Helmholtz Zentrum Berlin

BESSY III

The Materials Discovery Facility

Taking Soft- and Tender X-ray Science and Innovation to a New Level

Pre-Conceptional Design Report

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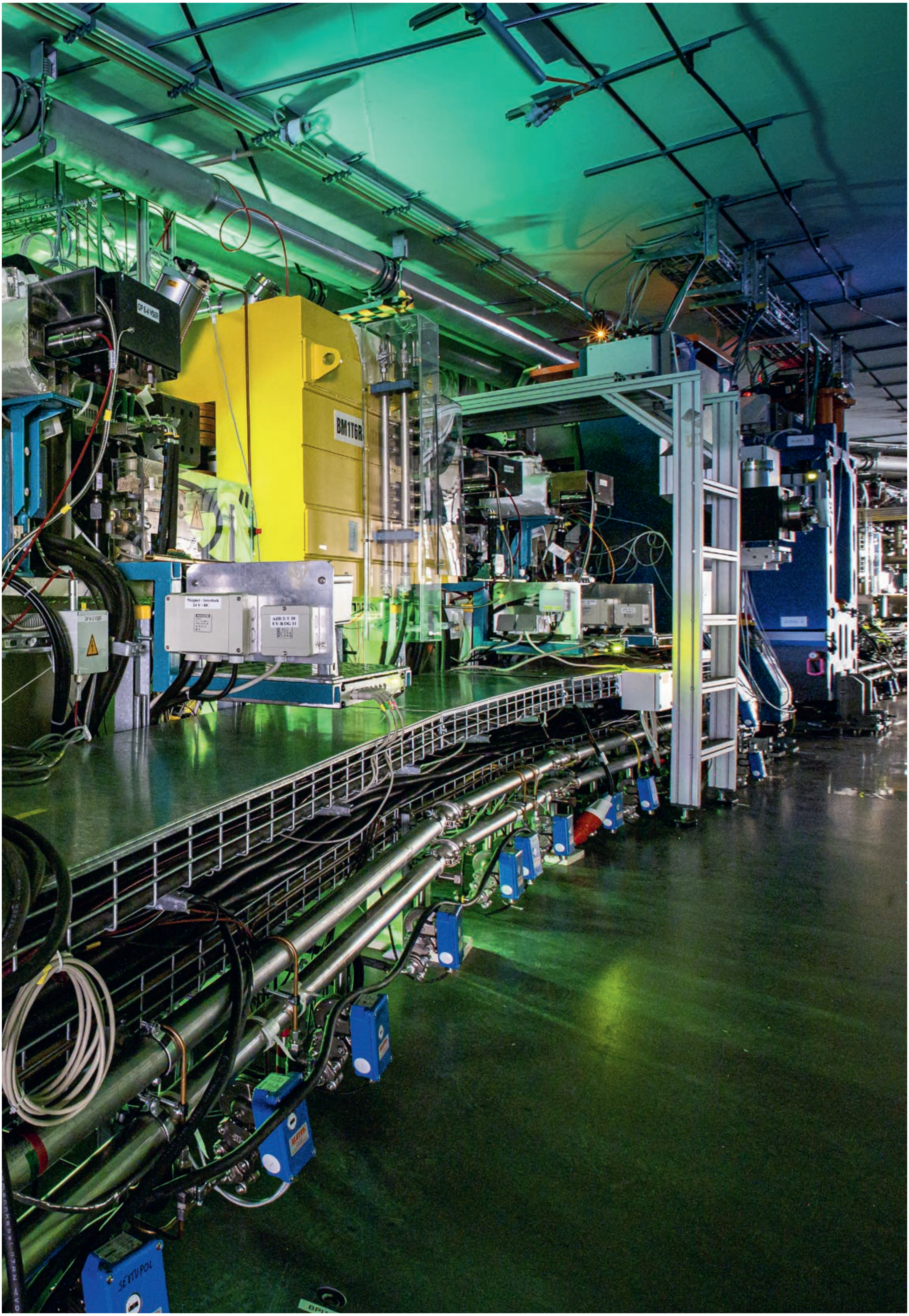

Executive Summary

BESSY III will be a world-leading synchrotron radiation facility for soft-to-tender X-rays, operated by Helmholtz-Zentrum Berlin (HZB). It will offer the German, European and international user community from academia and industry powerful experimental capabilities for materials research, and thereby drive materials discovery to address major societal challenges, in particular the quest for a climate-neutral society. **BESSY III**, integrated in the materials science campus Berlin-Adlershof, will provide unique capabilities for the materials and energy science community.

BESSY III will be a fourth-generation synchrotron light source based on a multi bend achromat lattice, providing synchrotron radiation of highest brightness and coherence in the soft-to-tender X-ray region for spectroscopy and microscopy at the nanoscale. The electron energy and ring circumference will be increased compared to BESSY II (2.5 GeV and 350 m, resp.) to meet the demand for a higher flux of tender X-rays, while maintaining the complementarity to the hard-X-ray sources PETRA III / IV and ESRF-EBS. In combination with advanced undulators and highly automated beamlines, photon beams of unprecedented quality will be available for both high-resolution and high-throughput studies, including dynamic investigations down to the picosecond time scale.

The capabilities of a bright photon source will unfold their full potential for unveiling materials properties by an efficient link to complementary techniques. Therefore, **BESSY III** will be embedded in the research campus Berlin-Adlershof and facilitate multimodal studies with laboratories operated by HZB and partners. A particular emphasis will lie on the development of specialized equipment and sample environment for *operando* investigations to study “materials at work”.

A key partner of HZB in the development of **BESSY III** is the Physikalisch-Technische Bundesanstalt (PTB) that will operate a sector of the new facility. Their globally unique expertise in metrology and quantitative materials science will not only enhance the economic impact of **BESSY III,** but also enable the installation of quantitative measurement capabilities at instruments beyond the PTB sector, which will permit otherwise unattainable insights into materials properties.

The combination of (i) the extremely bright soft X-ray source, (ii) the integrated research campus and (iii) the quantitative measurement capabilities will make BESSY III a world-leading facility for materials discovery used by universities, non-university research institutes and industry.

The scientific focus will lie on fields that contribute to achieving a climate-neutral, sustainable society (i.e. green energy production and storage, catalysis and green information technology) as well as life sciences. Soft-to-tender X-rays are indispensable in these fields for the study of electronic properties, which determine the functionality of materials. Dedicated *operando* equipment and an early involvement of industrial collaborators will ensure high economic relevance and innovation potential of the research. The optimisation of the **BESSY III** facility with respect to the focus fields will be driven by HZB's research groups, its key partners and the involvement of the user community.

BESSY III will make full use of the digital capabilities available at the time of operation, along the whole chain from photon generation to data collection and analysis. HZB is committed to plan, to build and to operate the **BESSY III** facility as a gold standard for large scale research facilities, and to make **BESSY III** the place to be for an international and diverse community of scientists and technologists.

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1. Materials Discovery at BESSY

HZB Photon Facility Strategy and the HZB Research Campus

Climate change mitigation and a growing world population urgently require a transition towards a globally sustainable, resilient, and climate-neutral society. Scientific and technological breakthroughs will be key to improving energy efficiency, ensuring a sustainable energy supply, and ultimately achieving carbon neutrality across all societal domains. As laid down in the recently published key issues paper for the promotion of materials research of the German Federal Ministry of Education and Research[1], materials are a prerequisite for any technological progress and thus a decisive economic factor. Solving this challenge thus requires research and development of new materials and radical new technologies for renewable, carbon-neutral energy conversion and energy storage processes as well as systemic green hydrogen solutions.

For materials discovery and developing tailored functional materials, understanding the electronic structure and ultimately controlling reaction pathways and processes are vital. For a wide range of applications, in particular for energy and quantum materials, the electronic structure is the key property that determines the functionality. Due to their ability to probe the electronic, chemical and spin structure, modern microscopic and spectroscopic methods using soft-to-tender X-rays that allow *in-situ* and *operando* investigations are an indispensable tool for materials research.

The BESSY II synchrotron radiation source at Helmholtz-Zentrum Berlin (HZB) is an internationally leading facility playing to its strengths in the soft X-ray regime, with the mission to enlighten and enable materials discovery, develop solutions to the societal challenges of this century, like Energy, Information and Health, and enable research and innovation along the entire value chain. BESSY II's long-term strategic development is guided by the center's programmatic research, the involvement of HZB's strategic partners, the scientific environment as well as the BESSY II user community as a whole. Within this framework, the areas of catalysis/electrochemistry, energy materials, as well as quantum and correlated materials discoveries, but also new bridges between basic research and industry.

BESSY II has now been in operation for more than 20 years and will be operated until 2035. With a recently formulated upgrade program BESSY II+ competitiveness on highest international level will be maintained. For the years after 2035, its successor source, **BESSY III,** needs to be ready for operation. Maintaining BESSY II competitive while bridging to **BESSY III** requires maintenance and modernization measures as well as the provision of new research opportunities within the guidelines

- **Expanding capabilities in the field of electrochemistry and catalysis with the ambition to provide worldwide leading, industry relevant experimental possibilities; here, CatLab serves as a blueprint for the further development,**

- **Leadership in quantum and correlated materials by upgrading instrumentation,**

- **Keeping competitiveness in Life Sciences by implementing fast and efficient high-throughput methods,**

- **Continuously developing and implementing novel accelerator operation and instrumentation concepts as well as access modes, and**

- **Maintaining the facility's leadership as a key enabler of metrology with synchrotron radiation and strongly develop and roll out materials metrology capabilities together with PTB and BAM.**

HZB has committed itself to become greenhouse gas neutral by 2035. BESSY II, as any large-scale infrastructure, consumes a significant amount of electrical energy. Dwindling resources, together with rising energy costs and climate change are all requiring mid- to long-term strategies for reliable, affordable and carbon-neutral energy supplies. Important steps towards a more energy-efficient operation of the facility are therefore essential parts of BESSY II+ and will pave the way towards a sustainable **BESSY III.**

The BESSY II+ upgrade program – which has been evaluated by an external panel of international renewed experts and leaders in synchrotron science in October 2022 – will not only enable continued outstanding scientific research and innovation at BESSY II, but also initiate developments that are of great importance for the design of **BESSY III. BESSY III,** integrated in the materials science campus Berlin-Adlershof, will provide unique capabilities for the national and international materials and energy science community by synergetically combining

- **a state-of-the-art 4th generation synchrotron radiation source,**
- **an integrated facility approach embedded in the materials research campus at Berlin-Adlershof, and**
- **quantitative and metrological materials science capabilities, which are leveraged by the world-leading expertise of Physikalisch-Technische Bundesanstalt (PTB).**

The interlocking plans for the BESSY II+ upgrade program and the successor source **BESSY III,** which are co-ordinated in terms of scientific foci and methodological developments, reflect the strategic relevance for HZB of the availability of modern soft-to-tender X-ray microscopic and spectroscopic methods at its Adlershof campus. ↘ Figure 1.1 shows the roadmap for the further development of the synchrotron radiation sources at HZB .

This roadmap, aligned with the national Helmholtz-Photon Science roadmap and the European LEAPS Strategy for the future development of large-scale research facilities in the field of synchrotron radiation, fits seamlessly into HZB's strategic campus development which aims at concentrating all research activities and infrastructures on one site – in Adlershof. In the medium term, additional laboratory and office space will be created there, with a focus on internal and external networking and the creation of transfer and innovation spaces. Both will contribute directly already for BESSY II and are indispensable for **BESSY III. BESSY III** will be the key pillar for new materials and technologies for the entire science and technology park Adlershof. The realization of BESSY II+, followed by **BESSY III,** will be a lighthouse and an attractor for bright minds from science and industry to keep Berlin and Germany within a leading European position.

In all campus development projects, HZB is committed to finding or creating sustainable solutions which are on the forefront of international developments.

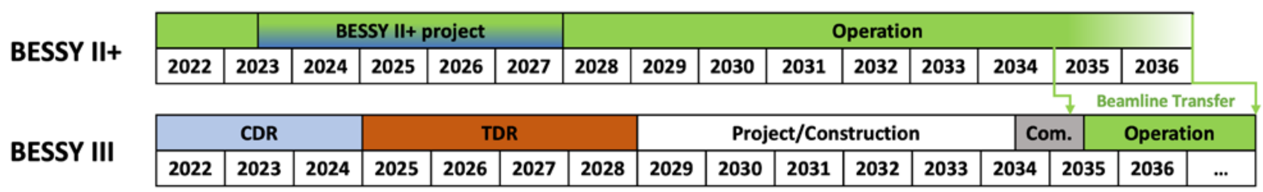

Figure 1.1: Roadmap for the further development of the synchrotron radiation sources at HZB which includes the transfer of beamlines and instrumentation from BESSY II+ to **BESSY III**

2. Mission and Motivation

BESSY III will become a world-leading facility for soft-to-tender X-rays enlightening the way for materials discovery and development of disruptive technologies. **BESSY III,** integrated in the material science campus Berlin-Adlershof, will provide unique capabilities for the national and international materials and energy science community by synergetically combining

- a state-of-the-art 4th generation synchrotron radiation source,
- an integrated facility approach embedded in the materials research campus at Berlin-Adlershof, and
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Climate change mitigation and a growing world population urgently require a transition towards a globally sustainable, resilient, and climate-neutral society. Scientific and technological breakthroughs will be key to improving energy efficiency, ensuring a sustainable energy supply, and ultimately achieving carbon neutrality across all societal domains. As laid down in the recently published key issues paper for the promotion of materials research of the German Federal Ministry of Education and Research[1], materials are a prerequisite for any technological progress and thus a decisive economic factor. Solving this challenge thus requires research and development of new materials and radical new technologies for renewable, carbon-neutral energy conversion and energy storage processes as well as systemic green hydrogen solutions.

Materials discovery requires dedicated synthesis capabilities, sophisticated analytical tools and theory support that enable the understanding and tailoring of the electronic structure and its dynamics on relevant length and time scales, often under realistic chemical and physical conditions for the processing of the materials *(in-situ)* or while in operation *(operando)*. The availability of soft X-ray synchrotron radiation (SR) is key to this investigation. While complementary hard X-ray sources such as PETRA III/IV and the ESRF-EBS focus on the atomic structure of the material, soft-X-rays are indispensable to provide deep insights in the functionality of a material by probing electronic structures and properties. Already at BESSY II, HZB is pursuing an integrated approach where investments into beamline and end station infrastructure as well as synthesis and complementary off-line characterization capabilities will create opportunities for new materials discoveries. However, as functional materials are increasingly heterogeneous on nanometer length scales, the investigation of such materials is often hampered. **BESSY III** will overcome this limitation and provide previously unavailable analytical capabilities for the efficient investigation of very small or inhomogeneous samples by means of nanoscale studies with high spectral sensitivity. The 4th generation soft-to-tender X-ray source will surpass the performance of BESSY II by orders of magnitude, especially in terms of spectral brightness, coherence, and smallest spot size. The new facility will allow time-resolved, *in-situ* and *operando* studies of materials and devices with full polarization control under real operation conditions, focusing on spectroscopic and microscopic methods matched to the desired applications. Based on these features, **BESSY III** will serve a broad user community from applied to curiosity driven research.

Already today, and increasingly in the future, more than just a state-of-the-art photon beam is required for scientific investigations to have real impact. Our surveys with experts from different user communities, partner institutions, and among the HZB scientists showed that the success of the research relies on multimodal experimental approaches, consisting of state-of-the-art, science-driven SR-instrumentation and sample environments combined with correlative off-line (lab) methods, complex material synthesis, and (near) real-time data processing in an integrated research environment at a materials science campus.

Consequently, **BESSY III** will be integral part of the HZB's Wilhelm-Röntgen Campus Adlershof (WCRC) and embedded in the Science and Technology Park in Berlin-Adlershof. At **BESSY III,** users and user consortia will not only be able to apply for beam time at the SR source, but also for access to the laboratory infrastructure linked to **BESSY III** on the integrated campus, thus significantly accelerating the development of new materials. **BESSY III** will come to life with a rigorous digitization of the entire scientific workflow, optimized data acquisition and analysis systems and sustainable data curation. It will benefit from IT infrastructure coordination, undertaken on multiple, large scale levels, e.g. national NFDI, DAPHNE, FAIRmat, ErUM-Data, European EOSC, ExPaNDS and global RDA. Active participation in these coordinated activities will add FAIR value to scientific data acquired at **BESSY III**. This research environment on the WCRC as embedded in the Science and Technology Park Adlershof will make **BESSY III** a unique and powerful analytical tool for materials research – a materials discovery facility.

The **BESSY III** concept is leveraged by the long-standing strategic partnership of HZB and the Physikalisch-Technische Bundesanstalt (PTB). In co-operation with the Bundesanstalt für Materialforschung und -prüfung (BAM), PTB will further expand its activities. Metrological measurements as conducted by the PTB for quantitative materials science will be implemented at **BESSY III,** tailored to the structural complexity of advanced materials down to nanometer length scales for applications in optics, semiconductor electronics, quantum technology, photovoltaics, energy storage, catalysis, or biotechnology. This includes the maintenance of a quality management system as well as measurement standards traceable to the international systems of units SI. Implementing metrological methods at the **BESSY III** instruments allows for a traceable quantitative sample characterization, thus adding unique value for academia, non-academic research institutions and industry.

Berlin is one of Europe's leading centers of science and research, one of the main focus areas being medicine, medical technology and biotechnology. Through its co-operation, especially the Joint Berlin MX-Laboratory, HZB is embedded in the Life Science Campus Berlin. Targeting the needs of this community, **BESSY III** will provide opportunities to better understand fundamental biological processes by examining organisms over multiple spatial scales to bridge hierarchical levels from molecules to cells to organs. Examples are the structure of proteins, the biology of diseases, the structure and function of the nervous system, and drug and therapy development. Nanometrology opens up the way to measure the size, shape and structure of nanoparticles in dispersion, e.g., for biomedical applications.

The Science and Technology Park Berlin-Adlershof operated by WISTA is the chosen location for **BESSY III.** The profile-defining coupling of **BESSY III** to the HZB research program, the further expansion of the long-term collaboration with MPG, PTB and BAM, and the embedment into the Adlershof Science and Technology Park, Germany's largest and most successful science and technology park guarantees the success of this endeavor. In Berlin-Adlershof, various research institutes, the natural sciences departments of the Humboldt-Universität zu Berlin (HUB) as well as many high-tech companies benefit from the inspiring neighborhood and drive innovation processes. In this stimulating environment, surrounded by the vibrant setting of Berlin as a city of science, the **BESSY III** facility will become a driver for the development of new technologies and for enabling world-leading technology companies. This ensures worldwide visibility and impact and will stimulate the further development of Berlin and Germany as a leading place for high technology and innovation.

The **BESSY III** facility needs excellent and dedicated people on all levels in administration, in technical and engineering support, for user operation and scientific leadership, to guarantee a a worldwide leading position. The **BESSY III** project in its development and implementation phase offers great perspectives to attract and develop the needed talents on all these levels. Already today HZB is very active and forward looking in the field of developing and attracting a diverse workforce and to promote women and minorities on all levels of qualifications. This is laid down in HZB's center strategy and demonstrated by the fact that HZB, as the first non-university research organization in Germany, successfully passed an auditing process and is now "VIELFALT GESTALTEN" (Shaping Diversity) certified. All the gained know-how and the established processes will allow to develop **BESSY III** in the best possible way.

The **BESSY III** facility will be built and operated in a sustainable manner. To achieve this, all feasible options for energy efficient and sustainable construction and operation, energy recuperation and on-site energy generation must be used to keep the carbon footprint as small as possible. In particular, we strive for the German Sustainable Building Council (DGNB) or rather BNB certification for the construction of the **BESSY III** facility.

HZB VISION AND MISSION

OUR VISION

TOWARDS A BRIGHT FUTURE: HZB 2030+

Our vision of HZB 2030+ is shaping a sustainable future by developing technological solutions based on novel materials.

OUR MISSION

WE DRIVE MATERIALS DISCOVERY

We strive to achieve a climate neutral society through science and innovation. This is why we drive materials discovery, create new sustainable technologies and empower the research community in realising this goal.

3. Strategic Relevance

Materials and Energy are the DNA of HZB. With a focus on energy applications, we research new materials – from the exploration of fundamental properties of matter to the discovery of functional materials and concepts. We develop these materials into devices and scalable technological solutions. All these steps are based on the development and operation of state-of-the-art facilities for our research, our partners and the international user community from academia, non-academic research institutions and industry. Understanding the electronic structure of materials and ultimately controlling the evolution of reactions and processes is key to tailoring functional materials and devices. For this, *in-situ* and *operando* microscopic and spectroscopic methods, as provided by a state-of-the-art soft-to-tender X-ray light source facility, are key enabler. Furthermore, quantitative measurements ("materials metrology") permit a reliable comparison of data from different techniques and thus strongly increase the informative value of multimodal approaches if non-simultaneous (including non-synchrotron) methods are used.

Up to now, HZB's BESSY II synchrotron radiation source, with its focus on the soft X-ray range, is ideally suited to provide these capabilities to a large and multidisciplinary user community, including the life science community. More than 1200 user proposal are submitted per year, resulting in about 800 beamtime campaigns at the 40 beamlines in user operation, and approx. 500 verified publications per year. The interconnection of HZB research with user operation provides the basis for strong scientific support for BESSY II users, ranging from the development of special accelerator operation schemes, undulators, beamlines, instruments and dedicated sample environments, to the evaluation and interpretation of the data. BESSY II is the European radiation standard for synchrotron radiation metrology and is used by PTB for a fast variety of metrology applications, especially for industrial users at 7 dedicated beamlines. BESSY II has now been in operation for more than 20 years and will remain in operation until at least 2035, overlapping with the friendly user operation phase of **BESSY III.** The further development of BESSY II requires an ambitious strategic upgrade program, for which the areas of catalysis / electrochemistry and quantum and correlated materials have been identified as strategic priorities where investments will not only create new opportunities for materials discoveries, but also new bridges between basic research and industry. The program will enable continued outstanding scientific work and innovation at BESSY II, as well as initiate developments that are of great importance for the realization of **BESSY III.** It will therefore serve as a scientific and methodological bridge between BESSY II and **BESSY III.** It also seamlessly fits into the strategic development of HZB's Adlershof Campus WCRC with its aim to further develop it into an inspiring research site, an integrated research campus, hosting HZB's in-house research. Additional laboratory and office spaces are being created in the mid-term here, with a focus on internal and external networking and the creation of transfer and innovation spaces. On the long term, the new **BESSY III** is a key element for the sustainable development not only for the WCRC, but for the Science and Technology Park as a whole, where it will act, as BESSY II has done, as a flagship and attractor for smart minds from science and business. In summary, **BESSY III,** embedded in the Science and Technology Park Adlershof, is pivotal to secure HZB's leading position in the science system, i.e., to

- **drive materials discovery and development by building and operating unique research facilities for in-house and user community research**
- **create technologies by completely novel thin-film approaches for a carbon-neutral society**
- **continuously innovate and aspire to reach the next Technology Readiness Level**

- **empower the research community by leveraging synergies in the Berlin-Brandenburg scientific ecosystem and with the most innovative partners worldwide.**

BESSY III is part of the “National Strategy for the Further Development of Accelerator-based User Facilities for Research with Photons and in High Electromagnetic Fields (Helmholtz Photon Science Roadmap)” [2], which sets out the strategic planning for the development of the Helmholtz Association’s accelerator-based user facilities of these fields. This National Strategy is embedded in the planning of other European light sources [3] through the framework of the League of European Accelerator-based Photon Sources (LEAPS), with the aim of achieving strong synergies and optimizing necessary complementarity between Europe’s facilities. Within this framework, the synergetical combination of a 4th generation soft X-ray source, embedded in the integrated research campus Berlin-Adlershof, and leveraged by the expertise of PTB in the field of metrology sets **BESSY III** apart from other light source projects in Europe, and thus fulfills the strategically relevant smart specialization of the facility. In particular, it ideally complements the proposed future hard X-ray photon source PETRA IV, as detailed in the Helmholtz Photon Science Roadmap, and the ESRF-EBS upgrade of the ESRF on European level [3].

