
thereof maintenance costs	1.753,5
thereof noncash expenditures	2.599,0
GSI investments	
continuing investments	1.320,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	

Table 45: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

GSI costs	8.789,0
- noncash expenditures	2.599,0
+ continuing investments	1.320,0
+ ongoing individual large investments > € 2,5 million	0,0
GSI cash expenditures	**7.510,0**

Table 46: Program personnel capacity by center (FTE), planned for 2021.

GSI part personnel	37
Scientists/Engineers	24
Scientific support personnel	13
for information only: corresponding LK I contribution GSI	127
Scientists	50
Doctoral students	56
Scientific support personnel	21
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

As GSI is currently not active part of PoF III, no personnel is listed here.

12. IBC

12.1. Overview

The Ion Beam Center (IBC) at HZDR is a worldwide leading center for research and application of ion beams in materials science. Various ion sources, microscopes, implanters, and accelerators are combined in a unique user facility that delivers a broad diversity and variety of ion beams of almost all stable elements with an energy range from a few ten eV to 60 MeV. In PoF III, the energy range of the IBC has been extended to low-energy ions down to a few eV, following recent requests for modifications of ultrathin films, surfaces, and 2D materials. In addition to broad beam irradiations, the IBC also offers unique focused ion beams (focused liquid-metal ion sources and helium/neon ion microscopes) as well as highly charged ions for the local modification of surfaces.

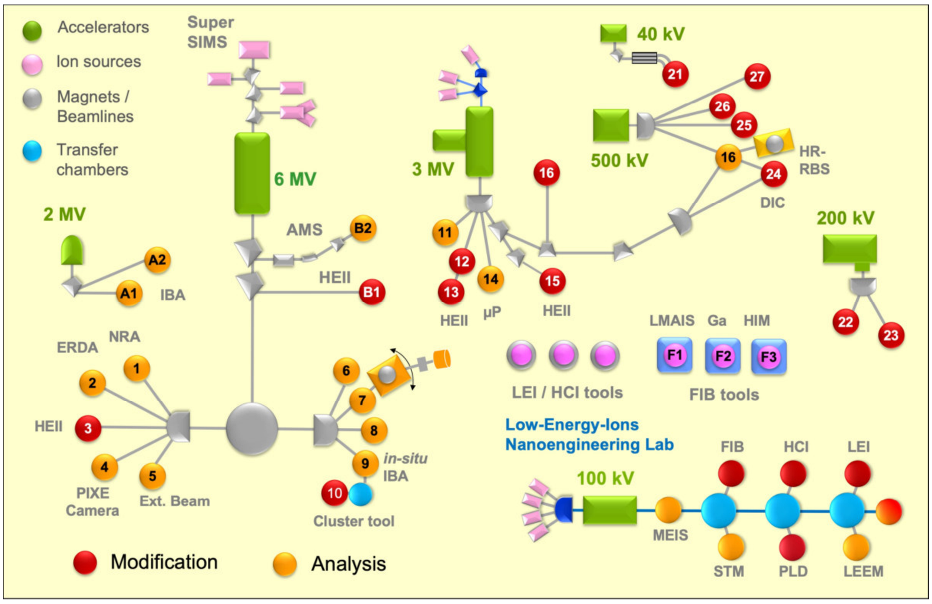

Figure 13: Floor plan of the Ion Beam Center (IBC) at HZDR.

12.2. Research Environment and Current Activities

Within the Program MML, the IBC is the major facility for providing eV to MeV ion beam modification of materials. Ion implantation beyond the solubility limit as well as the creation of non-equilibrium phases provide means to achieve new materials functionalities. For this purpose, a large variety of ion species are available. Focused and highly charged ions are used for pattern creation down to the atomic level. Recently, 2D materials have increasingly been addressed by making use of the new Low-Energy-Ion Nanoengineering Lab. In addition, ion beam analysis is being pushed to the limits of achievable lateral resolution. This MML-related research strongly relies on capabilities, which are not available anywhere else.

Starting in 2019, the IBC is coordinating the European Integrated Infrastructure project RADIATE, in which 18 ion beam centers in Europe are joining forces to provide users with access to 11 European ion beam infrastructures and to develop ion-beam-based techniques for analysis and material modification beyond the state of the art. The main objectives of this project are to provide flexible and efficient access to the ion beam infrastructures, to open them for new communities and young researchers, to increase the visibility of ion beam facilities in Europe, and to extend the cooperation between the European ion beam laboratories. Furthermore, the IBC is partnering with the ion beam center of the Jozef Stefan Institute in Slovenia in the framework of the Helmholtz European Partnering project CROSSING. The IBC is involved in two work packages of this project, related to correlative microscopy and to the realization of a virtual joint ion beam center providing access to international users.

Within the Helmholtz Association, the IBC is participating in the projects Helmholtz Energy Materials Characterization Platform (HEMCP) and Helmholtz Energy Materials Foundry (HEMF), where both analytical techniques and ion beam modification are used and provided for R&D into energy materials.

The IBC established its outstanding status on an international level over the last decades through the following characteristics:

- The IBC has been providing ion beam techniques as a user and competence center for ion beam research and applications for more than 30 years. With approx. 14,000 user beamtime hours and around 500 users per year, the IBC is an international leader, continuously supported by numerous national and European projects and by industry.
- The IBC activities rest on two pillars: ion beam analysis (IBA) and ion beam material modification (IBMM). Experienced beamline scientists and operators are supporting users from academia and industry in using ion beam techniques in various research fields for fundamental and applied research.
- With accelerator mass spectrometry (AMS), a method with the currently lowest detection limit, quantitative analysis of trace elements and long-lived radionuclides is offered for research in the life sciences, geology, oceanography, archaeology, and astrophysics. Routinely, analysis of the following radionuclides is provided: ^{10}Be, ^{24}Al, ^{36}Cl, ^{41}Ca, and ^{129}I.
- Users of the IBC can take advantage of add-on services, such as sample preparation and processing in a cleanroom environment, structural analysis by electron microscopy/ spectroscopy or X-ray techniques, and specific software tools for the simulation of ion processes or for data analysis.
- The IBC profits from a very strong theoretical in-house support in density functional theory (DFT), molecular dynamic (MD), and kinetic Monte Carlo simulations.