The continuous development of these user facilities is essential for the international competitiveness of both these facilities and the scientific community using them. This has been emphasized in a strategy paper published in 2020 by the Committee for Synchrotron Radiation (KFS) – the body elected by the German user community to represent user interests and being a partner for strategy developments with the BMBF. The KFS stated: “German research at synchrotron radiation sources is world-leading. In order to maintain this position, the KFS recommends investments in the further development of the sources. The KFS therefore supports the PETRA IV and **BESSY III** projects.”

4. Scientific Motivation

4.1 From Materials Discovery to Innovation

HZB strives to achieve a climate neutral society through science and innovation. We therefore drive materials discovery, create new sustainable technologies, and empower the research community in realizing this goal. Fully in line with the key issues paper of BMBF [1], HZB is developing models for an improved collaboration between academia, non-academic research institutions and industry and for the accelerated transfer of ideas into technologies and products. **BESSY III** will enable materials discovery with a key focus on materials, devices and systems that promise innovations for efficient energy conversion, use, and storage, as well as new paradigms for information technology. Importantly, it will cover the whole span from fundamental to applied investigations to achieve both a high innovation potential and an efficient transfer into economy and society. Therefore, a strong emphasis will be on *operando* investigations and application- (and thus industry-) relevant sample environments and processes.

The major benefits of the **BESSY III** light source are introduced in ↘Section 4.2, before the scientific motivation of **BESSY III** with respect to the focus areas energy, quantum and information technologies as well as life science is discussed in ↘Section 4.3. The relevance of **BESSY III** for metrology as performed by Germany's National Metrology Institute PTB is set out in ↘Section 4.4.

4.2 Scientific Opportunities by Bright Soft X-rays

Experiments with soft X-rays are an indispensable tool for materials research due to their ability to probe the electronic, chemical and spin structure by spectroscopic techniques or spectral imaging. For a wide range of applications, in particular for energy and quantum materials, the electronic structure is ***the*** key property that determines the functionality. Using 4th generation SR sources, extremely bright coherent X-ray beams are obtained that enable fast experiments with very high spatial, temporal and energy resolution as well as chemical, magnetic or even orbital angular momentum [4,5] state specificity, relying on full polarization control of the X-rays. At the same time, brighter X-ray beams offer a larger flexibility regarding the sample type, size and environment than many lab-based techniques, thereby enabling *operando* and *in-situ* studies under a broad range of experimental conditions. Apart from materials science, soft X-ray SR is also very well suited for the studies in life science, where high spatial resolution and chemical sensitivity are equally important.

The structural complexity of modern materials, often containing inherent or tailored nanoscale structural elements, as well as the need to expand the capabilities of *operando* and *in-situ* studies, requires experimental possibilities beyond those of today's SR sources. In collaboration with its users and partners, HZB has developed a concept for a successor source that matches the requirements of the mission-oriented scientific focus fields. The following paragraphs give an overview of key technical gains of **BESSY III.**

#high-res-spectro (high-resolution spectroscopy)
BESSY III will continue BESSY II's tradition of providing world-class spectroscopic techniques based on variable, even circular polarization, and further develop these capabilities by combining them with nanometer spatial resolution, based on the capability of 4th generation light sources to focus the probing beam down to the diffraction limit of the respective X-ray photon energy (↘Section 6.1.1). Using nano-focussing optics (↘Section 6.1.3), established spectroscopic techniques such as absorption, photoemission (incl. ARPES) or fluorescence spectroscopy will be offered in a scanning mode, with spot sizes of roughly 10 nm, i.e., a factor

1000 smaller, and a brightness that is at least 100 times higher than at BESSY II.

Complementing these capabilities for high spatial resolution, **BESSY III** will offer Resonant Inelastic X-ray Scattering (RIXS) with very high energy resolution (1 – 3 meV at 1 keV), an order of magnitude better than the highest-resolution RIXS beamlines today (↘Section 6.1.3).

#high-res-imag (high-resolution imaging)

Beyond spectroscopy as described above, microscopy and spectro-microscopy with nano-focusing will be enabled at **BESSY III,** e.g., scanning transmission X-ray microscopy with variable linear and circularly polarized X-rays (STXM). Driven by life science applications, a scanning microscope that detects backscattered electrons and employs Focused Ion Beam milling (FIB-STXM) is in development already at BESSY II. Using **BESSY III's** high brightness and coherence, 3D images with isotropic 10 nm resolution will be routinely attainable, also for thick tissue specimens. These high-resolution imaging capabilities will be embedded in a hierarchical imaging pipeline which is described in ↘Section 4.3.3 for life science (see also ↘Figure 4.4), but have many potential applications also in other fields.

Furthermore, coherent imaging techniques such as soft X-ray holography, ptychography and Bragg coherent diffractive imaging (Bragg-CDI) will be enabled, relying on the increase in coherence of roughly two orders of magnitude (at 1 keV) compared to BESSY II (↘see Figure 6.2). Using dedicated optics, the total gain in coherence at the final focus can be pushed to more than four orders of magnitude. These coherence-based techniques will enable imaging with very high spatial (sub-3 nm in 2D, sub-10 nm in 3D) and high temporal (ps-ns) resolution at magnetic sensitivity based on polarized light.

#dynamics and processes

Dynamic experiments in a wide range of time scales will be possible at **BESSY III**. In particular, the possibility to perform dynamic studies (even in *operando*) with time scales of order of magnitude from µs to s will be strongly improved due to the enhanced brightness and coherence of the source. Also, stochastic dynamics down to the µs range will become accessible by the coherence-based techniques.

Experiments at faster time scales and adjustable repetition rates will profit from HZB's expertise in developing advanced schemes of accelerator operation (↘Section 6.1.1) which will enable dynamic experiments down to a few 10 ps or potentially a few ps (rms) in special operation modes, complementary to FEL and table-top X-ray sources. The "Transverse Resonance Island Buckets" (TRIBs) operating mode [6], recently developed at HZB, generates a second orbit for an additional fill pattern which opens up, e.g., the possibility of MHz alternation of the helicity of the photon beam [7] (↘Section 6.1.1). It could be envisioned to couple TRIBs operation with a bunch length manipulation scheme based on the development of normal conducting higher harmonic cavities. Such a scheme could provide simultaneously two different bunch lengths, maintaining the needed lifetime for the low emittance beam in combination with some short pulses in the sub-10 ps regime.

#tender X-ray range

BESSY III will offer up to 5 orders of magnitude increased flux in the tender X-ray range based on the larger electron energy of 2.5 GeV (↘Section 6.1.1), specialized undulators (↘Section 6.1.2) and the development of multilayer grating monochromators (↘Section 6.1.3). Thus, all resonant techniques will be able to access absorption edges (also at circular polarization) that are difficult or impossible to access at BESSY II. This includes L-edges of 4*d* elements or M-edges of Lanthanides and the technologically relevant 5d element Hafnium, the K-edges of Si, P and S as well as many biologically relevant ions such as Ca, K, Mg and Na. Thereby, the range of interesting materials that will be studied at **BESSY III** expands significantly. The increased flux in the tender range will also enable better access to buried interfaces, necessary for layered materials.

#quantitative material science

At **BESSY III,** quantitative material science will be enabled by the partnership of PTB and HZB, yielding highly reliable data of materials properties. Apart from using calibrated instruments, metrological standards also imply the reproducibility of the sample preparation process and careful metadata acquisition, elevating the quality of data made available in FAIR data archives. Quantitative data sets permit a reliable comparison of data from different techniques and thus strongly increase the information content of the ↘#multimodal approach described below. Moreover, a direct comparison of experimental data to data from simulations or digital twins is possible, thereby leveraging the potential of computational materials design for future materials development.

The machine design of **BESSY III** incorporates the requirement for a fully calculable source (↘Section 6.1.1), allowing truly metrological standards at the PTB beamlines. Additionally, the close collaboration of HZB and PTB will facilitate the implementation of quantitative measurement conditions also at other instruments at **BESSY III** which will have a decisive impact on the importance of **BESSY III** for a broad community from industry, academia and non-academic institutions.

#high throughput, #automation, autonomous experimentation

Higher photon flux, a much higher coherence, advanced undulators and faster detectors at **BESSY III** (see ↘Chapter 6) allow for many orders of magnitude faster data acquisition than at BESSY II. E.g., full NEXAFS spectra will be measured within less than a second rather than several minutes. Additionally, comprehensive automation of the entire workflow will render high-throughput approaches feasible, which are capable to meet the demands imposed by vast parameter spaces of sample compositions and sizes as well as operational and sample preparation conditions. Thus, it will be possible to measure hundreds or even thousands of samples per day with automated spot adjustment, a reliable quality of data and minimal loss of beamtime. In addition, AI methods will support sample preparation and parameter selection, decision making during the experiment (↘see Section 6.3) and real-time data analysis during data acquisition. As outlined in ↘Chapter 7, autonomous experimentation, combined with rapid access modes, is crucial to make SR-based measurements attractive for industry.

#multimodal experimentation

Multimodal experiments, yielding a thorough material and process understanding, will be provided in various forms:

(i) The combination of multiple techniques at the same beamline, requiring specialized endstations and/or beamline designs.

(ii) Subsequent measurements at different beamlines and endstations requiring standardized concepts for sample handling and manipulation as well as experimental modules with specific environments (e.g. high pressure, liquids, cryogenic temperatures).

(iii) The combination of SR-based and lab-based techniques, extending the concept of transferable modules to complementary techniques.

(iv) The combination of experimental and simulation data enabling quantitative results.

#operando and in-situ studies

The facility will focus strongly on providing dedicated infrastructures for *operando* and *in-situ* studies. Samples and devices in operation, mimicking realistic manufacturing and operating conditions observed with spectroscopic and microscopic measurements reveal device performance parameters. Static *in-situ* studies of materials under relevant conditions give access to the role of compositions, arrangements, and effects of the external forces. The focus on *in-situ* and *operando* measurements will use specialized instrumentation and sample environments at the endstation, but also requires an efficient link of the SR-based experiments with facilities for synthesis and complementary analytic techniques as discussed in detail ↘in Section 6.2.

4.3 Scientific Focus Areas

The focus of **BESSY III** is to provide optimal experimental capabilities for the key research fields:

- **Energy, in particular energy conversion and storage as well as catalytic processes for chemical energy conversion;**
- **Quantum and Information Technologies;**
- **Life Science.**

Motivated by examples from current research, the following subsections illustrate how experiments at **BESSY III** can drive progress in these fields. However, many scientific areas beyond those described here will equally profit from the capabilities offered by **BESSY III** – including topics which are not yet on the horizon of today's research. This is due to the overarching nature of many of the discussed aspects. E.g., catalysis is an ubiquitous principle in (bio-)chemistry, and research on catalysis thus covers a large wealth of topics. Similarly, materials metrology (as detailed in ↘Section 4.4) may be applied to very diverse scientific fields, and nano-structures are relevant for various classes of materials as well as for biological tissue, as mentioned above ↘in Section 4.2.

4.3.1 Energy

Energy Conversion and Storage

Motivation: For many years to come, transforming into and maintaining a sustainable energy economy will be one of the most urgent global challenges. The pressing need to accelerate this transformation will not be coped with by simply relying on scaling-up of today's technologies but crucially requires new, more efficient concepts for the production and storage of electricity as well as the carbon-neutral operation of vehicles: e.g., battery concepts with significantly enhanced energy densities, improved long-term stability and high sustainability will be needed, as well as solar cells with performances surpassing current state-of-the-art photovoltaic technologies. Solar fuel generating devices which directly convert solar energy into chemical fuels are an additional promising energy storage technology that can address the intermittence of solar irradiation and related energy production. Exploring novel concepts for such applications, based on abundant, non-toxic, easily manufacturable, and stable materials, requires a detailed microscopic understanding: Which physiochemical processes occur within the complex device structures, e.g., at interfaces? Are these processes favorable or disfavorable to the device's efficiency? Which mechanisms limit the long-term stability, and which device structures facilitate recycling? Answering these questions requires powerful, fast analytical tools that can observe processes during operation and rapid feedback loops connecting the analytical experiments with the synthesis of materials and devices.

Approach: Synchrotron facilities provide optimal conditions for experiments that aim at an atomic-scale understanding of processes under actual operating conditions, as they yield information on various length and time scales involved in these processes. The soft to ↘#tender X-ray range is ideally suited to obtain high-resolution data on electronic structure and chemical states that are essential for the device's performance. For example, SR-based studies of solar cells at BESSY II have revealed the origin of interface-related performance limitations [8,9], the absorber doping mechanism [10], as well as dynamic and hydrogen bonding effects on the electronic absorber structure [11], generating crucial insights to propose mitigation strategies as well as material and/or device design optimization routes. This knowledge advantage has played a significant role in achieving record-breaking efficiencies for perovskite tandem solar cells [12]. In case of batteries, spectroscopic studies at BESSY II have, e.g., shed light on the importance of a solid interlayer on electrolyte stability [13] and identified sulfide movement as a key origin of capacity fading [14] (comp. ↘Figure 4.1).

The study of energy devices demands a strong focus on providing dedicated sample environments for static *in-situ* and dynamic ↘*#operando* studies, suitable for the soft-to-tender X-ray range and being able

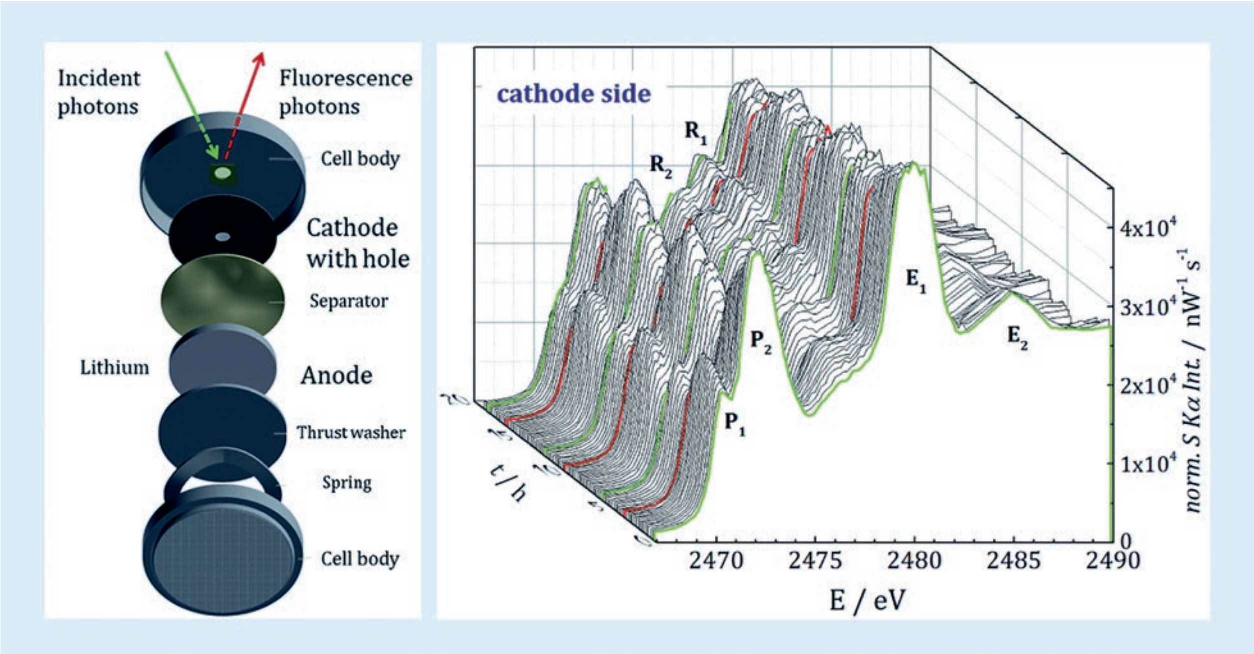


Figure 4.1: LiS battery investigated at BESSY II: *Operando* NEXAFS measurements in fluorescence yield at the Sulfur K-edge **(right)** using the Sulfur Kα signal normalized to a radiometric standard (denoted as norm. S-Kα Int.) on modified real battery coin cells **(left)**. The additional R1 and R2 peaks quantitatively reveal electrochemical temporal changes of Sulfur in the Lithium anode upon charge cycles (red and green lines)[14]. **BESSY III** will enable such ↘#quantitative measurements with enhanced acquisition speed, particularly for experiments in the ↘#tender X-ray range.

to simultaneously monitor device performance. For example, reusable generic battery cells that allow for decent current-voltage curves and an excellent interface for SR experiments will be provided. ↘#Multimodal approaches combining multiple techniques, such as spectroscopy, scattering, and imaging, either at one beamline, at different beamlines, or combining SR and offline methods, will play a central role in a thorough process understanding. Enabling such experiments will be a central guiding principle for **BESSY III**.

The capabilities of a high spectral brightness X-ray source will extend the accessible length and time scales of the processes that may be studied by the availability of nanometer-sized beams and the decreased measurement time, respectively (↘#high-res-spectro, ↘#dynamics). Thus, processes such as dendrite formation in batteries, the effect of local inhomogeneity on electro-catalytic efficiency of solar fuel devices, or charge carrier dynamics in solar cells can be studied. These experiments will also strongly profit from the better access to the ↘#tender X-ray range, which permits more significant penetration depth through the sample environment or into the device, e.g., for the study of buried interfaces. Furthermore, ↘#*operando* experiments that provide ↘#quantitative data, as envisioned for **BESSY III,** will lay the foundation for highly reliable and robust digital twins, which are expected to play a major role in accelerated technology development e.g. of batteries, and will thereby attract industrial collaborations.

In device-driven research, the speed of the overall cyclic process – encompassing design, synthesis, analytical measurement, and data analysis - is crucial to unfold significant impact in technological development. Combinatorial approaches, where the composition is systematically varied over the sample area, will tremendously accelerate the identification and optimization of new functional materials, e.g., for photovoltaic devices (↘#high throughput, ↘#automation). However, speeding up the overall process for device development also requires fast access modes, much more accelerated data analysis utilizing AI, and fast feedback loops to material synthesis. The latter will be achieved by a vital link between the X-ray beamlines and endstations with on-campus facilities for fabrication, processing, characterization, and performance testing of devices, including transfer under UHV conditions if required (see ↘Figure 6.10). This will also enable measurements of layered devices such as solar cells at intermediate steps of device fabrication.

Devices for energy production or storage must be stable over longer time scales, i.e., years to decades, to be economically feasible and environmentally sustainable. Thus, SR facilities must provide capabilities to investigate the long-term performance and possible degradation mechanisms. This will be achieved by accelerated aging tests and new access modes that allow the periodic analysis of samples at regular intervals using an automated cycling system.

Impact: **BESSY III** will combine dedicated measurement and sample environment capabilities with advanced beam properties to enable ↘#*operando* studies of processes in energy devices on a wide variety of length and time scales, embedded in associated facilities for synthesis and characterization. This will permit fast yet knowledge-based device structure optimization, e.g., by identifying essential loss mechanisms, scanning large parameter spaces for the optimal material composition, and evaluating degradation mechanisms. Thus, novel approaches for energy production or storage devices, including ideas that are yet to be proposed, can be efficiently probed for their potential to be developed into applications.

Catalytic Processes

Motivation: Catalysts are ubiquitous in many fields of economy, and it is estimated that they contribute directly or indirectly to approximately 35 % of the world's GDP [15]. Since they lower the energy required for an industrial process, ensure selectivity, and regenerate their original state after the reaction, they have enormous potential for saving both energy and material resources. Moreover, efficient catalysts are urgently required for the production of green hydrogen and its conversion into chemicals and synthetic fuels, and thereby constitute a fundamental component for achieving the global energy transformation (see also ↘Figure 4.2). The quest for finding novel catalysts, tailored towards high efficiency and selectivity, is therefore one of the key research questions of the coming decades. Specific research questions are: can we achieve a deeper understanding of reaction mechanisms and the key properties of a material that define its functionality? What is the nature of the active phase? How can results from the lab and an SR facility be translated into industrial applications? Importantly, the catalytically active states form only under reaction conditions, making ↘#*operando* experiments indispensable for answering such questions in catalysis research.

Approach: The application of soft X-ray ↘#*operando* spectroscopy will deliver essential insights into the catalytic active sites interacting with reactants and products moieties as well as their embedding scaffolds, interfaces or solution environments, due to the capability to probe to the electronic structure of (sub)surface states. Challenges are the generally complex structures of the active entities and the dynamic and metastable character of the active sites, requiring experimental access to a huge variety of scales, from nanometer and picoseconds relevant for processes at the active sites to millimeter and minutes/hours for processes involving catalyst particles (↘#high-res-spectro ↘#high-res-imag ↘#dynamics). ↘#*Operando* investigations using SR-based methods are well suited to address such challenges and have therefore led to many important findings in catalysis research in recent years [16], one example being the identification of the active site in ethylene epoxidation over silver catalysts at BESSY II [17].

To fully exploit the potential of SR-based experiments for catalysis research, dedicated instrumentation is required with respect to catalyst synthesis and sample environment using complementary facilities. Such instrumentation is currently being set-up at BESSY II and complementary laboratories on HZB's Adlershof campus WCRC as part of the CatLab project, operated jointly by MPG and HZB and aiming for innovations in catalyst design by using thin film technology. Thus,

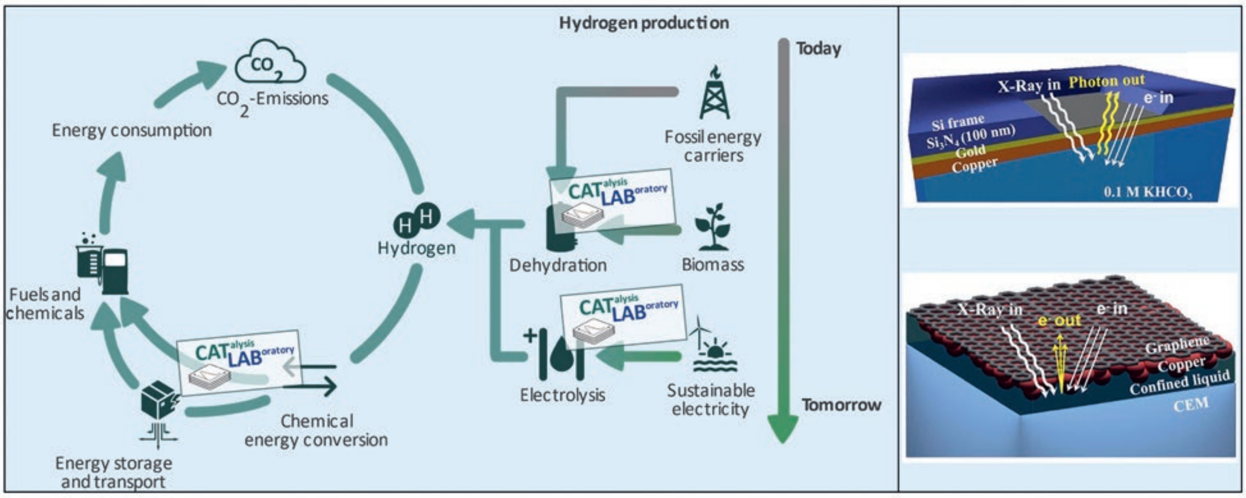


Figure 4.2: Relevance of catalysis in a CO_2 neutral energy system (left; illustration from the CatLab project); cells developed for ↘#multimodal and #*operando* catalysis research, designed to be used for soft X-ray photoemission (bottom right) and fluorescence spectroscopy (top right) [18].

BESSY III will be able to build on the experience gained over the coming decade to optimize experimental infrastructures for catalysis research. The investigation of electrocatalytic reactions, e.g., the hydrogenation of CO_2 [18], requires the development of dedicated electrochemical reaction cells (see also ↘Figure 4.2). Such cells have been used in a number of studies that elucidate reaction mechanisms of catalytic reactions [18–23].

The combination of various complementary techniques, i.e., a ↘#multimodal approach, is essential for a detailed atomistic understanding of the complex processes in catalysis. **BESSY III** will provide instruments which combine multiple techniques, e.g. ambient pressure X-ray and absorption spectroscopy to determine the electronic structure of the outermost surface (soft X-ray range) and the influence of the near surface region or the interface between active layer and the substrate (↘#tender X-ray range) combined with structure-determining methodologies like X-ray diffraction. Additionally, ↘#multimodal experiments using different instruments, including non-SR techniques such as TEM or SEM, will also be enabled by modular reaction cells that can be employed for both SR and offline measurements. The combination of X-ray spectroscopy and microscopy provides complementary information with respect to the electronic and geometric structure, respectively, which enables the elucidation of the reaction mechanism. X-ray diffraction and X-ray based microscopy techniques will strongly profit from the enhanced coherence of the X-ray radiation provided by **BESSY III.**

Studying the materials under reaction conditions is an indispensable prerequisite to obtain insights into the reaction mechanism. Therefore, novel ↘#*operando* reaction cells providing the required reaction conditions in terms of feed composition, temperature and pressure will be further developed. These reaction cells will enable the investigation of the active metastable surface states of the catalyst. Their correlation with the catalytic performance, measured simultaneously, will deliver insights into the heterogeneous catalytic reaction. All instruments will permit a sensitive determination of the functionality of the materials, by measuring the conversion of the educts and the selectivity of the products. Also the surrounding supporting laboratories and infrastructure will be well set up for these types of experiments, e.g., for high gas pressures, and a coupling to the synthesis tools is needed particularly in the case of thin film samples, where UHV transfer systems will prevent air exposure.

Impact: **BESSY III** will provide dedicated instrumentation to study the chemical states in particular of (sub-)

surface species which are involved in catalytic reactions, and thereby yield an atomistic understanding of the reactions mechanisms which is only accessible in ↘#*operando* investigations. This understanding will form the basis for developing and validating novel concepts and materials for a broad range of catalytic applications. Due to the immense importance of catalysis for various fields of economy, such research questions will remain highly relevant for decades to come. Collaborations with industrial partners at an early stage, as e.g. established in the CatLab project, will ensure a focus on the large-scale practicability of new concepts.

4.3.2 Quantum and Information Technologies

Motivation: The digital transformation, which affects nearly all areas of economic and everyday life, is an indispensable tool to tackle grand societal challenges such as the quest for a sustainable, carbon-neutral future. At the same time, the rapidly increasing electricity consumption of information and communication technology is in itself posing a challenge to the achievement of carbon neutrality, which implies an urgent need for disruptive energy-efficient concepts and the respective materials for computing and data storage. Can we find materials that enable spin-based, low-power electronics? Which material classes provide chances for breakthroughs in quantum and neuromorphic computing?

Approach: The key to answering these questions lies in the understanding of the electronic properties of candidate materials. Synchrotron-based spectroscopy therefore plays an important role in the investigation of the underlying quantum phenomena. For example, measurements at BESSY II first demonstrated 3D topological semimetals [24] as well as topological surface states hosted by a magnetic energy gap [25]. In the future, spatial resolution in the nanometer range will be an essential element of such investigations for two reasons: To investigate not only materials but (prototype) devices in operation, local access to the electronic properties is required to capture effects of electronic gating and voltage gradients over the device [26]. Furthermore, the relevant effects in quantum materials typically occur on very small length scales.

Promising candidates for electronics based on quantum materials are 2D materials and materials based on artificial heterostructures, since they may display high robustness (topological protection) and/or high sensitivity to external stimuli. Their properties can be tailored, e.g. by strain, magnetic order or ferroelectricity of the substrate or the various layers. Exploring the potential of such properties will rely on the measurement of electronic surface (or near-surface) states, where effects such as topological protection become manifest. Particularly interesting are 1D states which allow for lossless charge and spin transport. They appear near edges, e.g. between ferromagnetic domains, which are only experimentally accessible with spatial resolution in the low nanometer range. These effects can be measured by angle-resolved photoemission spectroscopy with nano-focus (nano-ARPES, ↘#high-res-spectro); an example is shown in ↘Figure 4.3. The measurement of their dispersion by scanning tunneling spectroscopy is not possible because they are inherently protected from backscattering, making angle-resolved photoemission the only investigation method, with nanometer spatial resolution as a prerequisite to be sensitive to edge states. While photoemission techniques are inherently surface-sensitive, penetration through a few layers is feasible at higher X-ray energies, even in an element-specific way.

Inherent spatial heterogeneity may also arise in systems that are chemically and stochiometrically homogeneous, if competing phases such as magnetic or charge order and superconductivity exist. This insight is a key contribution of soft X-ray research to the problem of high-Tc superconductivity in cuprate compounds and other systems with strong electronic correlations. Room temperature superconductivity at ambient pressure is considered one of the potential achievements with utmost technological impact. To measure excitations associated with the various ground states will require very high energy resolution: RIXS with 10^6 energy resolution at the Cu L-edge, combined with the spin sensitivity of polarized soft X-rays, will permit the study

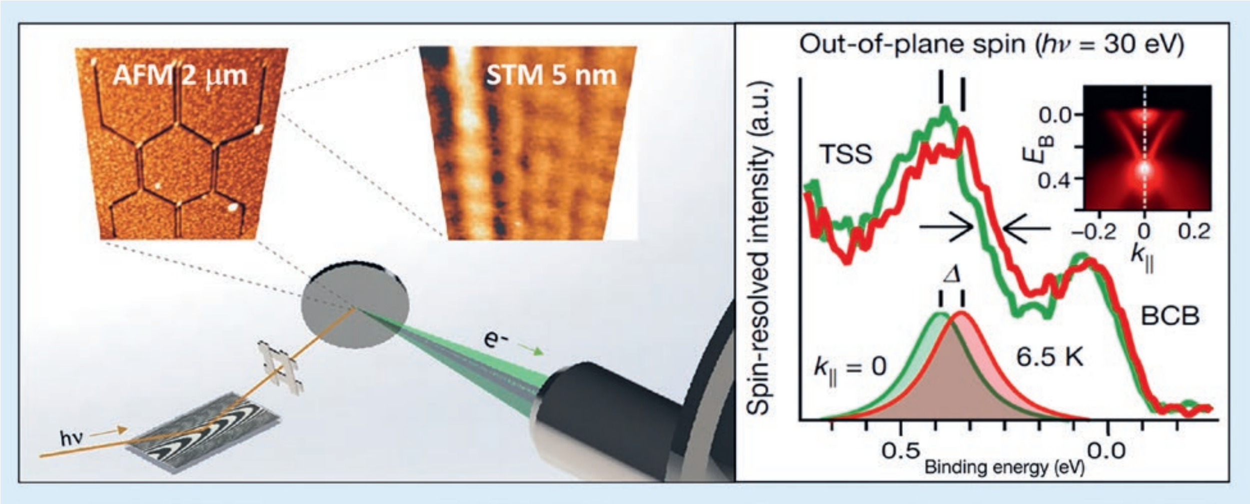


Figure 4.3: Nano-ARPES for quantum devices (**left**): This technique would permit to study, e.g., one-dimensional quantum spin Hall edge states, which cannot be investigated by ARPES so far. Such states appear in the layered topological insulator $Bi_{14}Rh_3I_9$ at positions where the sample has been scratched with a cantilever (see AFM and, as closeup, STM images, from [27]). **Right:** Topological surface states seen by spin resolved ARPES [25] in a layered spintronic candidate material. Spectra for different spin polarizations are shown in red and green, and the Dirac cone is displayed in the inset.

of meV-size spin gaps in such systems (↘#high-res-spectro). This will finally fulfill the long-standing dream to use soft X-ray RIXS as a complementary method to inelastic neutron scattering for the detection of spin excitations on relevant energy scales. Thus, interfaces and heterostructures with small sample volumes would become measurable for the first time.

Recently, the possibility to realize neuromorphic computing via nanometer-sized topological textures has come into the focus of quantum materials research. One possible concept is based on 2-dimensional skyrmions, the dynamics of which can be studied using X-ray imaging with nm spatial and ns to ps temporal resolution[28,29]. The challenge is in moving away from 2D towards 3D textures which would hugely increase the level of connectivity that can be realized, and thereby the achievable computational power of the neural network. An extensive wealth of topological textures is expected in 3D, one example being hopfions, whose study will require imaging capabilities of 3D inhomogeneous samples. To be able to manipulate such structures, their dynamic response to external stimuli such as electrical field pulses, spin injection and laser excitations needs to be investigated. In addition, topological structures based on ferroelectric rather than spin textures have been discovered, which are more compact and thus require imaging capabilities with a spatial resolution in the few nanometer range[30]. Such textures and their response to stimuli will become experimentally accessible at **BESSY III** using coherence-based imaging techniques which provide very high spatial (sub-3 nm in 2D, sub-10 nm in 3D) and high temporal (ps-ns) resolution (↘#high-res-imag, ↘#dynamics). Full polarization control and especially circular polarization are absolutely mandatory for all of these studies. The investigation of layered samples as well as prototype devices will require an efficient link of sample preparation and characterization to the synchrotron-based experiments.

Impact: By providing spectroscopic and imaging techniques with high spatial and spectral resolution as well as linear and circular polarization of soft-to-tender X-rays, **BESSY III** will identify promising candidate materials for novel computing applications based on quantum effects. The high brightness of the source will permit to develop such investigations towards ↘*#operando* studies of prototype devices, thereby taking a further step towards the technical implementation of the materials and associated phenomena.

4.3.3 Life Science

Motivation: Life science aims to unravel the complex processes that determine (human) physiology, starting at the molecular level and going up to the whole organism. Obtaining a sufficiently deep and detailed knowledge of these processes will enable a precise understanding of diseases and lead to finely tuned treatments that result in minimal side effects. For the example of a viral disease, we might ask: How does the virus enter a cell? Which molecules are involved, what are their three-dimensional structures and what is their role in the process? If we can answer these questions, we can aim at blocking this step with a drug that specifically targets these molecules, without affecting other cellular processes.

As the SARS-CoV-2 pandemic has demonstrated forcefully, humankind is constantly being exposed to new threats coming from the bacterial or viral world, where influenza and corona viruses are seen as one of the most likely causes for future pandemics. Climate change will furthermore expand the habitat of shuttle animals which are presently confined to (sub)tropical regions into Central Europe. Thus, research will need tools ready at hand that reveal the most important processes involved in the diseases and quickly identify active substances to block them. Beyond viral infections, many diseases such as cancer, heart disease and dementia remain poorly understood due to the complexity of human physiology. A key biomedical challenge for the future is to connect the underlying molecules responsible for these different diseases with the higher-level functions of the disrupted organism.

Approach: The investigation of the emergence of higher-order physiological functions will occupy biomedical researchers for many decades. It will require not only a catalog of the interacting components, but also knowledge of their spatial distribution within the cell or tissue, combined with integrative computational models of the process under study. This underlines a long-term need for a broad palette of different imaging techniques that are important for biomedical research [35,36]. They allow detection of different structures and molecules over a range of spatial scales and penetration depths. No single method provides all the information required to understand biological function, and so correlated #multimodal imaging will be critical for decades to come [35].

Synchrotron radiation will play an important role in enabling this multi-scale spatial analysis of biological function, since it provides unique imaging capabilities across a broad range of resolutions. For example, micro-computed tomography is used to examine organ

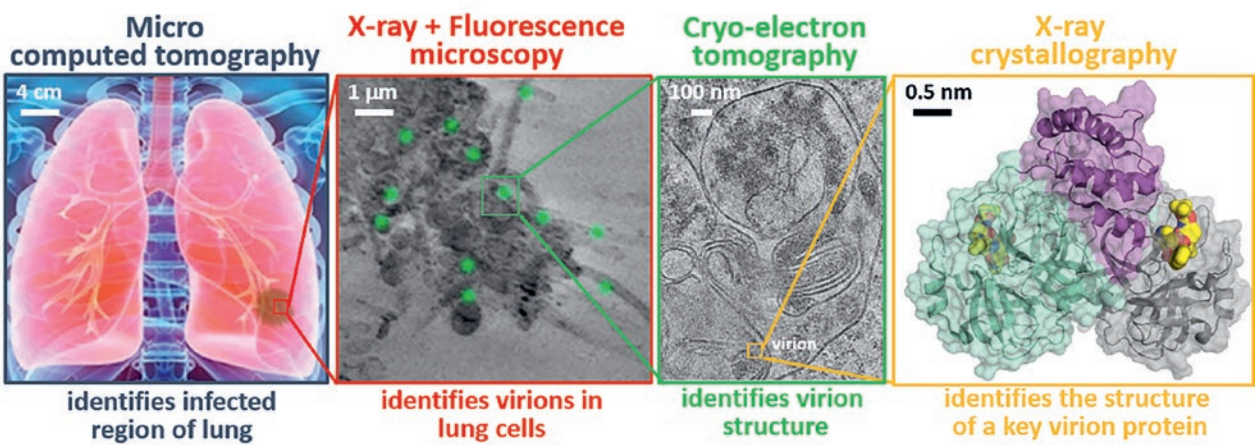


Figure 4.4: Hierarchical imaging pipeline for life science, illustrated by the study of a viral lung disease [31–34].

structure, X-ray microscopy with 10 nm spatial resolution to examine cellular ultrastructure (↘#high-res-imag) and high-resolution X-ray crystallography to examine the molecular structures of the individual components down to the atomic level. ↘Figure 4.4 provides an example how these capabilities can be combined and complemented by TEM, available at partner laboratories on campus, to form a hierarchical imaging pipeline that can be used for the study of viral diseases. This example can easily be generalized to other types of diseases, and similar experimental capabilities can be employed for the study of healthy tissue, e.g. of neural connections that give rise to brain functions such as memory.

Importantly, SR offers the ability to examine specimens in their native (or at least near-native) state, that is within cryo-preserved tissue samples not subjected to any form of chemical fixation, staining or dehydration. This is a key advantage, since such procedures, which are a prerequisite for most other imaging modalities, are well known to induce significant ultrastructural defects. Furthermore, the natural contrast afforded by soft X-ray radiation eliminates the need for any a priori knowledge about which structures of interest should be stained. An illustration is the identification of early stages of coronavirus entry: Here, transmission soft X-ray microscopy enabled detection of dark-rimmed vesicles which formed inside of late endosomes within minutes of coronavirus infection, thereby drawing attention to the late endosomes as a key organelle in viral uptake[32].

Macromolecular crystallography (MX) enables researchers to determine three-dimensional structures of biological macromolecules and their interaction partners to atomic resolution. With the advent of the computer program AlphaFold[37], the focus in MX is shifting from the determination of structures of individual macromolecules to the determination of complex structures. This can be either protein-protein complexes or protein-small molecule complexes, such as metabolites of potential drug candidates. Large-scale screening experiments such as the one pioneered at the HZB fragment screening facility will play an ever more important role[38]. A further increase of sample throughput to about one sample per minute (↘#high throughput) will allow screening of large chemical libraries within short time periods, e.g., up to 5000 compounds within a few days (a factor of 50 – 100 more than at BESSY II). Combined with automated analysis of the huge experimental data content (↘#automation) such experiments will significantly reduce the time it takes from an initial binding hit to the development of a first inhibitor, which may then be further analyzed for its pharmacological properties.

While recent developments in cryo electron microscopy have essentially taken up most of the structural work on large macromolecular assemblies and complexes, high resolution experimental structures of individual components will still only be available via MX. In particular, it will be necessary to investigate samples which can only be produced in very small amounts and which can only be crystallized into very small crystals. Being able to routinely obtain diffraction data from crystals with an edge length of 5 µm or less will enlarge the space of viable samples for MX and contribute to a more complete catalogue of protein structures to be determined. Such experiments will be performed in a large variety of sample environments.

Furthermore, while all of the current structural methods provide more or less static pictures of the molecules studied, evolution of biological processes matter. Adding relevant time resolution to macromolecular structures means being able to observe the molecular ↘#dynamics in order to create molecular movies, e.g. of certain enzymatic reactions. This will undoubtedly deepen the understanding in enzymology and be of high biotechnological relevance. These approaches, pioneered at XFEL sources, rely on individual diffraction patterns from very small crystals and require very high intensity beams.

Impact: At **BESSY III,** high-resolution X-ray imaging and high-throughput macromolecular crystallography will constitute essential elements of a versatile toolbox for life science and thereby also strengthen the highly active local life science community (e.g. MDC, Charité, Berlin University Alliance). Using this toolbox will deepen our understanding of biological processes, in particular also molecular processes involved in diseases, such that faster and more targeted drug search becomes feasible. Based on a thorough general understanding of such processes and the establishment of substance libraries, this will also enable not only a very quick response to the emergence of new pathogens but also development of drug therapies to treat major diseases such as cancer and dementia.

4.4 Metrology for Innovation

Motivation: Metrological measurements using SR offer unique characterization tools in the X-ray range, yielding ↘#quantitative data with known uncertainty [39]. Such accurate data sets form an indispensable basis for many industrial applications and have been gaining relevance in research since they enable a deeper materials understanding and leverage ↘#multimodal approaches. The Physikalisch-Technische Bundesanstalt (PTB) has established, over the course of several decades, a global leadership position for metrology with SR, offering experimental capabilities specifically tailored to the increasing demands of industry, academia and non-academic research institutions. Primary source standards for this endeavor are currently the BESSY II storage ring (EUV to X-ray range), where PTB operates eight beamlines, and the Metrology Light Source (MLS, THz to EUV regime). Both sources are operated by HZB in a long-standing and highly fruitful collaboration which shall be continued for the successor sources of both facilities.

Approach: The first pillar of PTB's current and future activities with SR is radiometry, i.e. metrology of electromagnetic radiation[39]. This requires the accurate measurement of the storage ring parameters such as the electron energy, polarization, the electron current and the bending magnetic field, and thus needs to be an elemental part of the planning for the new source. Besides source-based radiometry, detector-based radiometry with cryogenic electrical-substitution radiometers as primary detector standards has also been established by PTB[39], allowing the output signal of any kind of photodetection system to be accurately calibrated. Radiometry forms the basis for calibration services and scientific co-operations with external partners. Examples refer to the characterization of space instruments for solar and atmospheric research or to photon diagnostics of free electron lasers.

Based on its capabilities in radiometry, PTB offers, secondly, various measurements for industry at the MLS and its BESSY II beamlines. Industrial projects are related to the development and characterization of X-ray detectors, e.g. with DECTRIS AG, or optics for X-ray astronomy, in particular with the company cosine and the European Space Agency ESA, up to measurement techniques for EUV-lithography. After 20 years of development, optical lithography in the extreme-UV (EUV) at the wavelength of 13.5 nm today forms the technological basis worldwide for the production of the most sensitive areas of high-performance components in the semiconductor industry. PTB accompanies this development, which was awarded the German Future Prize for Technology and Innovation in 2020, with more than 6000 beamtime hours and a funding volume of currently more than 1.5 million Euro per year. While at the MLS the at-wavelength metrology of optical components is in the foreground, the work at BESSY II mainly relates to the development of new metrological methods for the characterization of semiconductor nanostructures in the EUV and soft X-ray range (see ↘Figure 4.5). When working with industrial customers and collaborators, state-of-the-art measurement capabilities are indispensable premises. Therefore, to maintain PTB's leading position in metrology for industry in the coming decades, upgrades of both SR sources used are crucially required.