The current scientific activities performed at the IBC can be divided into three main fields:

- Fundamental understanding of ion–matter interaction with the aim of controlling ion-induced modification of materials on the nanometer scale, e.g. studies of the charge and energy loss of highly charged ions in graphene, and self-organized patterning of surfaces by low-energy ion irradiation.
- Synthesis of functional materials and nanostructures by ion irradiation and implantation.
- Ion beam analysis with ultrahigh spatial resolution, laterally and in depth, e.g. implementation of He backscattering spectrometry and secondary-ion mass spectrometry in a He/Ne ion microscope, unprecedented elemental sensitivity with AMS.

A further mission of the IBC is the commercial exploitation of ion beam technology with partners from industry. The high beamtime demand for ion beam services from industry has led to the foundation of a spin-off company, the HZDR Innovation GmbH, in 2011, which provides ion beam services and technology transfer to industrial partners. The close collaboration between IBC and HZDR Innovation GmbH is considered as a reference model for developing innovative strategies towards an effective contribution of the Helmholtz large-scale facilities to economic innovation. Currently, more than 30% of the total IBC beamtime is used for commercial ion beam services. The income is used to keep the ion beam infrastructures up to date.

12.3. Content and Objectives

12.3.1. Expected Achievements and Development Potential

In the PoF IV period, the IBC will concentrate on the following scientific research and technical development activities:

- Commissioning of the Low-Energy-Ion Nanoengineering Lab and provision of beamtime for users at this facility
- Commissioning of a 1 MV tandem accelerator to strengthen the research activities and user operation in AMS

- Development of a microscope based on proton-induced X-ray emission (PIXE) with sub-micrometer resolution used for correlative microscopy [milestones IBC.4, IBC.5]
- Planning of a competence center for high-energy ion beams in materials research and medicine

In the PoF III period, the energy range of the IBC has been extended to ultralow energies with the establishment of the new Low-Energy-Ion Nanoengineering Lab. The aim of this facility is to broaden and advance experiments with ions of low (10 eV) to medium (< 500 keV) energy interacting with surfaces and thin layers and to enable new experiments with cluster and hyperthermal ion beams. By using highly charged and cluster ions, the total deposited energy into the solid is extended beyond 10 eV/atom in a depth of only a few nanometers close to the surface, leading to material states far from equilibrium. Combined with *in-situ* preparation and characterization by chemical and structural analysis before, during, and after ion processing, the study of ion-induced modifications of surfaces, 2D materials (e.g. graphene, boron nitride, transition metal dichalcogenides), and thin films becomes possible without deterioration. In the current PoF period, this new facility will be opened for user service, attracting users from new and interdisciplinary fields, e.g. for studying doping and defects in 2D materials [IBC.1].

After the installation of the 6 MV Tandetron, the IBC started a small activity in 2011 on AMS, which, in the first years, led to many applications in particular in environmental and geosciences. In 2017, HZDR decided to develop this area in addition to materials research into a third pillar of the large-scale user facility. Hence, in 2018, a joint TU Dresden–HZDR professor position was announced in order to establish interdisciplinary research and applications of natural and anthropogenic fingerprints of rare isotopes and trace elements. After the position has been filled, the group size will be enlarged and a dedicated 1 MV AMS device will be ordered [IBC.2]. In this way, HZDR increases its competences and capabilities in the field of AMS, e.g. to especially attract a broader user community from geo- and environmental to astrophysical and other fundamental sciences. Future steps in the development of the HZDR AMS facility include the integration of a laser detachment system and the development of an advanced secondary-ion mass spectrometer (Super SIMS) for stable isotopes.

In 2015, an Orion Nanofab (a He/Ne ion microscope) was installed and opened for user operation. In the last years, the analytic capabilities of the NanoFab have been extended, enabling the chemical analysis of surfaces with a lateral resolution of 30 nm. These methods can be used for correlative microscopy, including the He ion microscope with a resolution of 1 nm and electron-based microscopy methods. Current activities at the He ion microscope (HIM) aim at developing a scanning transmission ion microscope (STIM) within the EU Research and Innovation Action project npScope. The STIM is of particular interest for the analysis of nanoparticles, ultrathin films, and 2D materials. It will start user operation in PoF IV [IBC.3].

In collaboration with the Universität der Bundeswehr München, a competence center for high-energy ion beams in materials research and medicine is being planned [IBC.6]. Five different application areas are foreseen: radiation medicine, radiation safety and biology, materials science, astro- and environmental physics, and technology transfer to commercial customers. In view of the decommissioning of the 14 MV accelerator at the MLZ in 2020, after 50 years of operation, a user community is currently discussing the science case for a dedicated medium-energy ion beam laboratory making use of a new 14 MV accelerator with potential proton post-acceleration for medical applications. Given the long-term strategic mission of such a center, establishment within the Helmholtz Association and thus within the IBC is preferred.

12.3.2. Milestones

Table 47: Milestones for the IBC.