Materials metrology, the third pillar of PTB's activities at MLS and BESSY II, refers to the metrological characterization of materials and is becoming increasingly important, not only for applications in optics or semiconductor electronics but also for quantum technology, photovoltaics, energy storage, catalysis, or biotechnology. Methods used at MLS are IR spectrometry (SNOM) and photoemission tomography and at BESSY II and prospectively at **BESSY III** XRR, (GI)SAXS,

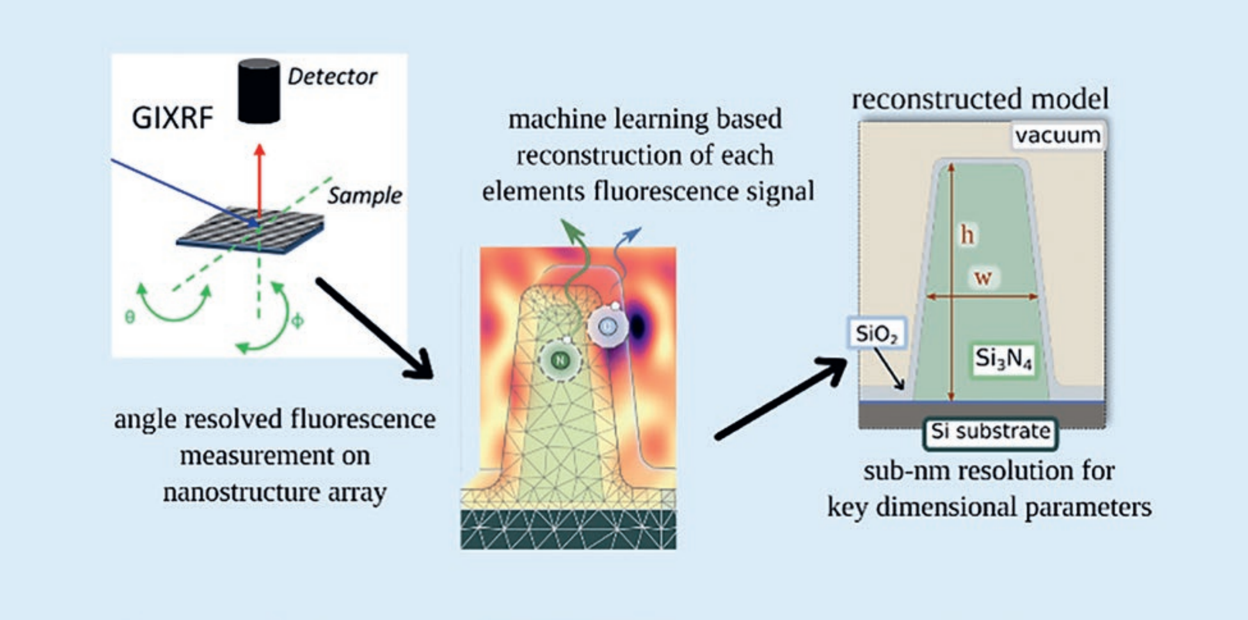


Figure 4.5: Materials metrology for periodic nanostructures: The high-precision reconstruction of a Si_3N_4 grating structure, including uncertainty analysis, is derived from GI XRF data from BESSY II and machine learning [40]. Better beam properties (photon flux, brightness, coherence) would permit detailed investigations of more complex structures.

and reference-free XRF. Apart from PTB, also the Bundesanstalt für Materialforschung und -prüfung (BAM) is strongly involved in materials metrology with its own beamline at BESSY II, which offers X-ray fluorescence analysis, micro computed tomography (Micro CT), X-ray topography, detector calibration as well as reflectometry, and is closely linked to industrial services. Driven by the structural complexity of modern materials, PTB and BAM advance their methodology towards the characterization of materials at the nanoscale and increasingly investigate materials under realistic conditions, i.e., ↘#*operando*, *in-situ* or even in-synthesis. Therefore, the applied methodologies will greatly profit from the availability of smaller focal sizes as well as higher brightness and coherence of a 4th generation light source (↘#high-res-spectro ↘#high-res-imag).

Materials metrology relies not only on ↘#quantitative data from analytical measurements, but also on a thorough quality management for sample synthesis and characterization including careful metadata acquisition. Establishing the necessary complementary techniques and an overarching FAIR data management system will have high priority for PTB, BAM and the general user community at **BESSY III**. Such data sets are ideally suited for the comparison with modelling approaches, which also form a key component of the materials metrology strategy. An example of nanometrology, combining SR data with machine learning algorithms, is shown in ↘Figure 4.5, the specific example being of high relevance for the development of the next generation of integrated electronic circuits.

Impact: Using **BESSY III** as primary source standard, PTB will be able to expand its global leadership position in metrology with SR radiation. The availability of these experimental capabilities is urgently needed in many fields of high relevance for the future economy of Europe, including semiconductor industry and sustainable energy technologies. Making use of the advanced source properties, ↘#quantitative measurements offered to industry, academia, and non-academic research institutions will be extended towards investigating complex structures on the nano scale as well as materials and devices under real operating conditions. Accurate experiments, offered by PTB, BAM and also HZB, will unleash the full potential of ↘#multimodal approaches at **BESSY III.**

5. The BESSY III Approach

Goal: As stated in ↘Chapter 2, **BESSY III** strives to achieve uniqueness through the triad of combining (i) a 4th generation light source, (ii) in an integrated research campus with (iii) capabilities for metrology and quantitative measurements. The first part of the triad is a world leading 4th generation soft-to-tender variable polarization X-ray source of highest photon beam quality that covers the requirements of the focus fields: Energy, Quantum and Information Technologies, Life Science and – as overarching principle – Metrology. The choice of the target spectral range and polarization result from the importance of electron and spin structure for the scientific focus fields and provides complementarity to the other large-scale research facilities in Europe (LEAPS) and of the Helmholtz Photon Science Roadmap[2], PETRA IV – focus on structure and crystallography – and DALI – focus on low energy electrodynamics with THz rays.

Approach: The main requirement for the accelerator and undulator design is to increase spectral brightness and coherence in the soft X-ray region to support ↘#high-res-spectro, ↘#high-res-imaging, ↘#dynamics and to improve the performance in the ↘#tender range compared to BESSY II, where HZB, PTB, BAM, and collaborative research groups are currently operating 47 beamlines (38 of them fully parallel). To extend the beamline offer into the tender regime, an increase of the ring energy compared to BESSY II is indicated. Although higher ring energy would be better for coherence and brightness, the investigation of electronic structures requires methods like angle-resolved photoemission (ARPES) in the VUV range and XAS on e.g. Li, B, C, N, O in the soft X-ray range, which are indispensable elements for all focus fields as is the EUV range for the PTB. Hence, as revealed by the ↘Figures 5.1 and 5.2, the core energy range of **BESSY III** must be around 1 keV reflecting an increased demand for experiments

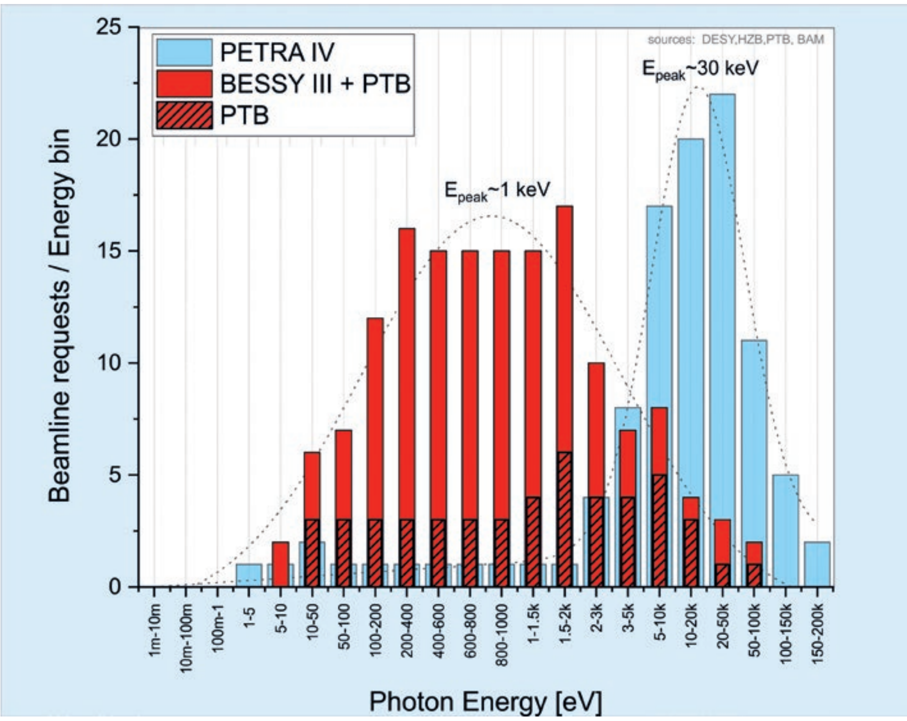


Figure 5.1: Histograms of experimental branches for **BESSY III** as derived from the science case and a survey among users (red bars) including the requests from PTB/BAM (shaded). Same numbers at PETRA IV (as of 3/2022, courtesy K. Bagschik (DESY)) reveals the complementarity of the two leading light source upgrades in Germany.

in the ↘#tender range compared to BESSY II. Comprehensive design studies for the accelerator system (↘see Section 6.1.1) suggest an energy of 2.5 GeV for the **BESSY III** storage ring to take account of the conflicting requirements. We have developed a tentative scenario on the basis of expert workshops and internal surveys which also includes the requirements of PTB and BAM as well as a certain number of open ports reflecting the need for curiosity driven research and industry needs with movable user endstations.

For this purpose, requested beamlines with their energy ranges were sorted into energy bins and compared with the PETRA IV beamline portfolio treated in the same way, and ↘Figure 5.1 shows the clear complementarity of the PETRA IV and the tentative **BESSY III** beamline portfolio. Indispensable applications at photon energies down to the VUV range but also access to hard X-rays as required by our partners PTB and BAM will be provided by special insertion devices. Bending magnets (SR-dipoles) will be designed as primary radiation standard for ↘#quantitative purposes of the PTB but e.g. also as broad band sources for ↘#multimodal approaches for catalysis [41]. In the core photon energy range around 1 keV, **BESSY III** will provide highest brightness and coherence like other modern 4th generation SR facilities worldwide (see ↘Chapter 6) based on multibend achromat (MBA) technology as proposed in ↘Section 6.1.1. Using this design, 2–3 orders of magnitude (depending on energy) gain in coherence and brightness from the source for the majority of applications is predicted. Together with innovative optics and detectors this will lead to up to even 4–5 orders of magnitude more X-ray photons on the sample compared to BESSY II. To realize the demanded *in-situ* and ↘#*operando* approaches, new concepts of endstations, detectors (↘Section 6.2.1) and sample environment (↘Section 6.2.2) are being developed. Because the overarching need for ↘#multimodal approaches is based on the combination of SR methods and complementary lab experiments, the embedment of **BESSY III** into a laboratory environment within an integrated research campus is mandatory. Digitization as an inseparable component of **BESSY III** will cover the whole scientific workflow, smart and fast data acquisition, automated and remote operation as well as AI guided autonomous research as described in ↘Section 6.3.

Impact: **BESSY III** will enable scientific breakthroughs in the aforementioned focus fields, in materials science and beyond. Thereby **BESSY III** will continue the success story of science with photons in Berlin-Adlershof over future decades and meet the demands of the user community for soft-to-tender X-rays clearly complementing the ranges offered by PETRA IV (see ↘Figure 5.1), DALI and EUXFEL on the Helmholtz Photon Science Roadmap [2]. Added value, especially for the German industry, comes from activities of the PTB at **BESSY III** and the planned upgrade of the MLS. Their ↘#quantitative methods will establish materials metrology for ground-breaking new technologies.

#	Name	Photon Energy	Main Methods	Main Applications
1	VUV to Hard	5 eV – 20 keV	XPS, HAXPES, NEXAFS, STXM XPS, HAXPES, NEXAFS, STXM	Catalysis, Energy (Storage, Batteries, Solar Fuels)
	DIP	20 eV – 1.5 keV	UPS/XPS, NEXAFS, EXAFS, XPS, UPS, ARPES	Energy, Catalysis
2	Soft & Tender	100 eV – 4 keV	PES, HAXPES, TXM, XAS, XPCS Resonant Scattering, CDI	Energy (Batteries), Quantum Energy, Quantum
	DIP	2– 14 keV	Diffraction/ EXAFS/XRF, NEXAFS	Energy, Quantum, Catalysis
3	XUV to Soft	60 eV – 1.5 keV	BElChem, XPS BElChem, XPS	Catalysis, Chemistry Catalysis, Chemistry
	DIP	2 – 14 keV	XRD/ EXAFS, WAXS, SAXS, HAXPES	Quantum, Energy Quantum, Energy
4	Magnetic Imaging	150 eV – 2 keV	Lensless Imaging, X-ray holography, XPCS STXM, Resonant Scattering, 3D mag. tomogr.	Quantum, Energy
	DIP	100 eV – 1.5 keV	XMCD, XAS with magnetic vector fields	Quantum, Energy, Catalysis Quantum, Energy, Catalysis
5	XUV Spectroscopy	5 – 200 eV	ARPES nano-ARPES	Quantum, Energy, Catalysis Quantum, Energy, Catalysis
	DIP	80 eV – 4 keV	NEXAFS, XPS	Catalysis, Energy, Quantum
6	Soft & Tender Imaging	180 eV – 8 keV	TXM, FIB-TXM Tender TXM, Tomography	Life Sciences, Energy Life Sciences, Energy
	DIP	20 eV – 1.5 keV	Soft X-ray Dynamics	Catalysis, Energy, Quantum
7	Inelastic Scattering	180 eV – 3 keV	RIXS meV@1keV RIXS	Quantum, Energy, Catalysis Quantum, Energy, Catalysis
	DIP	20 eV – 1.5 keV	Soft X-ray Dynamics	open port
8	Spectro Microscopy	100 eV – 1.8 keV	(S)PEEM, PEEM, Ptychography nano-ARPES	Quantum, Energy, Catalysis Quantum, Energy, Catalysis
	DIP	100 eV – 4 keV	Broad band soft + tender X-ray spectroscopy	open port
9	Macromol. Crystallography	5 – 20 keV	X-ray Diffraction X-ray Diffraction	Life Sciences Life Sciences
	DIP	80 eV – 2 keV	Soft X-ray spectroscopy	open port
10	Multimodal Spectroscopy	20 eV – 8 keV	Multimodal Spectroscopy Time-resolved spectroscopy	open port open port
	DIP	20 eV – 3 keV	Declined beamline, Multimodal spectroscopy	Catalysis
11	PTB: PGM/EUV	60 eV – 1.85 keV	Reflectometry / Scatterometry Reflectometry / Scatterometry	Metrology for Industry Metrology for Industry
	DIP PTB: FCM	1.7 keV – 11 keV	X-ray radiometry / X-ray reflectometry	Metrology
12	PTB: PGM/RFA	80 eV – 2 keV	X-ray spectometry X-ray spectometry	Materials Metrology Materials Metrology
	DIP PTB: white light	40 eV – 20 keV	Primary source standard **BESSY III**	Metrology
13	PTB: Tender X-ray	1 keV – 10 keV	µ-XRF / (GI)SAXS / Ptychography µ-XRF / (GI)SAXS / Ptychography	Materials Metrology, Energy Materials Metrology, Energy
	DIP PTB: XPBF/ESA	1 keV – 3 keV	X-ray optics for astrophysics	in-line Metrology for Manufacturing
14	BAMline	5 keV – 120 keV	Diffraction, XRF, µCT Diffraction, XRF, µC	Materials Metrology Materials Metrology

Figure 5.2: A tentative but yet incomplete beamline and method portfolio for **BESSY III** reflecting the scientific focus fields (Section 4.3) which are mainly based on methods from the soft-to-tender X-ray range. Successors of BElChem (XUV to Soft) and EMIL (VUV to Hard) are expressly aspired. The beamline requests from the PTB and BAM are shaded in light blue. Acronyms of methods see Glossary, (DIP) – dipole beamlines.

6. Technical Realization and Readiness

To realize **BESSY III** as the world leading facility for materials discovery, we aim to fulfill the triad of

- a state-of-the-art 4th generation synchrotron radiation source,
- an integrated facility approach embedded in the materials research campus at Berlin-Adlershof, and
- quantitative and metrological materials science capabilities, which are leveraged by the world-leading expertise of Physikalisch-Technische Bundesanstalt (PTB).

A thorough analysis of the possibilities of an in-tunnel upgrade of BESSY II to a 4th generation SR source has shown, that neither the required beam parameters in terms of energy and electron beam emittance, nor the capacity request in terms of number of available straight sections for the integration of insertion devices, can be fulfilled. In addition, as the radiation shielding of BESSY II is a monolithic concrete block being integral part of the BESSY II slab, any necessary modification of the radiation shielding to gain flexibility in the machine design would result in unacceptable long shutdown times without any usable photons of minimum 3 years. This is especially unacceptable in view of PTB's obligations with regard to its legal mandate of providing metrology applications to support industry.

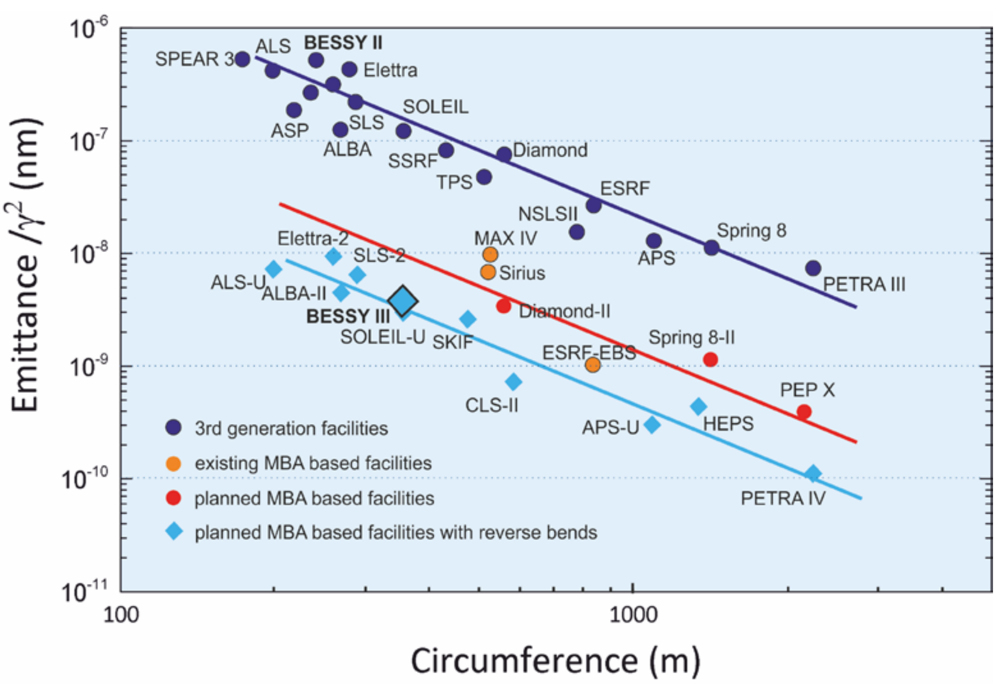


Figure 6.1: Emittance landscape of existing light sources and upgrade plans worldwide. Dark blue: 3rd generation sources in operation; Orange: existing 4th generation facilities; Red: upgrade proposals based on MBA technology. Light blue: upgrades based on latest MBA designs; big diamond: **BESSY III.** (adapted from R. Bartolini, 2022).

This new light source must support the scientific focus fields described in ↘Chapter 4 and must be within the parameter ballpark of worldwide discussed upgrades of SR-facilities depicted in ↘Figure 6.1. Such a globally competitive soft-to-tender X-ray large-scale facility can only be realized as a green-field facility complementing the surrounding WCRC campus environment of the HZB in Berlin-Adlershof.

The required new quality of such a flagship project can only be achieved if three technical areas are optimized to state-of-the-art technologies: photon beam generation, experimental instrumentation and infrastructure as well as digital tools for data management and automation.

Generating photon beams of unprecedented quality

The scientific motivations presented in ↘Chapter 4, but especially ↘#high-res-spectro, ↘#high-res-imag and ↘#dynamics ask for unprecedented photon beam qualities, which can only be provided by a 4th generation light source tailored for the soft-to-tender X-ray range. Further design criteria are (i) diffraction limited radiation at a photon energy of 1 keV and (ii) highest spectral brightness at 1 keV on the first harmonic of the undulators because this matches the photon beam emittance to the low electron beam emittance and promises highest polarization degree for elliptical insertion devices.

When it comes to the accelerator parameters, our approach is based on a contemporary MBA design and innovative magnet technology that lays the foundation for **BESSY III** to approach or even exceed the parameter ballpark of current and future upgrades worldwide (↘see Figure 6.1) keeping our light source competitive for the next decades and further scientific challenges to come. Details of the lattice design development and its technical subsystems as well as intriguing new accelerator physics concepts will be discussed in detail ↘in Section 6.1.1.

Based on the very low emittance of the electron beam, we will generate the photon beam with innovative

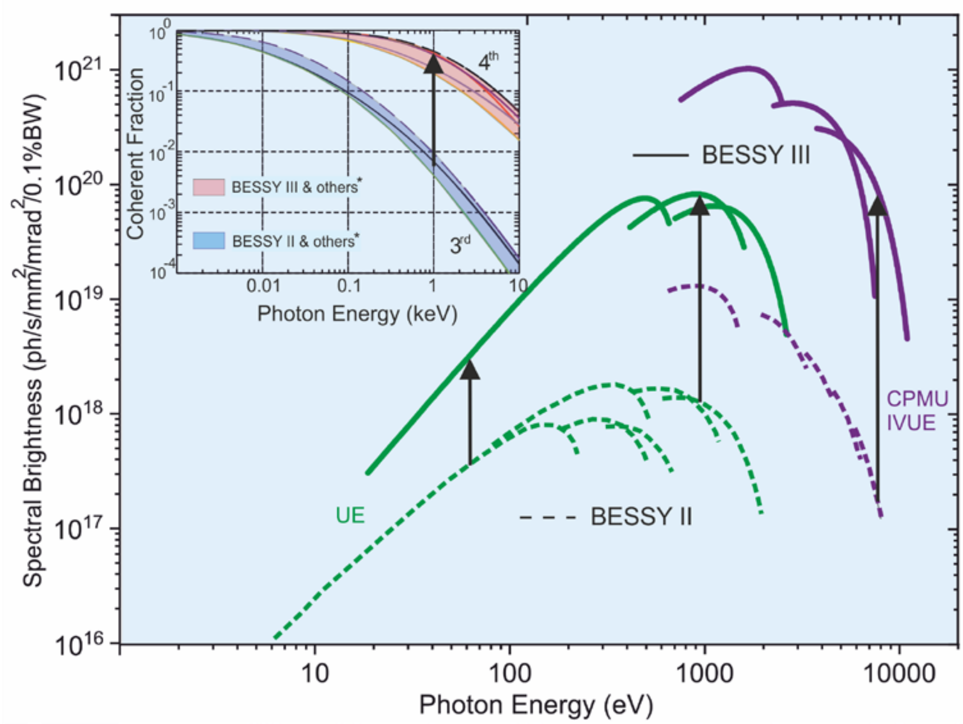


Figure 6.2: Target energy ranges, spectral brightness and coherent flux properties of a future **BESSY III** SR source as a flagship project in Berlin-Adlershof. Black arrows indicate a predicted gain in spectral brightness of one (in the VUV), two (soft X-ray range) and three (tender X-ray range) orders of magnitude. UE – elliptical undulators, CPMU, IVUE – invacuum undulators, ↘see Section 6.1.2. Inset: The arrow marks a two orders gain in coherent flux expected at the (diffraction limited) design energy of 1 keV. *Coherence curves from BESSY II / **BESSY III** and other medium energy upgrade projects (MAX IV, ALS, SOLEIL etc.).

undulator concepts described in ↘Section 6.1.2, like double period devices (DOPU) as well as in-vacuum undulators CPMU, IVUE that fully cover the energy range demanded in ↘Figure 5.1 at highest possible spectral brightness and coherent flux, see ↘Figure 6.2. However, in all focus fields the requirement for variable linear and circular polarization is mandatory, so that the majority of IDs must be elliptic. Arrows in ↘Figure 6.2 connecting spectra from elliptical undulators of BESSY II and **BESSY III** indicate here up to 2 orders of magnitude gain in transverse coherence at 1 keV and up to 3 orders spectral brightness enhancement in the ↘#tender X-ray range. This regime has been widely uncharted territory so far at BESSY II e.g. for 4d (L-edges) and 5d (M-edges, e.g. Hf) element spectroscopy for quantum devices (↘see Section 4.3.2) as well as Sulfur K-edge spectroscopy to understand batteries in ↘#*operando* as shown ↘in Figure 4.1.