	Year	Milestone
IBC.1	2022	Start of user operation of the Low-Energy-Ion Nanoengineering Lab
IBC.2	2022	Commissioning of a dedicated 1 MV accelerator for AMS
IBC.3	2023	User operation of the STIM
IBC.4	2023	Replacement of the Van de Graaff accelerator by a 3.5 MV Singletron for sub-micrometer ion beam analysis and correlative microscopy
IBC.5	2024	Installation of a PIXE microscope as a user facility
IBC.6	2025	Involvement in the preparation of a competence center making use of a 14 MV accelerator in collaboration with UniBW München

12.3.3. Planned Investments/Upgrades of the Facility

In the PoF IV period, several new investments are planned for the IBC:

- DREAMS, a dedicated 1 MV accelerator for AMS (2022)
- Replacement of Van de Graaff accelerator by a 3.5 MV Singletron (2023)

12.4. Life Cycle Analysis

In the last ten years, several ion beam instruments and end-stations have been replaced or upgraded, thereby extending their lifetime:

- Operation of the 6 MV Tandetron accelerator (installed in 2011) is foreseen until 2040.
- No replacement is planned until 2030 for the 3 MV Tandetron, which has been running since 1998. In 2019, a new wafer handler was installed by the HZDR Innovation GmbH.
- The Van de Graaff accelerator (installed in 1962) will be replaced in 2023 by a 3.5 MV Singletron.
- The 500 kV implanter (installed in 2015 and partly financed through HZDR Innovation GmbH income) has an expected lifetime of 30 years and is now increasingly taking over the implantations formerly performed at the 200 kV implanter (installed in 1994). Hence, the decommissioning of the 200 kV implanter is planned for the PoF IV period.

12.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 48: IBC - Ion Beam Center Resources (HZDR), planned for 2021. The costs include general and administrative costs, internal services etc.

HZDR costs (TEUR)	**10.247,5**
thereof personnel costs (including personnel of infrastructure)	6.511,4
thereof material costs	1.261,0
thereof electricity	668,3
thereof maintenance costs	500,7
thereof noncash expenditures	2.475,1
HZDR investments	
continuing investments	1.477,6
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0,0

Table 49: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

HZDR costs	10.247,5
- noncash expenditures	2.475,1
+ continuing investments	1.477,6
+ ongoing individual large investments > € 2,5 million	0,0
HZDR cash expenditures	**9.250,0**

Table 50: Program personnel capacity by center (FTE), planned for 2021.

HZDR part personnel	40
Scientists/Engineers	13
Scientific support personnel	27
for information only: corresponding LK I contribution HZDR	122
Scientists	65
Doctoral students	28
Scientific support personnel	29
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 51: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
HZDR	2.382,1	35	0,0	0
Scientists/Engineers	1.011,52	10	0,0	0
Scientific support personnel	1.370,57	25	0,0	0

IV. HIGH-FIELD FACILITIES

The study of the behavior of matter and materials in strong magnetic and electric fields as well as in ultraintense optical fields is a rapidly advancing research area in the Helmholtz Association and worldwide. It is enabled by recent advances in high-field pulsed magnets (with magnetic fields up to 100 T), accelerator-driven coherent long-wavelength sources (with electric fields up to 100 MV/cm), and compact high-power solid-state lasers (with intensities exceeding 10^{21} W/cm^2), for which the inventors of the corresponding enabling technology (chirped pulse amplification) were awarded the 2018 Nobel Prize in Physics. Compared to the research pursued at photon, neutron, and ion facilities, here scientists are concerned primarily with the interaction of matter and materials with the classical electromagnetic field (in contrast to single light quanta or transient Coulomb fields in heavy-ion collisions). This interaction either alters the physical properties or initiates quantum or collective excitations. For example, pulsed high magnetic fields allow for the systematic manipulation of material properties in order to decipher the underlying fundamental processes and provide insights for optimizing novel materials for future applications. These include for instance strongly correlated electron systems, such as inorganic and organic superconductors and magnetic materials, topological semimetals, novel semiconductors, and nanostructures. High electric fields generated by FEL and superradiant long-wavelength beams provide the means to study the time-resolved dynamics of collective electronic, magnetic, and vibronic (phonon) excitations in condensed matter, or field-initiated or -mediated processes in chemical and biological systems. The interaction of ultraintense lasers with matter, creating extreme temperatures, pressures, densities, currents, strong transient and quasi-static fields, energetic particle acceleration, and ultrafast radiation generation, involves both relativistic and non-linear phenomena. The scientific interests range from studying extreme conditions in the laboratory, which is of e.g. astrophysical relevance, to creating new particle and radiation sources for basic research as well as medical and industrial applications. Experiments making use of highest electromagnetic fields are especially important in the Topics MML-Matter and MML-Materials and also contribute heavily to the Topics MT-ARD and MT-DMA.

Within the Program MML, two facilities at HZDR – the ELBE Center for High-Power Radiation Sources (ELBE) and the Dresden High Magnetic Field Laboratory (HLD) – are operated as user facilities for a national and international science community, serving more than 450 users per year. Moreover, there is a strong connection to the Helmholtz International Beamline for Extreme Fields (HIBEF), which will be a user-dedicated beamline at the European XFEL.

- The ELBE center develops advanced radiation and particle beam sources for research on matter and materials under extreme conditions and in highest electromagnetic fields. The superconducting-accelerator-based infrared FEL sources, superradiant THz sources, and secondary neutron, gamma-ray, positron, and electron beams are in routine user operation. Novel ultraintense laser-driven sources are being developed and coupled with the ELBE accelerator to provide a worldwide unique platform for advanced accelerator research. The strong-field THz radiation contributes prominently to research in MML-Matter. Moreover, experiments at the ELBE neutron and gamma-ray beams and the associated low-background Felsenkeller laboratory give new thrust to multidisciplinary astrophysics.
- The HLD develops and operates world-class pulsed high-field magnets, including user magnets with fields up to 95 T, for modern materials research. It is the only installation in Germany and one of the four large user facilities in Europe that operate high-field magnets in combination with advanced measurement techniques; the other partner facilities are located in Grenoble, Nijmegen, and Toulouse. Together, they form the European Magnetic Field Laboratory (EMFL) infrastructure. The HLD provides state-of-the-art and in part unique experimental capabilities for a broad portfolio of techniques allowing high-resolution measurements, which are central to the

research in MML-Materials. The combination of infrared radiation produced by FELs at ELBE with pulsed-field magnets is worldwide unique.