Only a proper transport and final shaping of the photon beams by tailored soft-to-tender beamlines based on innovative monochromators and optic concepts, that preserve the polarisation state, enables users to benefit from a next generation electron storage ring. Our approach to achieve that, supported by full ↘#automation of controls, diagnostics, AI and modern data management, is described in ↘Section 6.1.3 by a selected example (↘#high-res-spectro). A glimpse into state-of-the-art X-ray optics for even further orders of magnitude higher transmission in the ↘#tender regime is also shown there. State-of-the-art beamlines tailored for such high performance will lift particularly high end imaging with coherent beams (↘#high-res-imag) to a new level but will also boost, by more photons, ↘#*operando* techniques as well as ↘#high throughput materials discovery.

Experimental instrumentation and infrastructure

Experiments at a future large-scale research facility such as **BESSY III** will differ significantly from today's status. Even in the early years of BESSY II (1999) user groups arrived with trucks loaded with endstations which were prepared at the home institute and then used for 1–2 weeks at a beamline. Ever since the situation has completely changed and will continue to change even more dramatic in the next decades. The reason is the enhanced complexity of the experimental questions, the setups and its technical challenges as well as the generally required much higher data acquisition speed. This has significant impact on the instrumentation itself, which e.g. for nano-foci, includes highly stable components controllable in UHV at the nanoscale (e.g. diffractive, refractive or capillary focusing) together with active feedback systems to stabilize the X-ray (or laser beams – ↘#dynamics) and automated sample positioning on the nanoscale (↘#automation). In sum, all this requires highly specialized fixed endstations and high-end detectors, a tailored but versatile sample environment and also surrounding – beamline-near – as well as complementary laboratories for the preparation or the execution of ↘#multimodal studies (↘see Section 6.2). All this will lift both, the design of the experimental infrastructure and the seismic, acoustic and thermal stability requirements to a new technical level compared to third generation sources. Such challenging issues beyond the machine will be best addressed in the context of the construction of an integrated research campus embedded in the ever growing high-tech environment of the science campus Berlin-Adlershof (WISTA) as discussed ↘in Section 6.2.

Data and Automation

The digitization pillar of **BESSY III** endorses three aspects of experimentation

(1) Automated and remote: covers IT environment for basic device control, data acquisition and handling, scientific computing. High standards of availability, reliability, ease of use, fundamental to these operation modes are mandatory for all components to be integrated or adapted. Experimenting remotely will hardly mean any disadvantage.

(2) **Smart and autonomous:** manual, simple raster scans are no more adequate to vast parameter spaces, faint signals or rare events. Intelligent data acquisition will utilize various knowledge sources to detect regions of interest rapidly and safely. Robust data analysis and -evaluation will justify trust in complex automated sequences and decisions no more supervised by humans.

(3) **Data quality and quantity:** Sample complexity and tiny structures push predictions of simulations and machine learning beyond validity limits. For decisive hypotheses verification the 4th generation light source beam is required. Detailed, precise and ↘#quantitative quality data have to be acquired to provide the urgently needed unambiguous ground truth, in large and dense FAIR databases.

For implications of (1)–(3) on data management and automation ↘see Section 6.3. On the general level of digital HZB, material research at **BESSY III** can leverage the achievements of the ubiquitous digital transformation process of the society. For material design and characterization, relevant data pools are already well orchestrated[42–44], available to research institutes and industry. To analysis and planning they add data-driven models and guidance by physical understanding. For **BESSY III** it is relevant, that HZB is well embedded into this rapidly growing global digital infrastructure, see ↘Figure 6.9 (overarching red text). Distinction of the domain specific IT infrastructure, as described ↘in Section 6.3, from the hosting general IT helps to define project scope and phases.

6.1 Generating Photon Beams of Unprecedented Quality

6.1.1 Accelerator Systems

Goal: The primary objective for the accelerator systems is in first order to develop a concept of an electron storage ring and its radiation sources, i.e., bending magnets and insertion devices, which will deliver the SR parameters requested by the scientific motivation, summarized in ↘Chapter 4 and 5. Absolutely mandatory is the request to provide highest brightness at 1 keV photon energy with diffraction limited radiation and free choice of polarization state (see ↘Figure 5.1 ↘#high-res-spectro, ↘#high-res-imag, ↘#tender) and to keep the requested beamline capacity, listed in detail in the beamline portfolio (see ↘Figure 5.2). An overarching goal, but also limiting boundary condition for our greenfield concept, is to keep the footprint, i.e. the circumference, of the accelerator systems reasonable small in order to make it fit on the only accessible and suitable free site in Berlin-Adlershof to stay embedded in Germany's most successful Science and Technology Park Adlershof. Secondary goal of the storage ring design is to keep to some extent BESSY's flexibility, based often on non-linear beam dynamics, and combine it with the more restrictive MBA structure, to allow for proof-of-principle experiments and/or advanced operation modes to support ↘#dynamics studies as it is done at BESSY II and MLS. Different from other SR facility upgrades is the essential aim to provide radiation sources usable as a primary radiation standard for ↘#quantitative metrology purposes, satisfying the needs of the PTB. In times of climate change and primary energy shortage due to geopolitical tensions, it goes without saying, that sustainability and an energy efficient layout are overall objectives for the design of the accelerator systems.

Expertise: HZB's expertise for design, construction and reliable and efficient operation of large-scale research facilities is successfully proven by BESSY I, BESSY II and the MLS. Moreover, the eagerness of improving the running facility as a whole, but also individual hardware components as well as exploring the facility's beam physics limits set the base for quite a few pioneering developments within the field of storage ring based SR-sources. This lays the foundation, not only for HZB's worldwide reputation, but also for the concept of **BESSY III.**

For example, HZB developed in the 2000ies in an EU wide collaboration the 500 MHz EU-HOM-damped cavity[45], now commercial available from from RI Research Instruments (RI) under license from HZB, which is used by many 3rd generation light sources and also foreseen at many MBA upgrades. Within SEAlab & Supralab, see ↘Figure 6.11, the fruitful collaboration, especially with RI, continues also on superconducting RF systems.

The introduction of top-up injection, not initially planned for BESSY II, lead to the development of a very robust radiation protection concept [46] and highest injection efficiencies of 95 % and above [47]. First experimental studies of a non-linear kicker injection [48] pushed the idea of transparent off-axis injection, which was realized at MAX IV and SIRIUS and will become an often chosen injection concept at 4th generation light sources.

Operation and development of BESSY II and MLS always supported integration of timing capabilities [49] by exploring non-linear operation regimes as low-α or TRIBs operation. Short pulses have been made accessible by femtoslicing [50] down to 100 fs (FWHM) photon pulse length or low-α operation with 1 ps to 15 ps electron bunch length [rms], pioneered at BESSY II [51]. The MLS [52], developed by HZB, is the first electron storage ring optimized for low-α operation and its flexibility allowed, just recently, a first proof of principal experiment of steady-state micro-bunching (SSMB) [53]. The VSR concept [54, 55] aims for simultaneous generation of short and long electron bunches by introducing a beating scheme with higher harmonic RF systems, which are currently under development in two hardware projects, one as normal conducting cavity system [56] and the other as high-gradient cw superconducting one [57].

For timing experiments, the pulse repetition rate is a crucial parameter. At BESSY II different separation schemes have been developed to provide different repetition rates, e.g., a fast rotating photon beam chopper [58] or the pulse picking resonant excitation scheme [59]. The latest and most promising development is the TRIBs operation, which generates a second stable orbit for storing an additional, flexible and adjustable, fill pattern [6,60,61]. Pioneering proof-of-principle experiments have shown that TRIBs allow for completely new experimental capabilities, as MHz helicity flipping of X-rays from an undulator [7], opening new possibilities for XMCD experiments. A first successful proof-of-principle test [61,62] at the 330 pmrad 7-MBA 3 GeV MAX IV ring motivates to investigate TRIBs as an operation mode for **BESSY III** [63].

Approach: The main target parameters for the **BESSY III** storage ring are listed in ↘Table 6.1 and compared to BESSY II.

In order to fulfill the request for highest brightness at 1 keV, delivered by the 1st undulator harmonics, and a broader span of photon energies into the tender X-ray region, the beam energy must rise from 1.7 GeV to 2.5 GeV (see ↘Figure 6.2). This increase in energy is also beneficial for our strategic partners BAM and PTB which requires access to hard X-ray beams. In addition, the emittance must decrease from 5 nm rad to 100 pm rad to provide diffraction limited radiation up to 1 keV photon energy, which can only be fulfilled with a state-of-the-art MBA magnetic lattice. Due to the available space on the envisaged site, only 350 m of circumference, i.e. 22 m length for one section, is available, which makes the design a challenging task. Due to the capacity request for IDs, see beamline-portfolio in ↘Figure 5.2, a 16-fold periodicity is needed and in addition each sec-

Parameter	BESSY III	BESSY II
Energy	2.5 GeV	1.7 GeV
Emittance	100 pm rad	5 nm rad
Circumference	~ 350 m	240 m
# of straights	16 with 5.6 m	16 with 5.0 m
Stored current	300 mA (500 mA)	300 mA

*Table 6.1: Main objectives of **BESSY III** and main parameters of BESSY II.*

tion should provide at least one additional bending magnet source up to 20 keV. Two of the 16 straights will be used for injection and the RF system, so that 14 are left for insertion devices. A straight length of 5.6 m is defined to enable installation of long undulators to push the flux and the brightness at dedicated beamlines and for double undulators and double canted undulators, as implemented with the EMIL setup at BESSY II, to provide multiple source points for ↘#multimodal studies. A stored average current of 300 mA is the baseline design, but within detailing on radiation safety, impedance budget, vacuum system and RF system dimensions an increase to 500 mA could be envisaged.

First attempts in lattice design, like a 16-period 9MBA based on the ALS-U design or a 18-period 5MBA resulted in very ambitious magnetic specifications, which have triggered a discussion about the hardware limits and technical realization. Within the conceptual design phase CDR, the decision has been made to follow a more conservative ansatz for the whole accelerator complex and rely on already existing or reliable to scale accelerator technology and concepts. It will be upon the subsequent CDR/TDR phase to assess the technical risks and redefine the technical ambitions, which could enable lattice improvements.

For **BESSY III**, the fundamental RF system will be realized with up to six 500 MHz EU-HOM-damped cavities, providing 2 MV to 3 MV total voltage compensating the energy loss per turn of about 0.350 MeV in bends, giving an energy spread of 0.9 x 10^{-3}. It will provide sufficient overhead for energy acceptance, redundancy for reliable operation and for the additional ID losses, expected to be up to a factor two higher than with the bare lattice. Defined by the fundamental RF system and the momentum compaction factor α of the lattice, which was chosen not to be less than 1.0 x 10^{-4} for stability reasons, the zero current bunch length is expected to be around 10 ps (rms). Using a normal conducting active HHC system at 1.5 GHz, currently under development by a collaboration of ALBA, DESY and HZB [56], it is foreseen to lengthen the bunches by a factor of 3–5 to increase Touschek lifetime and to mitigate impedance issues. All cavities will be driven by reliable individual solid state amplifiers with an integrated digital-low-level RF system.

A well mature off-axis TopUp injection scheme, based on a 4-kicker or non-linear kicker injection scheme, is foreseen for **BESSY III**, setting strict demands on the dynamic aperture of the lattice. The injector system will be composed of a triode-gun at 100 keV with pulsed grid modulation for flexible bunch pattern generation, a 100 MeV to 150 MeV pre-accelerator injector LINAC with individually powered 3 GHz LINAC sections for redundancy and a low emittance, fast ramped 1 Hz booster synchrotron, placed in the same tunnel as the storage ring.

For the magnet optics design of the main storage ring the magnet specifications, listed in ↘Table 6.2, have not been driven to technical limits and are based on state-of-the-art conventional iron yoke electromagnet technology for multipoles. Wherever possible, permanent magnets or hybrid magnets will be used, which are currently under investigation [64], e.g., within the PerMaLIC collaboration of LEAPS. The inner vacuum pipe diameter of 18 mm, in order to have good pumping capabilities, the integration of *in-situ* bake-out capabilities, the thermal load distribution, and a reasonable impedance budget, defines the minimum bore diameter of 25 mm of the multipole magnets, allowing for sufficiently strong gradients. The vacuum system in general

Magnet type	Max. Value
homogeneous dipole magnet	< 1.3 T
combined fct. bend (2 pole)	< 0.8 T and 15 T/m
combined fct. bend (4 pole)	< 0.8 T and 30 T/m
quadrupole	< 80 T/m
sextupole	< 4000 T/m
minimum spacing (yoke to yoke)	0.1 m
bore diameter	25 mm
inner vacuum pipe diameter	18 mm

Table 6.2: Technical limits for magnets used in the magnet optics design.

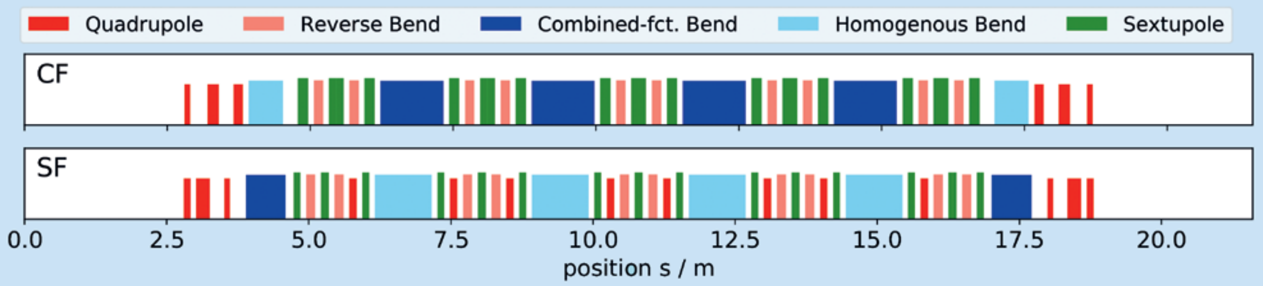


Figure 6.3: Combined function (CF – royal-blue – top) and separated function (SF – light-blue – bottom) MBA unit cell lattice.

will be based on NEG coated vacuum chambers with local ion-getter pumps at highest gas loads, i.e., mainly at the synchrotron radiation absorbers.

Sticking to the technical limits and keeping the circumference of ~350 m a 6-MBA compared to 7- or 8-MBA seems to be the best solution with respect to emittance and the momentum compaction factor. In order to deliver a robust design with good control of non-linear beam dynamics, also with regards to a possible TRIBs operation close to a 3rd resonance, we chose the Higher Order Achromat (HOA) approach, strictly fixing the phase advance between the two chromatic sextupole families within the MBA unit cell[65].

A special request for the optics design for **BESSY III** is the integration of radiation sources, usable as primary radiation standard for the PTB , i.e., an absolute calculable, predictable and traceable radiation source for metrology purposes ↘#quantitative. For that the deflecting magnetic field around the source point must be known to highest precision and be accessible for NMR probe measurements. As the measurement sensor itself requires spatial dimensions of (10 x 10 x 10) mm^3 volume, a purely homogeneous magnet field is required for this volume and at the source point along the orbit of the electron beam. This is best realized with a purely homogeneous dipole magnet, which must be included in the lattice. Due to symmetry reasons, we decided to include the homogeneous metrology bend right from the beginning in the MBA structure to have 16 completely symmetric cells as starting point. In principle, then there are two configurations, shown in ↘Figure 6.3, how the metrology bend can be implemented in a MBA structure.

In the upper configuration the separated function (homogeneous) bend (SF) is placed at the beginning and end of the MBA structure as matching bend. The inner unit cells of the MBA structure are set up with combined function bends (CF) with vertical focusing as mainly used in most MBA unit cells. In the lower drawing the configuration is swapped. The inner unit cell bends are homogeneous SF bends, and here an additional quadrupole is used for vertical focusing and the outer matching bend is realized as CF bend. The three basic blocks of a MBA lattice, the MBA unit cell, the dispersion suppression cell and the matching cell, have been studied carefully and set up under the same boundary conditions for both lattice types and then finally combined to a robust sector cell with reverse bends realized as transverse displaced quadrupoles[66,67]. An interesting result is that the integrated sextupole strength for the SF lattice, and so the sextupole length, is reduced by 50 % compared to the CF lattice due to more favorable β functions and dispersion at the sextupoles. Both lattice variants are nearly equal in total section length and fulfill the demands, stated in ↘Table 6.1.

First evidences indicate that the SF lattice, shown in ↘Figure 6.4, with homogeneous bends in the MBA unit cell is more robust in respect to non-linear beam dynamics and therefore provide higher lifetime, allow for better injection and eases the integration of the metrology bend and the bending magnet sources. With a field strength of 0.65 T the critical energy of the homo-

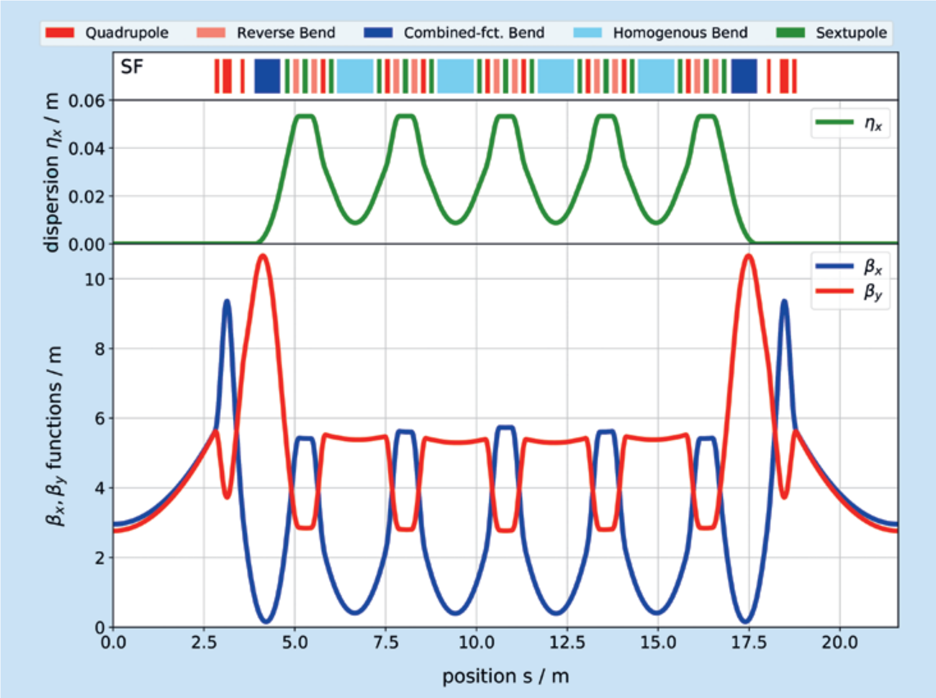


Figure 6.4: First baseline lattices for **BESSY III** based on a MBA unit cell with homogeneous bends – the SF lattice.

geneous bends will be at 2.7 keV, which suits the PTB very well, because it is similar to the metrology bending sources at BESSY II with 2.5 keV. Another option currently under discussion is to replace some of the homogeneous bends by longitudinal gradient bends, which could push the critical energy to higher photon energies. For example, a field strength of 2.2 T will result in a critical energy of 9 keV, better matching the catalysis & energy scientific needs. However, the impact of longitudinal gradient bends on the beam dynamics and the overall lattice parameters need to be studied carefully.

Based on the here presented magnet parameters and technical specifications, we are convinced that within the detailing technical design process of the CDR phase of the project, we will be able to maintain the competitive performance parameter of our lattice. All the overhead which will remain available in this process, we than can either use to target a even higher performance or to use it for the most sustainable and energy efficient machine design.

We decided to set equal and low β_x, β_y-functions in the straights to guarantee phase space matching between photon and electron beam emittance and keep the option for round beam operation, which will reduce further the zero current equilibrium emittance by $^2/_3$ down to ca. 70 pm rad with smallest spot sizes of 15 µm. Next planned steps are the analysis of collective effects as for example, intra-beam scattering, which could limit the reachable emittance, an adaption of the lattice for injection and a tolerance analysis including magnet and girder misalignment and magnetic field tolerances. The aim is to setup a framework for simulated commissioning. Therefore currently an online model and digital twin development is ongoing at HZB to improve the data handling and convert processes[68, 69] towards full ↘#automation).