- Associated to this Facility Topic the HIBEF beamline at the European XFEL (operated in the context of this user facility, but not as LK II) has been a major strategic investment during PoF III (cf. Volume II C, 2.2.1). It is a platform for research with highest electromagnetic fields at the High Energy Density Science (HED) instrument of the European XFEL, developed jointly by HZDR and DESY in conjunction with HI Jena and a large international user consortium. HIBEF includes an ultrahigh-intensity laser (based on DRACO), pulsed high-field magnets (from HLD), a high-repetition-rate high-energy laser for shock compression (from STFC, UK), and high-pressure diamond anvil cells (from the ECB beamline of PETRA III). Therefore, it has a strong link to ELBE and HLD as well as to the Facility Topic *High-Field Facilities*. HIBEF will come into full operation in PoF IV and is a centerpiece of much of the research on strong fields and extreme states of matter in the Topics MML-Matter and MML-Materials, with major experiments planned on vacuum birefringence, relativistic laser plasmas, compression dynamics, and the study of new phases of materials at high pressure and in strong magnetic fields.

In addition to the major user operations mentioned above, the high-field pulsed magnet and high-power laser research contributes heavily to related research activities in MML-Matter and MML-Materials. These include e.g. the development of compact beam transport systems for laser-accelerated ions for medical therapy in the Research Field *Health*, for the LIGHT project at the PHELIX laser (GSI MML Ion Facilities), and for magnetized plasma astrophysics at DRACO, HIBEF, and LULI (Ecole Polytechnique, France).

The Dresden Advanced Light Infrastructure (DALI) is being designed as a successor to ELBE, with the goal of extending the technical capabilities and availability of strong-field THz radiation, additionally integrating VUV, and therefore enabling new research directions. These include e.g. exploring the dynamics of and controlling chemical reaction pathways, for example in solution and at surfaces, resolving complex dynamics of biomolecular processes initiated by strong-field pulses, or coherently controlling collective phenomena and new phases, for example room-temperature superconductivity in condensed matter. DALI will also include high-power lasers and high-field pulsed magnets and further the present capabilities in extreme-conditions and magnetic-materials research. Scientific workshops are presently being conducted, and a CDR for the science case, followed by a TDR for the technical design, will be developed early in PoF IV.

13. ELBE (DRACO AND PENELOPE)

13.1. Overview

The ELBE Center for High-Power Radiation Sources is a worldwide unique user facility combining a superconducting linear accelerator (ELBE) with ultraintense petawatt lasers (DRACO and PENELOPE). Its mission is to develop accelerator- and laser-driven sources of radiation and particles for a broad international community of users (approx. 100 per year, limited by the inherent single-service mode of the facility) and for advanced technology developments within the Research Field *Matter*.

The ELBE linear accelerator operates in quasi-continuous (CW) mode, providing MHz pulse repetition rates at 100% duty cycle and with excellent time resolution. This allows for high-count-rate experiments with superior signal-to-noise ratio, making the secondary beams of neutrons, positrons, gamma rays, and single electron bunches world-class. ELBE uses the 1.3 GHz superconducting accelerator technology developed within the TESLA Technology Collaboration, but extended to CW operation. The ELBE linear accelerator drives two FELs operating in the IR/THz regime and two superradiant THz sources (coherent broad-band and narrow-band) with single- and few-cycle electromagnetic fields.

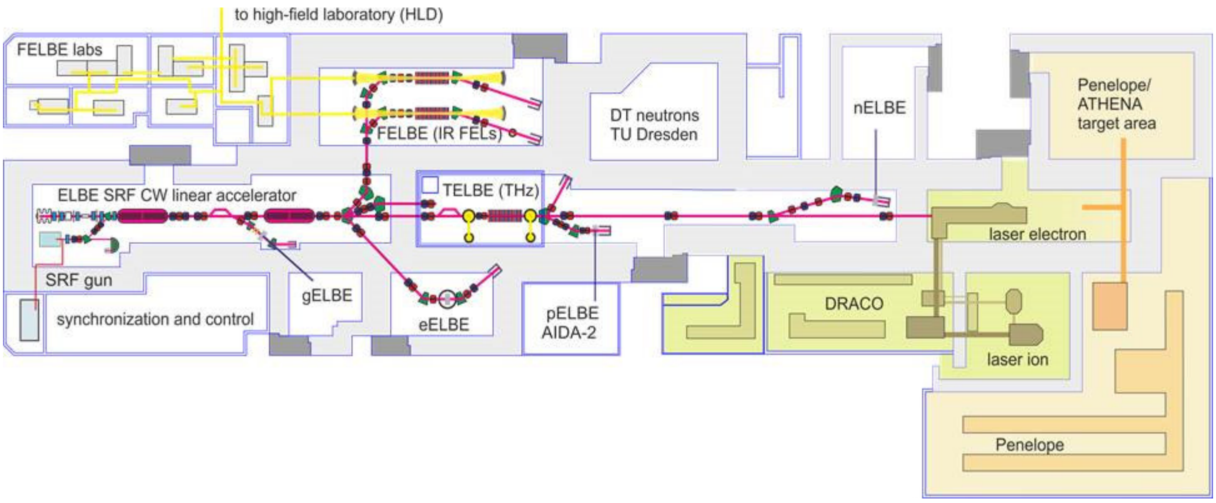

Figure 14: Layout of ELBE accelerator and beamlines: IR FELs (FELBE), superradiant THz (TELBE), positrons (pELBE), bremsstrahlung (γELBE), neutrons (nELBE), and PW lasers (DRACO and PENELOPE).

The combination with extreme optical fields available at the DRACO petawatt laser makes the ELBE center a worldwide unique facility for research with highest electromagnetic fields. The high-field research focuses on exploring matter and materials under extreme conditions and far from equilibrium.

All the ELBE beams are used extensively in the Research Fields *Matter*, *Energy*, and *Health* and complement the research capabilities available at other large-scale facilities within the Program MML. Accelerator and laser developments at ELBE are coordinated within the Topic MT-ARD. These activities focus on advanced beam diagnostics and high-power CW superconducting radio frequency (SRF) particle sources, establishing ELBE as a test bed for CW upgrades of international facilities, and on plasma acceleration within the new Helmholtz infrastructure ATHENA [milestone ELB.5]. Materials research using accelerator-based positron and gamma-ray beams encompasses *in-situ* studies of defect evolution during material fabrication and under varying environmental conditions within the Helmholtz Energy Materials Characterization Platform (HEMCP).

13.2. Research Environment and Current Activities

The ELBE center is a national large-scale facility designated by the BMBF for the ErUM framework program (former "Verbundforschung"), which sponsors joint projects with German universities in advanced accelerator physics and technology. On the international level, the ELBE center coordinates the European LEAPS CALIPSOplus project for modern light source research with accelerator-based sources, including transnational access for the scientific use of FELBE. Strategic partnerships with Helmholtz Centers, international laboratories, and universities have been established, and the user facility is integrated in European programs and projects for the further development of and user access to the ELBE center. Transnational access to the ELBE neutron and gamma-ray beams is granted through the EU FP7 program CHANDA and within the upcoming EU Coordination and Support Action (CP-CSA) ARIEL, which promotes nuclear-data programs for energy and nuclear-safety research. The EuCARD2 Integrated Activity Project supports advanced particle accelerator research and plasma particle acceleration in the Laserlab-Europe network and through the Weizmann–Helmholtz Laboratory WHELMI in Rehovot, Israel.

The ELBE infrared FEL facility FELBE covers a wavelength range from 5 to 250 μm and can be operated in CW or macro-bunched mode. The infrared beams from either FEL are distributed to seven optical user laboratories and to the HLD located adjacent to ELBE, enabling unique experiments with IR/THz radiation in pulsed magnetic fields of up to 70 T (in 150 ms pulses). FELBE's optical user labs feature scanning near-field infrared microscopy (SNIM), various setups for non-linear and time-resolved pump–probe spectroscopy, luminescence, and Fourier transform studies. The research profile of FELBE is intimately linked to the Topics MML-Matter and MML-Materials. Key investigations pursued at FELBE include ultrafast dynamics of low-energy excitations in solids, high-field-induced modification of electronic/vibronic or magnetic properties, or nanospectroscopic imaging of nanostructures[37].

Two sources of superradiant THz radiation (TELBE) provide beams ranging from broad-band radiation (0.1–3 THz) from a coherent transition or diffraction radiator to narrow-bandwidth tunable radiation (0.1–3 THz) from a short electromagnetic undulator. The CW SRF injector provides high bunch charges up to 200 pC at 200 kHz for high THz peak power. High-field THz radiation can be used to drive and study time–resolved dynamics[38]. Direct access to THz-driven changes of the electronic structure in different types of matter will be enabled by a time- and angle-resolved photoelectron spectroscopy (trARPES) end-station, which is currently under development [ELB.3]. This novel THz-ARPES method promises to shed light on the fundamental processes underlying e.g. Mott transitions, superconductivity, and catalysis.

The nELBE photoneutron source is the world's only fast neutron beam at a superconducting electron accelerator, enabling optimum conditions for energy-resolved neutron interaction measurements from 10 keV to 10 MeV using time-of-flight techniques. At the bremsstrahlung beam at γELBE, new phenomena of cross sections of photonuclear reactions and radiative capture are studied that have significant effects on reaction rates in synthesis processes of heavy elements in stellar environments. In this way, γELBE complements the studies of quiet and explosive stellar burning and big-bang nucleosynthesis reactions in the associated Felsenkeller underground low-background laboratory, which was set up in collaboration with the TU Dresden. The combination of Felsenkeller, nELBE, and γELBE offers unique opportunities for coherent studies ranging from applied nuclear physics and technology to fundamental questions[39] in nuclear astrophysics research, and is part of the new thrust in multidisciplinary astrophysics within MML-Matter.

ELBE also provides an intense source of positrons, which are used for high-resolution defect studies in materials. The Monoenergetic Positron Source (MePS) provides secondary positron beams of 2–20 keV energy for depth-resolved defect studies using positron annihilation lifetime spectroscopy. Especially, open-volume defects such as point defects, precipitations, and grain boundaries in metals, alloys, ceramics, polymers, and (ionic) liquids are addressed, and material porosities with sizes ranging from 0.2 to 35 nm can be characterized[40]. Two radioisotope-based

37 B. Pietka et al., Physical Review Letters 119 (2017) 077403
38 H. Hafez et al., Nature 561 (2018) 507
39 R. Schwengner et al., Physical Review Letters 118 (2017) 092502
40 A. Quintana et al., ACS Nano 12 (2018) 10291

installations, a slow-positron beam, and annihilation lifetime measurements are available for preparatory and complementary studies. A new apparatus for the *in-situ* characterization of defects (AIDA) during ion beam deposition is being commissioned for unprecedented *in-situ* research on dynamical effects of defect formation and annealing. Future research will focus on dynamical effects of defect migration and development by means of laser-induced charge carrier manipulation, high- and low-temperature annealing, and ion irradiation.

A direct electron beam is used for high-timing-resolution detector tests and irradiations of materials and devices. Technological developments for range verifications in cancer therapy with particle beams profit from cross-cutting activities (CCAs) within MML and the Research Field *Health*.

An additional focus of the ELBE center is to provide a leading high-power laser platform in the Program MT for advanced plasma accelerator and radiation source development with emphasis on low repetition rate but ultimate peak current[41]. In connection with ELBE's state-of-the-art synchronization system and independent beams for plasma probing, the facility offers studies of acceleration processes of electrons and ions in unprecedented detail[42]. It also serves as a model system for next-generation dense plasma probing at the European XFEL with HIBEF.