Impact: The concept for the accelerator complex, especially for the storage ring with its radiation sources, fulfills the demands raised by the scientific motivation described in ↘Chapter 4. As shown in ↘Figure 6.1, **BESSY III** will be in the forefront of 4th generation low emittance light sources in the soft-to-tender spectral range. It will deliver up to three orders of magnitude more brightness and allow for 10 nm foci on the sample – 3 orders of magnitude smaller compared to BESSY II. In addition, **BESSY III** will come with special features like the metrology sources for the PTB or bending

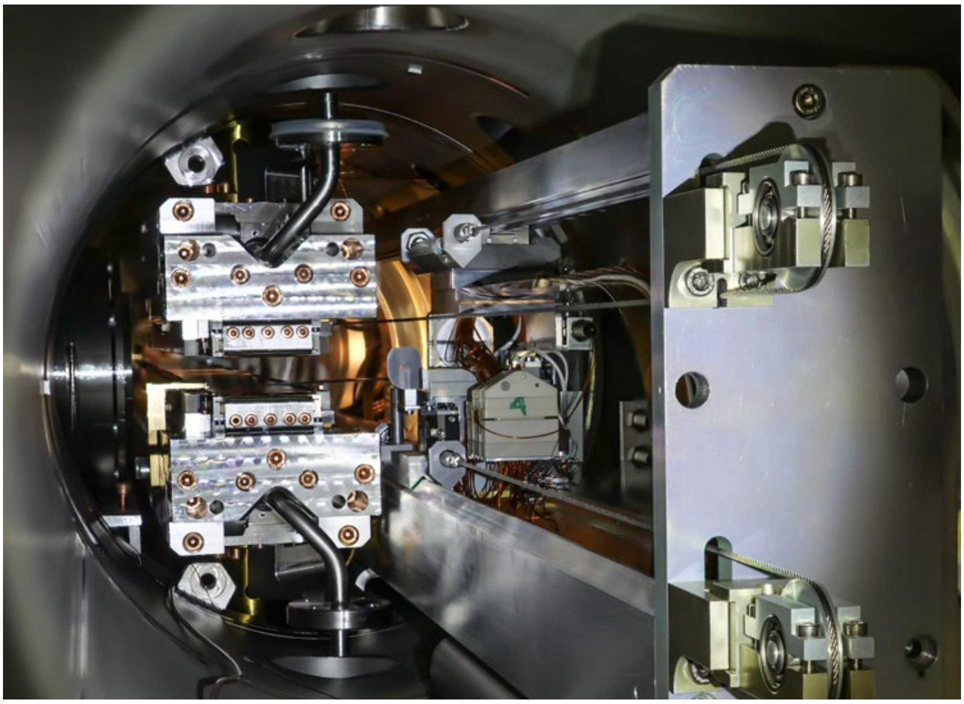


Figure 6.5: View inside the CPMU17 during the magnet field measurements. The magnet structure on the left side and the in-vacuum measurement bench on the right side are shown.

sources from ~10 eV to the 20 keV regime. If desired a 2nd stable orbit option by TRIBs for timing and other experiments can be integrated.

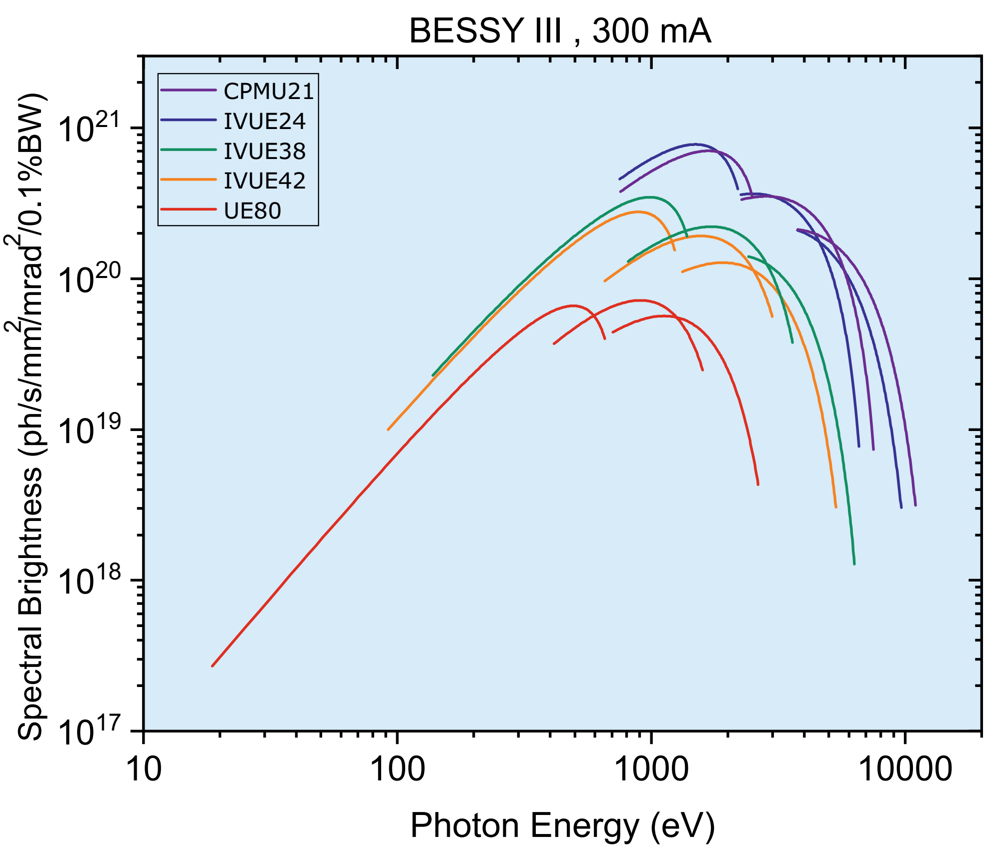
6.1.2 Undulators and Photon Sources

Goal: **BESSY III** aspires to make a broad spectrum of photon energies available to users, with a core range from soft-to-tender X-ray energies. Furthermore, full polarization control is being requested for ever higher photon energies. The goal is to design and build insertion devices (IDs) that will provide each beamline with a high flux, high spectral brightness and coherence tailored to their experimental requirements.

Expertise: HZB has a long and successful history in designing and developing innovative ID solutions, including APPLE-II devices, and the Cryogenic Permanent Magnet Undulator (CPMU) for the EMIL beamline[70]. The present culmination of expertise in the Undulator Group is the successful construction and measurement of cryogenic in vacuum devices, bringing cutting edge mechanical, electrical and cryogenic engineering together with state-of-the-art magnetic material science and magnetic measurement techniques (↘Figure 6.5)[71–76]. This drive for innovation continues with the development of an in-vacuum elliptical undulator (IVUE32), currently under construction for BESSY II[77–80]. The successful development of this technology will release the potential for **BESSY III** to offer polarization control across a broader energy range. Active research and development activities such as for the IVUE32, often undertaken in collaboration with partners from across industry, academia and non-academic institutions, illustrate that the Undulator group is well placed to contribute to the success of the next incarnation of BESSY.

Approach: The tentative beamline portfolio presented in the previous chapter, needs a corresponding likewise tentative ID portfolio, illustrated in ↘Figure 6.6, that covers a very wide photon spectrum, ranging from photons of a few eV to 120 keV. This energy range, even at the challenging margins, will be covered at **BESSY III** through the use of a wide variety of established and developing ID technologies:

- **CPMUs for the tender X-ray range;**
- **APPLE-II devices for the soft X-ray range;**



No.	Name	Photon Energy	ID or ID combination
1	VUV to Hard	5 eV – 20 keV	UE80 + CPMU21
2	Soft and Tender	100 eV – 4 keV	IVUE 42-24 (DOPU)
3	XUV to Soft	60 eV – 1.5 keV	U70
4	Magnetic Imaging	150 eV – 2 keV	IVUE42
5	VUV Spectroscopy	5 eV – 200 eV	UE140 or UE150
6	Soft and Tender Imaging	180 eV – 8 keV	IVUE38
7	Inelastic Scattering	180 eV – 3 keV	IVUE42
8	Spectro-Microscopy	100 eV – 1.8 keV	UE56
9	Macromolecular Crystallography	5 keV – 20 keV	CPMU18
10	Multimodal Spectroscopy	20 eV – 8 keV	UE80 + IVUE24

Figure 6.6: Example of tentative IDs for **BESSY III** beamlines and expected spectral brightness: U are planar devices, UE are APPLE-II devices, CPMU are cryogenic planar in-vacuum devices and IVUE are in-vacuum APPLE-II devices. The period length is specified in the name of the device in mm. The minimum gap for all in-vacuum devices (IVUEs and CPMUs) is 6 mm. The actual minimum gaps and lengths of BESSY II- IDs are used. A minimum gap of 13 mm is assumed for UE80. CPMU21 is 3.5 m long. All other IDs of **BESSY III** are assumed to be 5 m long

- **APPLE-KNOT or APPLE-LEAF type undulators for the VUV and soft X-ray;**
- **Novel Multi-Period Undulators for beamlines that require access to the very broadest spectrum BESSY III is able to offer.**

Photon energies from a few tens of eV up to the soft X-ray range can be covered by planar and APPLE-II undulators, such as U70 and UE56 or UE80. In-vacuum APPLE-II undulators, such as IVUE42 and IVUE38, with a minimum gap of 6 mm can provide photon energies from the soft X-ray up to the tender X-ray range. The core tender X-ray range can be accessed via CPMUs, such as CPMU21, CPMU17 or CPMU18. Detailing of the needed solutions to extract the high radiation power will take place within the CDR and TDR phase of the project, when the respective beamline design and the needs on photon energy range is more mature.

Extremely low energies even below 10 eV at **BESSY III** will require high-K undulators, which will radiate a great deal of power. APPLE-KNOT or APPLE-LEAF undulators direct the majority of this power away from the undulator axis, even in linear operating modes. This allows the majority of the heat load from these devices to be absorbed by apertures around the undulator axis [81–83].

Multi-Period Undulators can cover the energy range from 100 eV to several 1000 eV with a variable polarization. Multi-Period Undulators refer to undulator structures that contain multiple undulator magnet arrays arranged side-by-side. These arrays can be moved side-to-side, so that the appropriate period length can be chosen [84, 85]. For the purposes of **BESSY III,** a Double Period Undulator DOPU should suffice. For example, a DOPU with period length 42 mm and 24 mm can cover the energy range required for ↘#multimodal energy research.

In ↘Chapter 4 a strong case for multimodal beamlines is laid out. This demand can be fulfilled with two undulators installed consecutively into the same straight, in a similar fashion to the EMIL straight at BESSY II, which requires correspondingly long straight sections. Cooling and interlock concepts to protect small vacuum chambers and beamline components will be carefully adapted in the CDR and TDR phase based on operational experience with the EMIL straight section and high power wigglers at BESSY II. Apart from the strong requirement of the PTB, there are several other requests for bending magnet sources from the catalysis, energy and quantum communities (↘see Figure 5.2). Accordingly, at least one dipole per MBA cells is planned as photon source (↘see Section 6.1.1). The request of BAM and PTB for photon energies from 5 keV to 120 keV can be met with a WLS with a magnetic field corresponding to a critical photon energy of 30 keV.

Impact: The undulators are part of the essential infrastructure of a future **BESSY III** and are an indispensable prerequisite for achieving its scientific goals. The continuing development work for in vacuum elliptical undulators and double period undulators strengthen the leading role of HZB in the field of permanent magnet undulator design. Our history of collaboration with industry an academic partners illustrates our commitment to technology transfer following developments in the field of undulator design.

6.1.3 X-ray Optics and Beamlines

Goal: In order to fulfill the needs of the BESSY III users and of their research, the beamlines have to transport the light from the source to the experiment with as high transmission as possible while simultaneously delivering all required properties. This includes common parameters such as photon energy, photon flux, bandwidth and state of polarization as well as spot size on the sample. All of these parameters will have to be fully remotely controllable and the state of the beamline as well as that of the delivered photon beam will have to be included seamlessly into the (meta-)data of the user experiments. In combination with an automated and protocolled beamline quality assessment with sophisticated (online) diagnostics [86], this lays the ground for FAIR data collection and open science.

Expertise: We can built on the excellent expertise of the HZB in X-ray optics [87] and beamline design and construction which has been gathered since the set-up and operation of the BESSY II beamlines. In particular, the collimated plane-grating monochromator (cPGM) based beamlines [88] have a proven track record for robust and flexible operation simultaneously providing state-of-the-art performance. Taking full advantage of our X-ray optics design and metrology capabilities [89] as well as our unique grating production facility at HZB [90] we have developed new multi-layer optics (mirrors and gratings) allowing to extend the operation range of the cPGM with exceptional efficiency up to 5 keV [91]. Current investigations show that the photon energy limit can be extended to even higher energies while providing similar or higher photon flux as compared to double crystal monochromators (DCM) with a new multi-layer optics based cPGM design.

Rational beamline design strongly relies on photon source and beamline ray-tracing simulation tools. HZB is developing the corresponding software since decades. It is utilized all over the world and current developments include a refactoring based on modern cross-platform industry standards towards an open-source code. The corresponding speed-up of the simulations fosters the integration of AI methods for general beamline design optimization which is currently investigated in collaboration with DESY.

Approach: Based on the needs of the scientific focus areas in ↘Section 4.3, one can group the tentative beamline portfolio of **BESSY III** (↘see Figure 5.2) into the main categories ”classical”, ”tender” and ”special” with roughly similar quantities:

- **Beamlines covering the ”classical” soft X-ray range (approx. 100 eV to 2,000 eV)**
- **Beamlines which are geared more towards the tender X-ray range (up to 5 keV)**
- **”Special interest” beamlines demanding the broadest possible photon energy range or require very special conditions such as extreme spatial or energy resolution.**

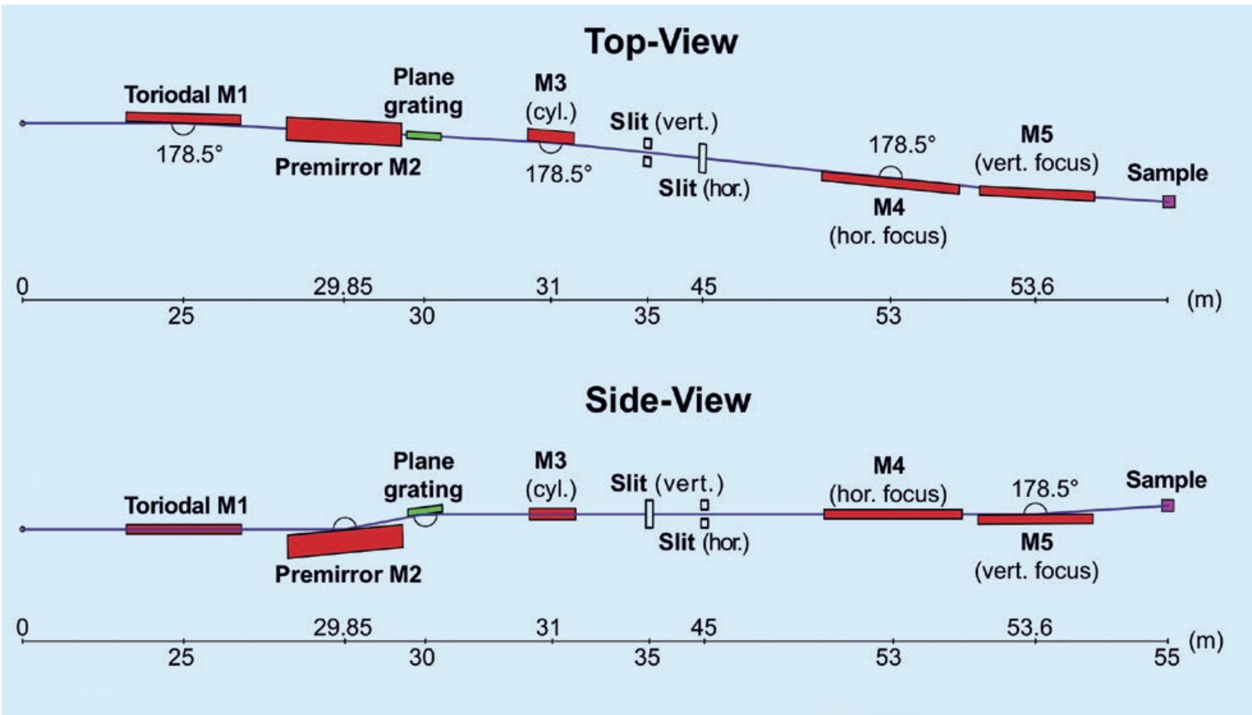


Figure 6.7: Scheme of the energy storage research micro-focus beamline for photon energies 100 eV to 4,000 eV.

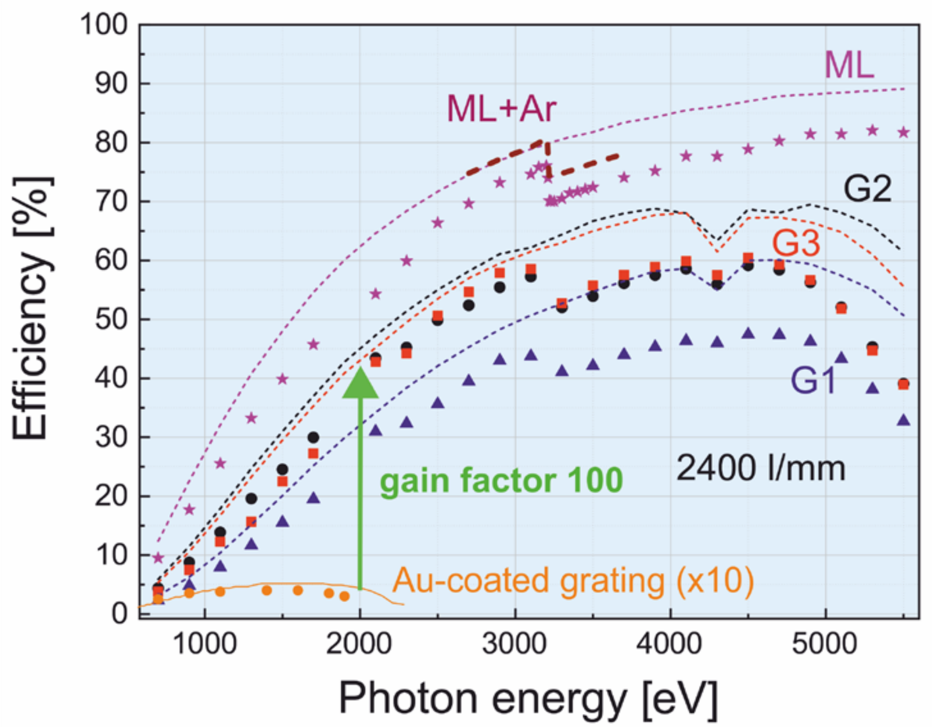


Figure 6.8: Calculated (lines) and measured (symbols) efficiencies of Cr/C multilayer optics (35 bi-layers) for a mirror (ML, pink; ML+Ar, dashed line, accounting for argon impurities) and three gratings with 2,400 l/mm (G1/G2/G3 with different blaze angles in blue/black/red, respectively). Adapted from[93]. Shown at the bottom is the efficiency of gold-coated gratings in use at BESSY II. Compared to these optics, the multi-layer optics gain two orders of magnitude above 2 keV.

The soft X-ray beamlines at **BESSY III** will be based on the proven cPGM design. For the tender X-ray range, multi-layer optics will serve soft-to-tender X-ray needs with one monochromator design that allows the users to benefit from increased capabilities and flexibility. This also gives enormous benefits for standardization by streamlining the portfolio of beamline designs and associated components. Beamline components will be considerably improved in terms of stability and repeatability compared to BESSY II and serve as standardized building blocks wherever possible.

Further dedicated components will realize the third category of beamlines where extreme performance for high-end applications has to be reached or complex ”two-color” operation (similar to EMIL nowadays[92]) is desired. The space available at **BESSY III** will allow long (90 m) beamlines necessary e.g. for providing few meV bandwidth at 1 keV photon energy with still sufficient photon flux (#high-res-spectro). For the hard X-ray beamlines (well beyond 8 keV) a standard DCM would still be the option of choice especially for applications where high photon energy resolution is key. Our concept for an energy storage research beamline (↘ Figure 6.7) serves as an example which addresses the scientific need for an extended photon energy range including tender X-rays by a modified cPGM design utilizing multi-layer optics. By simply adding a second multilayer coating in addition to the standard gold coating for both the pre-mirror as well as the blazed grating, the corresponding photon flux gains more than two orders of magnitude (↘ Figure 6.8) allowing to perform ”proof-of-principle” experiments up to 3 keV already at BESSY II. For the **BESSY III** beamlines even higher throughput is anticipated (by special IDs and adapted optics e.g. lower angles of incidence) allowing to utilize high photon flux even beyond 4 keV for ↘#high throughput experiments.

AI-methods for all beamline aspects (design/simulation, construction, set-up, commissioning, operation and maintenance) are currently intensively investigated to cover two ”Digital Twin” aspects of the **BESSY III** beamlines: (a) improved understanding by bridging the gap between theory based description and real behavior, providing *surrogate models* that can do realistic predictions and (b) support operation by intelligent re-alignment procedures and good *virtual beamline* *representations,* which also provide (remote) training and experiment preparation capabilities to the users.

Impact: Research applications at **BESSY III** will benefit from the fact that the proposed beamline design standard, the improved cPGM design with the multi-layer optics option, is able to cover the requested core photon energy range, soft-to-tender X-rays (see ↘Figure 5.1). A common beamline design that allows to fulfill the needs for both high-resolution spectroscopy as well as high-resolution imaging, being particularly demanding in terms of coherence preservation along the whole beamline up to the sample, will also be a very strong benefit for all other anticipated research applications at **BESSY III**. For these the required stability (on short and long time scales) and the necessary complete understanding of X-ray optics is a base requirement for predictable and repeatable measurement conditions which are highly relevant e.g. for automated ↘#high throughput sample screenings calling for high sensitivity paired with low quantitative uncertainty.

6.2 Experimental Instrumentation and Infrastructures

Following the requirements for scientific discovery at **BESSY III** described in ↘Chapter 4, especially the idea of a material discovery facility, infrastructure has to be provided that goes far beyond what a single piece of data acquisition equipment can do. The path we want to follow with the concept of integrated research is schematically described in ↘Figure 6.9 and explained in the following subsections.