Based on the upcoming fully diode-laser-pumped petawatt laser PENELOPE, the center hosts the novel Helmholtz infrastructure ATHENA_h with focus on compact light-ion acceleration, pulsed-magnet beam transport, applications in radiobiology (with a link to the Program *Cancer Research* in the Research Field *Health*), and warm dense matter physics. After its anticipated completion in 2022, ATHENA_h will operate as a user facility, supported by the ongoing collaborative and transnational-access (TNA) user program at the DRACO beamlines [ELB.5].

13.3. Content and Objectives

The major objectives for the ELBE center for PoF IV include: full implementation of the new beamlines and high-field sources; development of parallel multiuser operation to accommodate increasing demand; improvement of the electron beam performance (synchronization, pulse duration, bunch charge) to realize the full potential of the secondary sources; and maintenance of high-quality user services, while pursuing an active program of advanced accelerator and strong-field research. In addition, with the aid of the extended ELBE user community, the scientific staff and accelerator physics team of ELBE will complete the full conceptual design, followed by a technical design, of the DALI project [ELB.2, ELB.4].

13.3.1. Expected Achievements and Development Potential

Specific activities during PoF IV include the following:

- Completion of the AIDA positron beamline for dynamical studies of defect migration in charge carrier manipulation, annealing, and ion irradiation [ELB.1].
- Commissioning of the trARPES beamline at TELBE for user research to dynamically access electronic structure changes induced by THz-driven phase changes, superconductivity, and catalysis.
- Integration of DRACO petawatt operations into the external user program in conjunction with Laserlab-Europe and ATHENA.
- Coordination of the experimental program in nuclear astrophysics at the Felsenkeller underground laboratory with the international user operation of nELBE and γELBE.
- Improvement of the electron beam performance with upgrade of the SRF gun photocathode laser, reduced emittance, and increased bunch charge and stability [ELB.6].

41 *J. Couperus et al., Nature Communications 8 (2017) 487*
42 *L. Obst-Huebl et al., Nature Communications 9 (2018) 5292*

13.3.2. Milestones

Table 52: Milestones for the ELBE center.

	Year	Milestone
ELB.1	2021	User operation of AIDA for *in-situ* defect spectroscopy
ELB.2	2021/2022	CDR for DALI
ELB.3	2022	User operation of trARPES beamline of TELBE
ELB.4	2023	TDR for DALI
ELB.5	2023/2024	Start of ATHENA operation including external user access
ELB.6	2025	Improved stability of ELBE electron beam operation

13.3.3. Planned Investments/Upgrades of the Facility

During the PoF IV funding period, moderate investments are planned that aim at continuously modernizing the ELBE infrastructure. Moreover, the conception of DALI as a potential successor of ELBE will be further promoted.

13.4. Life Cycle Analysis

The ELBE accelerator is approaching 18 years of operation, but is still unique as a CW linear-accelerator-based secondary-radiation facility for routine user operation. New beamlines such as pELBE (since 2015) and TELBE (since 2016) have been added, continuously extending the scientific program. The advantage of CW SRF technology is recognized for many future projects, including CW upgrades of LCLS II, the European XFEL, and SHINE. In light of the experience with ELBE as an operating demonstrator of CW SRF accelerators, a continuing strong interest including broad international collaborations well into the next decade is anticipated. The ELBE center is therefore foreseen to have an operational life as an internationally competitive user facility until at least 2030.

The DALI concept is being explored as a possible replacement of ELBE, with a lifetime of another several decades. DALI builds in part on the rapid successes in the commissioning of the TELBE facility and the very promising future of pulsed-resolved high-repetition-rate measurement techniques. These include many emerging concepts to make use of strong-field THz radiation as a pump–probe technique reaching beyond solid-state physics to chemistry and biological sciences, including for example time-resolved ARPES, THz SNOM, and THz spectroscopy in the liquid phase. An option for extending the concept to the VUV range is under discussion. DALI further builds on the strong high-power laser infrastructure of the ELBE center and its connection to the HLD, with the vision of a broad scientific portfolio including the exploration of matter and materials under extreme conditions. After the completion of the CDR [ELB.2] and TDR [ELB.4], and if the required funding is acquired, an implementation of DALI could start in 2025.

13.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 53: ELBE (HZDR), planned for 2021. The costs include general and administrative costs, internal services etc.

HZDR costs (TEUR)	**10.844,1**
thereof personnel costs (including personnel of infrastructure)	5.644,4
thereof material costs	2.670,2
thereof electricity	1.339,4
thereof maintenance costs	539,0
thereof noncash expenditures	2.529,4
HZDR investments	
continuing investments	2.388,1
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0,0

Table 54: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

HZDR costs	10.844,1
- noncash expenditures	2.529,4
+ continuing investments	2.388,1
+ ongoing individual large investments > € 2,5 million	0,0
HZDR cash expenditures	**10.702,7**

Table 55: Program personnel capacity by center (FTE), planned for 2021.

HZDR part personnel	28
Scientists/Engineers	9
Scientific support personnel	19
for information only: corresponding LK I contribution HZDR	122
Scientists	65
Doctoral students	28
Scientific support personnel	29
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 56: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
HZDR	2.054,2	29	0,0	0
Scientists/Engineers	865,30	9	0,0	0
Scientific support personnel	1.188,93	20	0,0	0

14. HLD

14.1. Overview

The Dresden High Magnetic Field Laboratory (HLD) is one of the leading facilities for research with high magnetic fields worldwide. It is the only institution of its kind in Germany. At the HLD, researchers from all over the world use the HLD's leading-edge infrastructure for the generation of highest possible non-destructive magnetic fields and its dedicated experimental instrumentation to carry out advanced materials science experiments under extreme sample conditions, primarily in physics, chemistry, and engineering. The majority of the research projects aims at deciphering the fundamental properties of novel materials with the goal to reach an in-depth understanding and, by that, to use and optimize the material properties for future applications.

As a user facility of the HZDR, the HLD benefits from central administrative and technical services such as the central department for research technology. The HLD has an in-house design and development program for pulsed magnets and gigawatt pulsed power supplies, for which it operates its own specialized workshop. The continuous improvement of these installations with respect to maximum field, maximum power, and longevity is an important objective. A broad portfolio of partially world-unique pulsed-field magnets, with temporal field profiles as shown in Figure 15, is offered to users. This includes dual-coil systems reaching magnetic fields up to 95 T (figure inset). The in-house system competence puts the HLD team in an ideal position for developing dedicated high-field equipment for the European XFEL (HIBEF project). The HLD scientists are also intensively engaged in the development of novel experimental techniques specifically adapted for the challenging use in the hostile environment of pulsed magnetic fields. Besides high-resolution electrical transport, magnetization, dilatometry, and ultrasound measurements, this also includes resonant methods such as electron spin resonance (ESR) and nuclear magnetic resonance (NMR). These experimental techniques are available over a broad temperature range down to millikelvin temperatures. The combination of infrared radiation produced by FELs for the near-to-far infrared wavelength range of the neighboring ELBE facility with pulsed-field magnets is worldwide unique and allows the performance of unparalleled magneto-optical and ESR experiments.

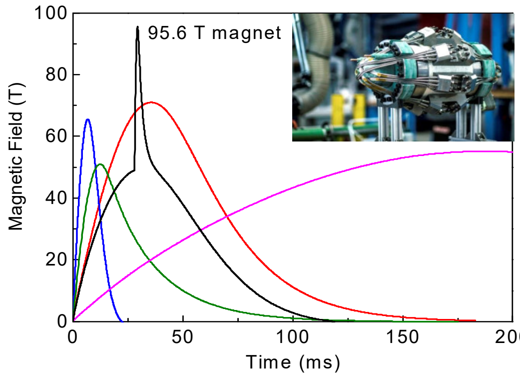

Figure 15: Temporal field profiles of the pulsed-field magnets of the HLD.

Access to the HLD is regulated through a peer-reviewed proposal system, which is centrally managed by the European Magnetic Field Laboratory (EMFL, see below). Expert support is provided by highly skilled research scientists, who have often also developed or improved the user-requested experimental infrastructures. In many cases, the close collaboration between local contacts and users leads to common scientific projects. The user demand for magnet time at the HLD has increased significantly (by about 10% per year), reaching 121 user projects in 2018 (350 users per year). All research and technological activities within the HLD are embedded in the Program MML.

14.2. Research Environment and Current Activities

The HLD maintains a highly active cooperation with the Dresden materials sciences community in the framework of the local science network DRESDEN-concept, in particular with TU Dresden, IFW Dresden, and the two Max Planck Institutes for the Physics of Complex Systems (PKS) and for Chemical Physics of Solids (CPfS). The user facility plays an important role in a number of joint DFG collaborative research projects, for example in the cluster of excellence

Complexity and Topology in Quantum Matter (ct.qmat). Beyond these activities, the HLD cooperates with many German universities and has tight bonds to all materials-science-based Helmholtz Centers within the Program MML.

The HLD cooperates closely with all other high-magnetic-field user facilities in Europe, the Dutch High Field Magnet Laboratory (HFML) in Nijmegen, and the French Laboratoire National des Champs Magnétiques Intense (LNCMI) with two sites in Grenoble and Toulouse. The four laboratories supplement each other in their complementary technical infrastructure for the generation of static magnetic fields up to about 38 T (Grenoble and Nijmegen), pulsed non-destructive magnetic fields up to about 100 T (Dresden and Toulouse), and semi-destructive fields up to about 200 T (Toulouse), each combined with a wide variety of advanced high-resolution experimental techniques. In an effort to serve the international user community even better, the partner labs established a single distributed research infrastructure, the European Magnetic Field Laboratory (EMFL)[43], legally founded in January 2015 as an international non-profit organization under Belgian law (Association Internationale Sans But Lucratif, AISBL). The successful implementation of EMFL was recognized by the “landmark” status in the 2016 roadmap list of the European Strategy Forum on Research Infrastructures (ESFRI). As a “landmark”, the EMFL is classified as a pan-European research infrastructure that ensures that scientists in Europe have access to world-class facilities, enabling them to do cutting-edge research. Strong synergies within EMFL have been achieved by common networking, sharing expertise in magnet design and experimental infrastructures, establishing joined committees, training staff, users, and students, and engaging in public outreach. Calls for magnet time are organized through a single EMFL entry point twice a year, and the proposals are evaluated by a single selection committee. Feedback and requests from the users are organized by a common user committee. The AISBL legal structure of the EMFL allows for the inclusion of additional partners. In 2016, the UK joined the AISBL, followed by Poland in 2019. Further parties are interested to join.

Beyond the strategic cooperation within Europe, numerous collaborations exist with university and non-university groups worldwide. The HLD is a chairing member of the Global High Field Forum[44], a consortium of the major high-field laboratories worldwide promoting science and technology with high magnetic fields.

Major current activities

The HLD is strongly engaged in consolidating and extending its role as a leading-edge user facility for research with high magnetic fields, in tight cooperation with its EMFL partners. Activities to this end comprise both the mentioned well-targeted magnet and power-supply design program and continuous advancements in the HLD experimental infrastructure according to the milestones and work program defined for PoF III. This combined approach allows for leading-edge signal-to-noise-ratio measurements in extreme fields and enables groundbreaking scientific results to be achieved. The HLD pursues a focused in-house research program at the forefront of materials science research both to fulfill its scientific mission and to attract world-class users.

14.3. Content and Objectives

14.3.1. Expected Achievements and Development Potential

The HLD will enhance its visibility significantly by demonstrating technical and scientific record achievements. The international research community will recognize the HLD as an attractive user facility for materials research at highest fields and as a strong and strategically important cooperation partner. In detail, the following goals are to be reached.