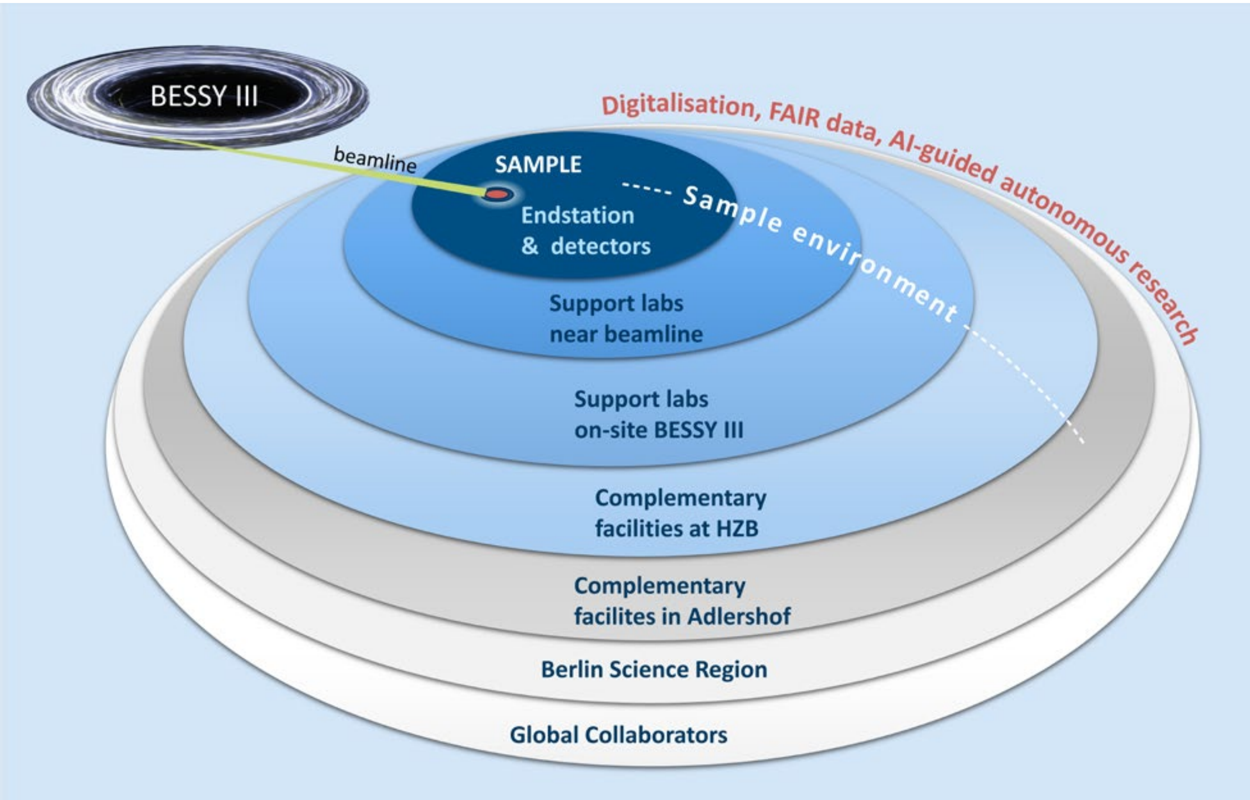


Figure 6.9: The envisaged research environment at **BESSY III** in a simplified sketch. Support labs and characterization toolsets augmenting the light source capabilities will be provided inside the integrated research campus (blue ellipses), complemented by Adlershof campus facilities, science environments of Berlin and international partner labs. Sample environment (white arc) is the overarching activity for organizing #multimodal approaches. Rigorous digitization will create a productive working style and scientific data of sustainable quality (red text).

High brightness X-ray beams from the source are incident on the sample within an endstation (dark blue area in ↘Figure 6.9), which in the soft-to-tender X-ray region is usually a complex UHV chamber equipped with sample manipulation capabilities, load-locks, spectrometers (electrons, photons and ions) and tailored detectors (↘Section 6.2.1). The endstation already contains components of an overarching sample environment that provides desired physical and environmental parameters and standardized components for sample transfer (see ↘Section 6.2.2).

In the immediate vicinity of an experiment, we provide beamline-near support labs that are indispensable for combinatorial approaches (↘#multimodal, ↘#operando, ↘#*in-situ*) to material discovery. Already existing blueprints for this kind of labs are BElChem[94] and EMIL[92] at BESSY II. In addition, general on-site supporting labs that can be used by the different focus fields (see ↘Section 4.3) such as Physics Labs (for experiment preparation, vacuum), Detector Labs (detectors and electronics), Chemistry labs (catalysis, energy, life sciences) and Bio labs (life sciences). These are planned as commonly usable facilities near the beamlines and endstations with on-site support from lab specialists.

The entire chain for the realization of ↘#multimodal approaches will be completed by complementary facilities embedded in HZB's research campus and farther by surrounding complementary facilities in Adlershof offered by our partners (e.g. cryo-EM at HUB). Like indicated in ↘Figure 6.9, the sample environment (↘Section 6.2.2) is an overarching activity organizing the way of the sample among different labs inside the integrated research campus (see ↘Section 6.2.4) accompanied by rigorous digitalization of all relevant components. Further added value will be generated by close collaboration within the science campus Berlin-Adlershof, the Berlin-Brandenburg region (TUB, FUB, the Universities of Potsdam and Cottbus) and global collaborations within LEAPS and facilities overseas out of the global SR-facility pool.

6.2.1 Endstations and Detectors

Goal: Owing to the complexity of experiments for materials discovery at a 4th generation light source and challenging UHV, stability and sample environment requirements, mainly permanent endstations adapted to the beamline, but also a few mobile endstations to be deployed at different beamlines, will be provided by HZB and within joint projects with collaborators. **BESSY III** will offer some open ports for external user endstations and for new ideas to come.

Expertise: The expertise for construction, operation and further development of experiment endstations at HZB is based on decades of experience in the operation of BESSY II and the cooperation with our partners, industry and the user community and ranges from THz to hard X-rays with a strong focus on UHV-based setups for soft X-ray applications. As of 2022, BESSY II already provides 55 endstations including 9 flexible setups that can be used at different beamlines at currently 6 open ports and with different methods[95]. Examples for permanent endstations which are adapted to the beamline, the undulator and special modes of the storage ring are e.g. ARPES 13 and 12[96], MAXYMUS (STXM)[97], (S)PEEM[98], DYNAMAX[99] as leading instruments in the quantum and information technology focus area. Being once a trailblazer in lensless imaging (see ↘Ref. [100]), BESSY II in-house and external users are yet limited in sufficient coherent flux to catch up recent progress at the emerging 4th generation sources, see ↘Figure 6.1. The BESSY II soft X-ray microscope TXM has excelled for life sciences and the Energy Materials *In-situ* Laboratory (EMIL)[70] combines soft and hard X-ray spectroscopic methods as a blueprint for future multimodal SR experiments.

While hard X-ray detectors are readily available now and not even particularly expensive, the low energy of soft X-ray photons will make these devices always more delicate. Using these for quantitative science will for the foreseeable future require great care and expertise in choosing the right detection and amplification scheme for the experiment, calibrating detectors and regularly keeping track of their performance. Despite

HZB has not been developing detector hardware in the past it provided beamline and tools to test them. Long term experience exists at the PTB to quantitatively calibrate detectors in the soft and hard X-ray range, e.g. for space missions (ESA and NASA) and industry (DECTRIS) (see ↘Section 4.4). There are collaborations of HZB and renowned well established detector groups (DESY, KIT, CERN) within the Distributed Detector Lab (DDL) to characterize soft-to-tender X-ray Detectors at BESSY II.

Approach: Our approach is to further improve permanent endstations developed over years at BESSY II and PTB/BAM, develop new ones and transform them into fully automated high-stability facilities at **BESSY III** with flexible sample environments and best possible adaptation to dedicated beamlines at **BESSY III.**

Prominent examples from the focus area quantum and information technology in ↘Section 4.3.2 are 1D states between ferromagnetic domains which can be only measured by nano-ARPES as depicted in ↘Figure 4.3. To address this at **BESSY III**, HZB is going for a high resolution beamline in the soft X-ray range (e.g. cPGM based, see ↘Section 6.1.3) and an endstation featuring nm refocusing capabilities e.g. with reflection zone plates (RZP) developed at HZB and a high resolution electron analyzer like at the ARPES 13 and 12 endstations [96], [101] at BESSY II. As mentioned in ↘Section 4.3.2, topological structures require imaging capabilities with a spatial resolution in the nanometer range and high time-resolution. Such textures and their response to stimuli will become experimentally accessible at **BESSY III** using imaging techniques which provide very high spatial (sub-3 nm in 2D, sub-10 nm in 3D) and high temporal (ps-ns) resolution. A recently launched new team at HZB [102] to visualize complex spin states and electronic textures under realistic "↘#operando" conditions is aiming at developing such coherent imaging approaches for **BESSY III** anticipating the orders of magnitude higher coherent flux, see ↘Figure 6.2, compared to the pioneering experiments [100].

Approaches in ↘*#operando* nano-spectroscopy with electro-chemical cells for catalysis (see ↘Section 4.3.1) are pursued on the way to **BESSY III** e.g. the MYSTIIC endstation, a new soft X-ray STXM endstation at EMIL based on the world leading STXM magnetic imaging MAXYMUS endstation [97] at BESSY II.

Driven by life science applications (see ↘Section 4.3.3), a novel scanning X-ray microscope endstation that detects backscattered electrons and employs Focused Ion Beam milling (FIB-SXM) is in development. Using high brightness and coherence, 3D images with isotropic 10 nm resolution will be routinely available that can be used also for ↘#high-res-imag in all other focus areas. Never before seen ↘*#operando* insights are expected employing TXM for battery materials (see ↘Section 4.3.1 and ↘Figure 6.1) in the ↘#tender range [93], where the gain in flux can be up to 5 orders of magnitude: 3 orders from the ID (↘Figure 6.2) and 2 more orders from the novel multilayer-coated gratings as revealed by ↘Figure 6.8.

When it comes to detectors, the approach is to continue existing collaborations within the Distributed Detector Laboratory DDL, LEAPS and global collaborators ensuring access to the latest sensor technologies for the start of **BESSY III** operation. On the route to **BESSY III**, HZB will provide infrastructure for testing and characterization of detector systems with a focus on soft-to-tender X-rays and BESSY II undulators and beamlines acting as multitools for a ↘#quantitative characterization of detectors together with the PTB. Within the DDL collaboration, HZB is establishing a photon test beam facility with a dedicated test station for soft X-rays.

Impact: Permanent and well adapted fully automatized experiment endstations will increase the performance of most of the experiments, e.g. a permanent X-ray holography endstation or nano-ARPES for ↘#high-res-imag and ↘#high-res-spectro, respectively. This will lower access barriers for inexperienced users and industry, who are just interested in answers to their scientific questions performing SR experiments but do not want to invest in learning instrument specifics or own equipment.

Detector activities on the way to **BESSY III** will result in higher image resolution and sensitivity for key methods like CDI, PEEM, TXM, RIXS, RXS etc. in the soft-to-tender

X-ray range and enable new levels of ↘#high-res-imag and #dynamics studies as well as ↘#operando imaging and metrology (↘#quantitative). Novel detectors will preserve the higher brightness from the machine and enable on-chip signal analysis and fast data management + AI (↘#automation) as well as ↘#high throughput and to manage huge amounts of data by smart reduction concepts.

6.2.2 Sample Environment

Goal: Sample environment for **BESSY III** experiment endstations and for the laboratories of the complementary facilities at HZB will play a crucial role for the scientific program of **BESSY III**. The overall goal here is to enable excellent scientific research at **BESSY III** by providing outstanding and tailored sample environment. In addition, we will maximize the use of the available beamtime by fast ↘#high throughput and automated (↘#automation) sample environment. Industrial cooperation and applied research will be fostered by sample environment solutions that enable investigations of components under realistic conditions and reflect the specific needs of our industrial users. The concept of the integrated research campus for **BESSY III** will be supported by standardized and modular sample environment interchangeable between end stations and complementary laboratories. Complex scientific topics such as advanced ↘#*operando*, complementary *in-situ* and ↘#multimodal studies profit from this integrated approach, for example in energy and catalysis related research, as presented in ↘Section 4.3.

Expertise: Developing and implementing excellent sample environment for neutron investigations and SR experiments has been a long time focus point at HZB. A dedicated sample environment group with broad experience on the wide spectrum of scientific fields as well as in developing versatile and more demanding experimental environments for soft-to-tender X-ray methods

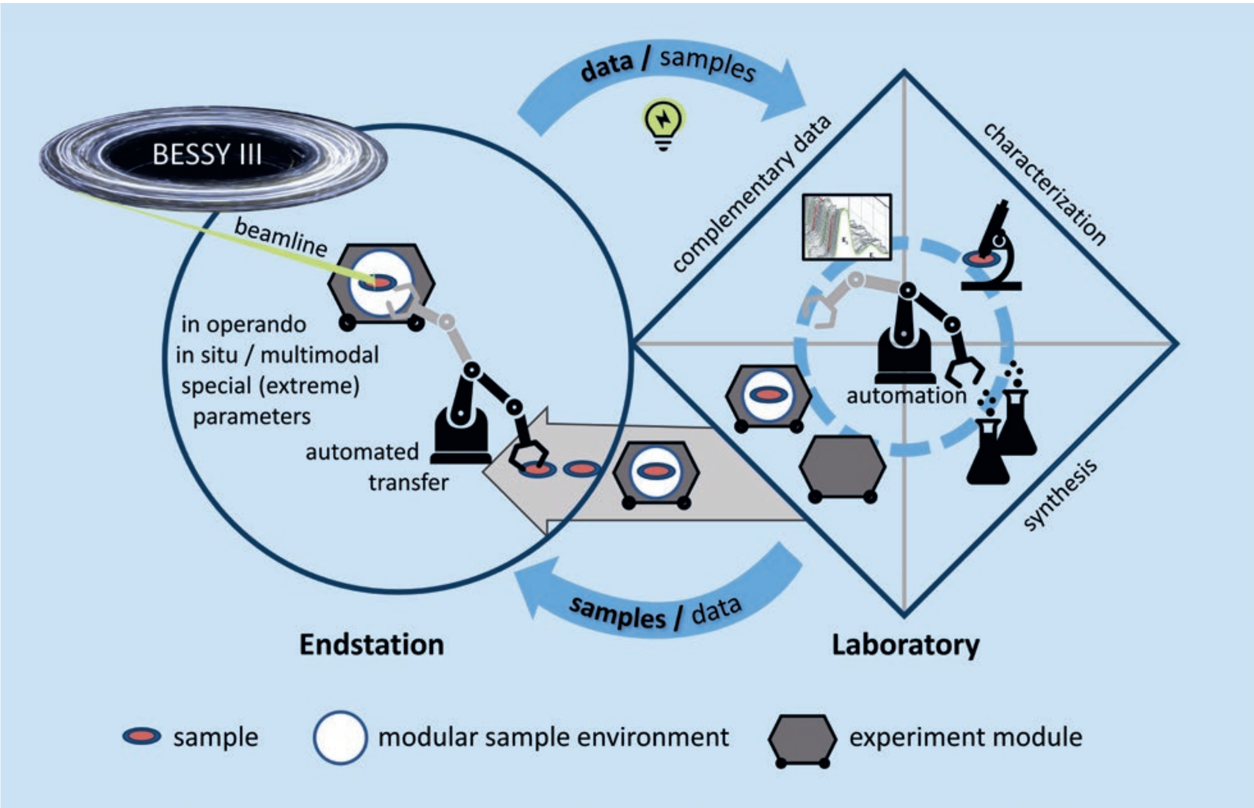


Figure 6.10: Integrated sample handling spanning complementary laboratories and **BESSY III** end stations. Standardized sample environment modules enable material transfer. Exchange of complementary data adds process tuning capabilities to the workflow.

has been formed at BESSY II. Available expertise covers e.g. *in-situ* and ↘#*operando* sample environments for electro-chemical and catalytic experiments, ↘#automation and nano-positioning for ↘#high-res-imag, but also extreme sample conditions like temperature, fields or pressure. New interchangeable sample environment modules for standardized soft X-ray endstations has been established for ↘#multimodal experimentation in the framework of the Berlin Joint Lab for Electrochemical Interfaces (BElChem)[94]. Tailored ↘#*operando* electro-chemical devices and sample environment infrastructure for optimization of battery cells has been built up. Novel reactor cells for gas catalysis based on micro-electro-mechanical systems (MEMS)-nanoreactor technology[103] are in development to combine high pressure catalysis with soft X-ray absorption spectroscopy for CatLab[104] and Care-O-Sene[105]. Within international projects and collaborations with various European photon sources (LEAPS), the HZB sample environment group plays a pivotal role in the development of new sample environment standards and novel equipment.

Approach: Our focus will be on state-of-the-art *in-situ* and ↘#*operando* sample environment for soft-to-tender X-ray investigations. We intend to combine a high degree of standardization with ↘#high throughput and complete ↘#automation. Standard sample holders and advanced sample environment modules, like generic battery cells as well as ↘#*operando* reactor cells, will be integrated into automated investigation routes (see ↘Figure 6.10). One branch of these routes is sample preparation, characterization and measurement of complementary data in the laboratory. Automation there might include commercial solutions[106]. The other branch covers X-ray studies at dedicated **BESSY III** end stations. There cutting edge technology, e.g. nano-positioning or extreme unique sample conditions, is required. Overall data exchange will be in standard format, e.g. NeXus, HDF5. Continuous sample tracking and FAIR metadata standards will be an integral part of all sample environment equipment.

Complete “sample processing” at the instruments covers sample identification, even fabrication, end station and off-line measurements and all-in data analysis capable of closed loop feedback optimization. To support time and spatially resolved experiments (↘#dynamics, ↘#high-res-imag), we will provide fast and precise positioning in the nanometer range. For experiments related to quantum and information technology research (see ↘Section 4.3.2), where extreme temperature and magnetic field environments are relevant, we will shift limits and extend today’s available parameter space.

Impact: Standardized sample preparation and handling procedures, complementary *in-situ* measurements, and automation robots will raise key investigations, i.e. in catalytic reactions (see ↘Section 4.3.1) or electro-chemical processes, on a superior level of rapid exploration. The establishment of more and better possibilities for X-ray investigations under ↘#*operando* conditions is bridging the gap between fundamental science and applications. Joint developments with international and industrial partners will further push international standardization for the benefit of the worldwide SR-user community.

6.2.3 Supporting Labs and Complementary Facilities

Goal: To round off the ↘#multimodal approach, **BESSY III** will provide access to beamline-near and onsite support labs, that host many basic material synthesis and characterization techniques as well as highly advanced laboratory-based instrumentation. These will allow extensive sample preparation and pre-characterization prior to SR based experiments. Even more important will be the opportunity of investigations with advanced complementary techniques in additional complementary facilities at HZB and on the Adlershof campus (see ↘Figure 6.9) that accompany related experiments at **BESSY III.**

Expertise: Apart from supporting labs (beamline-near and on-site) at BESSY II, HZB is already operating a number of CoreLabs, that will serve as blue-print for future complementary facilities related to **BESSY III**. The X-ray CoreLab provides a variety of X-ray diffraction instruments for thin film, (micro-)structure, texture, and residual stress analysis, as well as radiography and tomography, partly utilizing advanced metal jet X-ray sources. The quantum materials CoreLab provides instrumentation for solid-state synthesis, single-crystal growth, and the study of electric, thermodynamic, and magnetic properties at a range of temperatures (0.4 K – 800 K) and high magnetic fields (up to 14 Tesla). The CoreLab for Correlative Microscopy and Spectroscopy (CCMS) is dedicated to support research projects by means of state-of-the-art electron, ion and light microscopes. And finally, the Energy Materials *In-situ* Laboratory (EMIL)[70], located directly at BESSY II, combines soft-, tender- and hard X-ray spectroscopic methods with a variety of synthesizing, preparation and characterization methods and allows both simultaneous *in-situ* and ↘#*operando* measurements.

Approach: A state-of-the-art suite of beamline-near and on-site supporting labs as well as complementary facilities (CoreLabs) will be provided for **BESSY III** users. Moreover, by demand of partner institutions and the users, highly dedicated lab instrumentation will be supplied and be a part of the experimental campaigns. As an example from ↘Section 4.3.2, materials for future quantum and information technology will be nanometer-sized structures, prepared with advanced lithography techniques from 2D layered precursors. Development of such structured materials would greatly benefit from corresponding sample preparation facilities being available on-site. Necessary characterization techniques to be supplied would be suited scanning probe microscopy SPM and electron microscopy, the latter preferably combined with Lorentz microscopy and electron energy loss spectroscopy EELS, indispensable tools also for materials and metrology applications.

Comparable facilities will be made available for the systematic development of new materials, specifically those which are relevant, e.g., for energy storage or green hydrogen production. Here, it is important to provide on-site facilities for synthesis as well as equipment for electro-chemical experiments and off-line testing. For imaging of device prototypes, X-ray radiography and tomography instrumentation based on metal jet hard-X-ray sources will be provided. In each case, standardized sample environment and sample transfer to the **BESSY III** based analytics will support fast feedback loops for ↘#high throughput combinatorial materials and device optimization.

In any case, the detailed and reliable characterization of complex materials requires the combination of different complementary methods with and without synchrotron radiation on a common metrological basis (SI traceability), which will be further developed in cooperation with BAM and PTB, and thus an advanced on-site laboratory infrastructure for sample preparation and characterization. In the field of catalysis from ↘Section 4.3.1, first steps towards integrated research have already been taken by the recently started CatLab[104] project of HZB and MPG. Here, a novel synthesis approach based on thin-film technology requires dedicated on-site deposition tools with vacuum transfer to the experiment for *in-situ* investigations by techniques like XPS and XAS, accompanied by X-ray diffraction and electron microscopy at on-site labs.

The present MX activities at BESSY II may be regarded as an already long working, successful example for integrated research, with its highly efficient interplay of protein crystal synthesis, automatized sample selection and molecular structure determination based on international standardization. As mentioned in ↘Section 4.3, the latter is the final step of a hierarchical imaging pipeline in health and life science investigations discussed in ↘Section 4.3.3, that step-wise covers resolution length scales between a few microns (e.g., imaging of organs) and sub-nm (molecular assemblies). While **BESSY III** will provide X-ray microtomography, cryo-X-ray microscopy, and MX, the full imaging pipeline will be accessible on-site by including lab-based cryo-fluorensence microscopy and cryo-electron microscopy into a successor of the present CCMS CoreLab.