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43 http://emfl.eu
44 http://globalhiff.org/

Establish access to high pulsed magnetic fields at other large-scale facilities

The HLD will establish access to highest magnetic fields at other large-scale infrastructures, in particular at HIBEF at the European XFEL. The advance and transfer of HLD technology to the European XFEL will allow unprecedented high-field X-ray experiments to be performed, such as X-ray magnetic circular dichroism (XMCD) measurements in the 60 T range. This will open the doors to as yet inaccessible element-selective studies of complex materials under extreme sample conditions. The HLD will both design and manufacture key components, such as pulsed magnets adapted for X-ray optical experiments (the design for a biconical 60 T magnet is shown in Figure 16) and an advanced pulsed-power generator. These activities comprise the milestones [HLD.1] and [HLD.2].

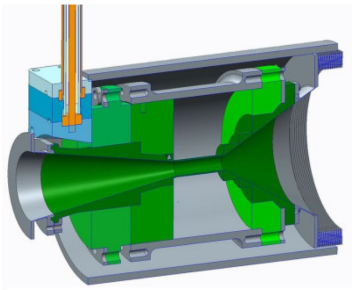

Figure 16: Design for a biconical 60 T magnet developed by the HLD.

Realize high-pressure experiments on sub-micrometer-sized samples

During the coming years, the HLD will expand its experimental infrastructure by providing the possibility to pattern materials down to sub-micrometer sizes using focused ion beams. This technique is ideally suited for structuring samples including electrical contacts so that the samples can be placed in a diamond anvil pressure cell. We will realize an experimental station for high-pressure studies of such samples in pulsed magnetic fields [HLD.3].

Reach world-record fields beyond 100 T

A particular challenging task is the design and successful realization of a 100 T pulsed magnet [HLD.4]. A possible design is based on three nested coils that would, at least in theory, allow fields up to 105 T to be reached with stress levels in the wire below those in the currently used double-coil 95 T magnet. Besides enabling research at ultimate field strengths, following this route in the next years will allow us to gain further knowledge in order to improve the coil performance also of more standard magnets, with the aim to increase their longevity.

Enable the first THz pulsed-field experiments with DALI

With the start of operation of the strong THz sources in the DALI infrastructure, envisaged at the end of the PoF IV period, unprecedented high-field THz spectroscopy experiments will become possible. For that purpose, a next-generation pulsed-field THz spectrometry lab will be realized at the HZDR [HLD.5], and a pilot experiment will be conducted.

14.3.2. Milestones

Table 57: Milestones for the HLD.

	Year	Milestone
HLD.1	2022	Realization of the HIBEF beamline for materials research experiments at the European XFEL
HLD.2	2023	Commissioning of a specially designed pulsed-field magnet for X-ray experiments at HIBEF
HLD.3	2024	Realize experimental station for high-pressure investigations of sub-micron-structured samples in pulsed magnetic fields
HLD.4	2025	Reaching world-record fields beyond 100 T by use of a new design
HLD.5	2027	Enable the first THz pulsed-field experiments with DALI

14.3.3. Planned Investments/Upgrades of the Facility

In the PoF IV funding period, moderate investments are planned that aim at continuously modernizing the HLD infrastructure, such as magnets, capacitor banks, and experimental stations.

14.4. Life Cycle Analysis

The HLD has been operating as a user facility since 2007. A substantial enlargement in 2011 to 2014 roughly doubled its size and available magnet time, with the facility becoming fully operational in 2017. The HLD and its technical infrastructure are realized on the latest technological level, featuring for instance the most-advanced capacitor banks worldwide. Based on these recent upgrades, the experience with the lifetime of other magnetic-field user facilities, the continuously increasing demand for magnet time in the last decades, and the growing number of scientific challenges in many research areas that are tackled with high fields, a further operation of the HLD for at least another 20 years is well justified. Through continuous improvements of the pulsed-magnet designs and the experimental infrastructure, an even longer operation will be possible and is anticipated. With respect to the recent major upgrades, no large investments are planned in the forthcoming PoF IV period.

14.5. Resources

The following tables show the costs (full costs) and the expected and current personnel allocated to the facility.

Table 58: HLD - High Magnetic Field Laboratory Dresden, planned for 2021. The costs include general and administrative costs, internal services etc.

HZDR costs (TEUR)	**7.695,1**
thereof personnel costs (including personnel of infrastructure)	4.339,9
thereof material costs	1.035,7
thereof electricity	186,9
thereof maintenance costs	212,9
thereof technical gases	303,4
thereof noncash expenditures	2.319,6
HZDR investments	
continuing investments	650,0
ongoing individual large investments > € 2,5 million financed through Helmholtz large investment budget	0,0

Table 59: Reconciliation of total program costs to cash expenditures (in TEUR). Noncash expenditures include depreciation, reserves, variations in receivables and liabilities.

HZDR costs	7.695,1
- noncash expenditures	2.319,6
+ continuing investments	650,0
+ ongoing individual large investments > € 2,5 million	0,0
HZDR cash expenditures	**6.025,5**

Table 60: Program personnel capacity by center (FTE), planned for 2021.

HZDR part personnel	26
Scientists/Engineers	14
Scientific support personnel	12
for information only: corresponding LK I contribution HZDR	122
Scientists	65
Doctoral students	28
Scientific support personnel	29
for information only: corresponding LK I contribution total MML	634
Scientists	347
Doctoral students	168
Scientific support personnel	119

Table 61: Current personnel resources, preliminary resources for 2019.

	Helmholtz Program		**Third-party funding**	
	TEUR	FTE	TEUR	FTE
HZDR	1.267,1	24	0,0	0
Scientists/Engineers	620,05	12	0,0	0
Scientific support personnel	647,00	12	0,0	0