Impact: HZB will offer a wide suite of supporting laboratories and complementary facilities inside the research campus that will support users of **BESSY III** in the full process of sample and materials synthesis, pre-characterization, and extensive investigation by lab-based experimental techniques complementary to the SR-based studies. This integrated approach will optimize

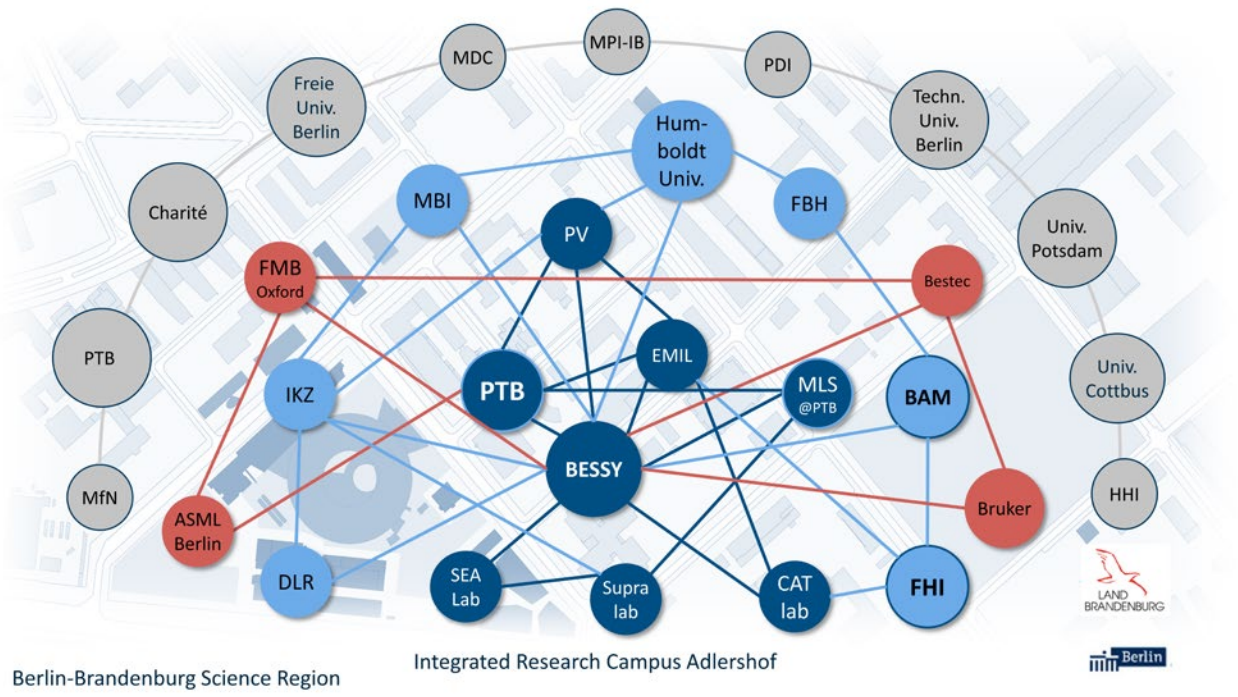


Figure 6.11: Schematic illustrating the SR-light source as part of the integrated research campus of the HZB and partners (dark and light blue dots) in Berlin-Adlershof. The embedding into the Science and Technology Park Adlershof enables networking with scientific on-site partners, more than 150 relevant high-tech companies (sketched by red dots) and a variety of scientific institutions (grey circles) in the Berlin-Brandenburg science region. SEAlab and Supralab are facilities for superconducting accelerator R&D at HZB.

the efficiency of any of the research fields pursued at **BESSY III**. It will therefore help speeding up innovation cycles which are necessary to address the pressing global challenges.

6.2.4 Research Campus

Goal: HZB currently operates two sites: the Lise-Meitner Campus LMC in Wannsee and the WCRC in Adlershof, with a strong renovation backlog and modernization delay in Wannsee combined with space potential in Adlershof. The HZB campus strategy is to relocate and concentrate its research focus and infrastructures from the LMC to the WCRC in Adlershof. The aim is also a development of the LMC for scientific research and knowledge transfer and gradually opening the site for third parties if necessary. The new light source **BESSY III** as the flag-ship project in Adlershof will be embedded in a dedicated laboratory environment near to the beamlines, which is complemented by a suite of material research infrastructures operated by HZB and its partner institutions PTB and BAM forming an integrated research campus within the Science and Technology Park Adlershof. In-house and external users can apply for beam time at the SR source, but also for access to additional HZB and partner infrastructure linked to **BESSY III.**

Expertise: Within the recent years, HZB has already gradually developed towards an integrated research campus within large projects like EMIL[92], CatLab[104] and also in close networking with the stakeholders PTB and BAM, which directly share large laboratories with BESSY II (see ↘Figure 6.11). The PTB laboratory at HZB and the MLS follow up on the experiments[107] on black-body radiation performed in Berlin more than 120 years ago. The combination of a National Metrology Institute (#quantitative) and a modern SR source remains unique.

Already with the start of the BESSY II project in 1993 at the science site Adlershof, numerous high-tech companies and in the course of the 1990s–2000 the natural science departments of the HUB as well as several Leibniz Institutes as MBI, FBH, IKZ and the Helmholtz partner DLR have settled here (see light blue dots in ↘Figure 6.11). All of them are having strong ties with HZB in joint projects, exchange of expertise and personnel as well as technical support. With the construction of BESSY II and the commissioning in 1999, more companies in Adlershof (e.g. red dots in ↘Figure 6.11) started a strong networking with BESSY II. Since the foundation of HZB in 2009, there are more than 12,000 registered order transactions of HZB with ca. 150 companies located on the WISTA campus and intense networking activities take place. Some of these companies are today global players in their fields, like FMB, BESTEC and others, see ↘Chapter 7.

Approach: Our approach is to further develop the existing campus WCRC in Adlershof and to integrate a greenfield facility **BESSY III** as flagship project to this campus as a key infrastructure. With Metrology as one pillar of the above mentioned triad and the direct embedding of Germany's National Metrology Institute (PTB) at **BESSY III** is worldwide unique. The Adlershof campus is located in the southeast of Berlin, near to Berlin airport BER (30 min by public transport) and 45 Minutes away from Berlin central station. The campus is embedded in an excellent transport infrastructure and thus offers the wide scientific landscape as well as non-scientific advantages of direct connection to the diverse metropolis. There are potential sites available where the footprint of the accelerator complex according to the tentative design in ↘Section 6.1.1 will fit in and even more laboratories can be integrated with potential further use of the BESSY II accelerator building after the transition to the new source **BESSY III**. The approach follows HZB's strategic campus development that the WCRC will further evolve as an integrated research campus with focus on materials discovery, hosting all of HZB's in-house research. Research activities from the LMC in Wannsee will be relocated to Adlershof. Additional laboratory and office spaces on the WCRC will be created with a focus on internal and external networking fully in line with the WISTA strategy for the future of the Science and Technology Park Adlershof as a whole.

Impact: HZB and various research institutes, the natural sciences departments of the HUB as well as many high-tech companies on the Science and Technology Park Adlershof mutually benefit from the inspiring neighbourhood and will keep driving innovation processes. The realisation of a **BESSY III** facility on the WCRC in Adlershof will also strengthen and support the strategy of the WISTA to further develop science in Adlershof (↘Figure 6.11) virtually along radial lines with strong connections to surrounding local centres of scientific and technical aggregation. **BESSY III,** with its integrated research capabilities, will certainly add attraction to Adlershof and raise respective interest of new partners. This way, HZB maintains and extends a unique science site in the German capital for the energy transition, quantum computing and other challenges of the future to come.

6.3 Data and Automation

Goal: Digital tools, perfectly tuned to the specific demands of the scientific focus areas, are required to fully exploit the new facility. ↘#high throughput optimized experimental conditions and ↘#automation preventing human errors minimize time to innovation and save resources. HZB is committed to interweave all data streams, linked with the operation of the light source, the experiments and the complementary facilities. Sample tracking, experimental conditions and sequences, data analysis and decisions, published results and curated FAIR data sets, will be covered and available to machine learning (ML) analysis.

Ubiquitous connectivity and high quality of service (QoS) will be provided everywhere to allow for reliable remote, automated and autonomous experimentation. Acquiring complete ↘#quantitative validated meta data describing experimental settings from X-ray energy, intensity, polarization, via instrument set-up like focal spot, timing, mechatronics, to sample life cycles tracked from synthesis, preparation to positioning, ambient and ↘#operando conditions will initially mean higher costs for hardware and installations, but will pay off in sustainable operation and allows to guarantee the necessary data veracity. Ultimately the digital

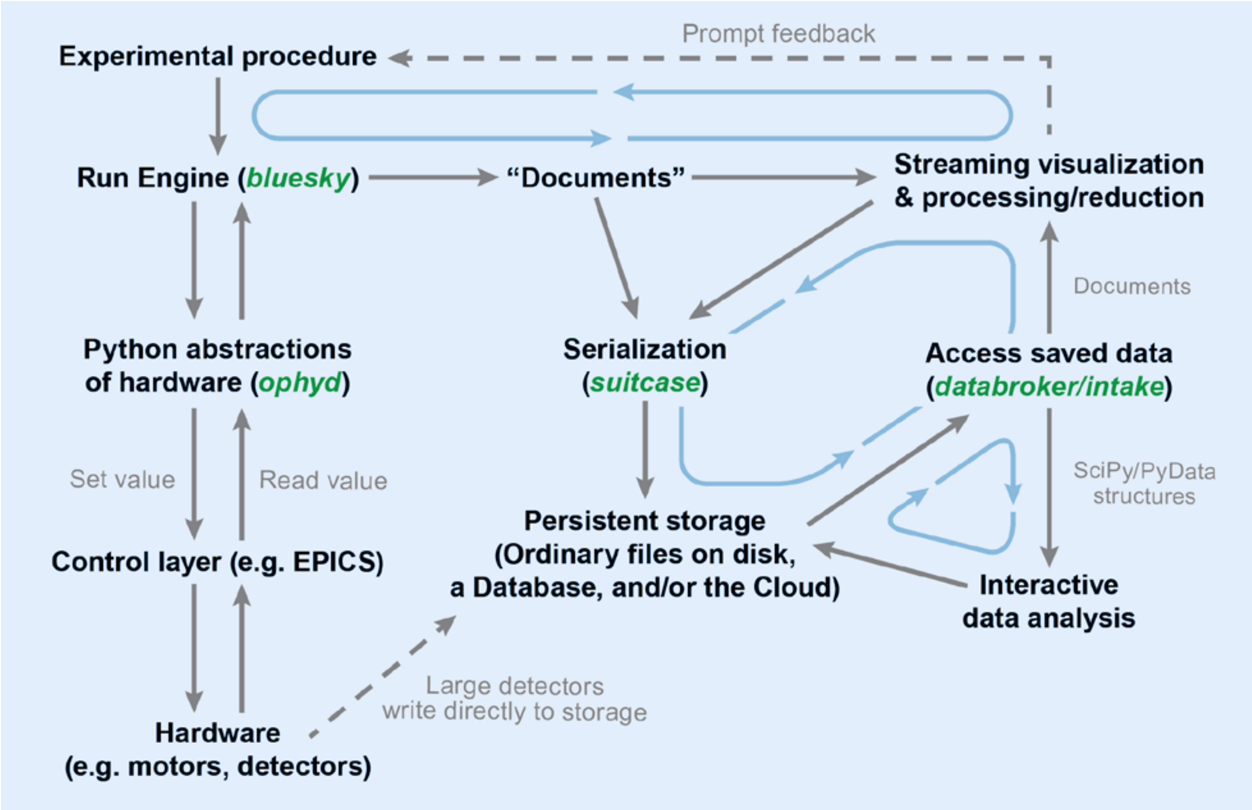


Figure 6.12: Sketch of the automation framework Bluesky [109] as a rich experiment control software ecosystem. Features include ophyd, a device abstraction layer overcoming the flat EPICS data model, bluesky, a run engine covering experiment design, data acquisition, -analysis and -handling flow control and databroker, providing native connectivity to nearly any extending python based scientific toolkit.

environment for **BESSY III** needs to be qualified for a continuous curation of ground truth data, providing a unique, valuable, and reliable repository of FAIR data, given back to the funding society.

Expertise: BESSY, as well as the PTB, participated early on in EPICS, today a well known international, lab spanning controls collaborations. Cooperation of this ever renewing, globally distributed group of open minded, helpful experts on the best technology of its time, boosts every participant's potential and has a compelling standardization effect. BESSY II and MLS controls groups still benefit from the innovative power of today's projects of scale, like ESS, ITER, LCLS II. Around 2019 a new collaboration, called Bluesky [108–110] emerged from the five US light sources and spreads around the globe. The Bluesky python ecosystem (↘Figure 6.12) is a powerful match to the controls requirements of beamlines and instruments, well suited to adaptive experimental data acquisition. Remote workflow management is supported by Tiled[11], a data access and management extension of the Bluesky constituent databroker, see ↘Figure 6.12. Adaptive Bluesky supports autonomous decision making. HZB has been an early European Bluesky adopter and is now a full member of the rapidly evolving global collaboration. HZB is strong in modelling the source, accelerator to beamline, improving operations with reinforcement learning, and deep learning surrogate models with reverse mapping ML methods.

Approach: The **BESSY III** control system, diagnostics and data acquisition hardware will form a distributed, fine-grained architecture, that accommodates the abundance of sensors, actuators, motors, robots and complex subsystems, required by the highly autonomous, remote controlled operation[112]. Components range from system on chip (SoC), front end, signal con-

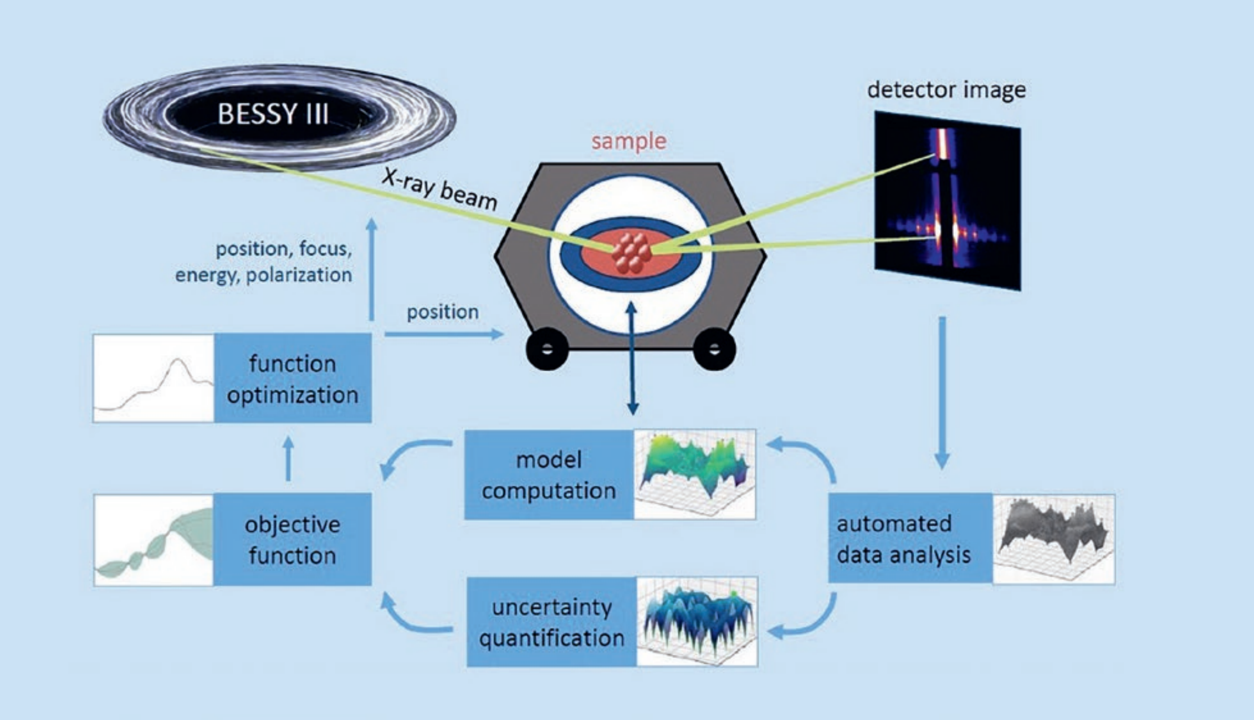


Figure 6.13: A schematic of autonomous experimentation balancing exploration, i.e. learning the landscape of the parameter space, approaching the objective function, and exploitation, i.e. attempting to rapidly achieve relevant results, trying functions as optimized. Sample model development and uncertainty removal are best guided by simulations and checked against FAIR data bases.

ditioning units, desktop and edge computing set-ups capable of near real time data analysis, to computer center rack systems, hosting a variety of virtual instances (Docker, Kubernetes, etc.), resource balanced with external cloud services. Since vast requirements on IT resources easily exceed HZB capabilities, **BESSY III** concentrates on performance critical installations at the instruments, and rely on shared, federated storage and compute infrastructures, emerging from DAPHNE-4-NFDI, ErUM-Data, ExPaNDS, EGI. Affiliation to these community approaches provides guard rails to best practices, supports exchange of solutions, while limiting back bounces from the IT infrastructure resource consumption on the carbon footprint. In protection of health and assets, safety (SIL), industrial control (ICS) and cyber security standards will be applied.

To make the best out of the digital toolbox, components need to be orchestrated and optimized on the applications, specific for **BESSY III** ↘#high-res-spectro, ↘#dynamics, ↘#*operando,* ↘#multimodal[113] etc. instruments. Integration, synchronisation and protection capabilities are guaranteed by software, timing and security interlock frameworks, provided by **BESSY III.** In addition, data access and manipulation software have to fulfill data policy standards and user experience expectations. Scientists taking advantage of the LEAPS light sources complementary opportunities, swapping facilities as experimental approaches change, want to be familiar with common data handling and portable and secure facility access interfaces.

Digital twins in its various forms (trained data, simulations, hardware substitution) and functions (integrity checking, process tuning, teaching, preparation and training) will be essential to the **BESSY III** software inventory and corner stone to robust operations.

High beam intensities focused on tiny spots easily destroy samples under study. Parallel data capture, via large and fast area and multi-channel detectors, will optimize processes and minimize beam time on target. Facilities have to tame the resulting data deluge, but scientists need to be certain, that intelligent data reduction discards only noise and background and signals are safely detected [114, 115]. Recent detector developments merge photon counting and charge integration into incremental digital read-out, enabling trigger-less, zero-suppressed image read out [116], handling very high photon fluxes in the detector and relaxing HPC data analysis.

Moreover, relevant signals must not be overlooked by autonomous adaptive processes, involved in tuning from coarse to fine, and reaching for high exploration speed. Multi-lenghtscale modeling, FAIR knowledge data bases, AI methods of decision making [117] will provide good predictive reasoning, the base for reliable #high throughput. Smart parameter scans (↘Figure 6.13) will be made available and tailored to e.g. ↘#multimodal applications, for a ↘#quantitative example see ↘Figure 4.5 [40]. In comparison with brute force methods, relevant sample states, compositions or orientations are more likely found [118, 119] by this methodology, even under ↘#*operando* conditions. Closed loop autonomous workflow that includes self-driving labs [106], e.g. in the synthesis and characterization part sketched in ↘Figure 6.10, will further accelerate targeted discovery of materials.

Impact: Digital means are key to optimal use of available beam time, saving operational costs. Cutting down unproductive dead times maximizes accessibility to the precious facility. Intelligent autonomous experimentation reduces the turnaround time from idea to scientific verification and demonstration of innovative applications. AI supported sample synthesis and handling reduces valuable material spending. A big share on digital tools within the overall project plan elevates sustainability of the facility significantly: most valuable in terms of relevance and longevity of scientific data acquired. A high degree of automation has a democratizing effect on science made available by this new light source. Costly expert training on instrument specifics is no more prerequisite for access to state-of-the-art X-ray experiments. Common remote operation tools and a familiar user access experience brings facilities to the scientists, saving travel time and energy.

7. Opportunities for Economy and Industry

Goal: Achieving direct economic and technological impact in key areas for climate neutrality requires a significant acceleration of innovation. This demands a deep integration of disruptive materials research and industrial technology development through establishing long-term strategic partnerships with industry partners. **BESSY III** aims at facilitating accelerated innovation cycles in three sectors as in ↘Figure 7.1.

Firstly, **BESSY III** will push the envelope in technological development during the construction phase, creating numerous opportunities for joint developments between HZB and industry. Secondly, the tailored lab environment and unique facility capabilities will attract leading industrial companies, making **BESSY III** an easily accessible and valuable tool for industry. Third, **BESSY III** will facilitate the establishment of longterm partnerships between HZB and industry in joint R&D projects to boost technology transfer and to enable the generation of start-ups.

Expertise: During the BESSY II construction and operation phases local SMEs, e.g. FMB, SPECS, BESTEC, grew to hidden champions and leaders in their market segment. Those companies have benefited from development partnerships and the opportunities to provide high-tech equipment to be operated successfully at BESSY II. The most prominent example of an industrial impact of BESSY II is the rise of a small technology firm FMB to the major international players in vacuum, beamline and endstation technology.

BESSY II regularly serves industrial users, in particular for drug development, residual stress analysis, development of photoresists for lithography processes, surface hardening or analysis of semiconductor devices. Moreover, HZBs partner PTB uses BESSY II to serve their various industrial customers (e.g. Zeiss SMT, ASML, DECTRIS) in metrology material purity analysis and radiometry. A prominent example is the development of resists and optics for EUV-lithography enabled

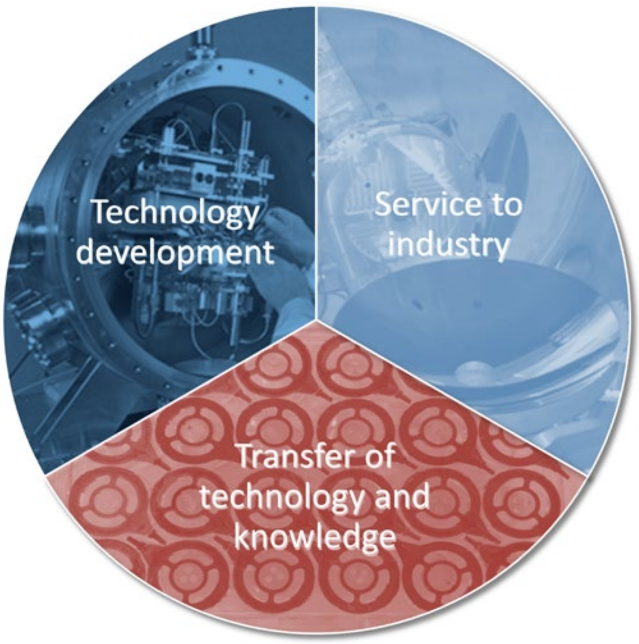


Figure 7.1: The three sectors of opportunities for economy and industry.

by our strategic partner PTB within their cooperation with Zeiss SMT and ASML. EUV-lithography is now the most advanced manufacturing technology for the fabrication of microprocessors.

BESSY II enables a dynamic ecosystem for innovation. Examples are X-ray microscopy development (Axilon AG), special sample holders for protein crystallography (Jena Bioscience GmbH and a spin-off, Crystal Factory Growth Biotech UG) or optical metrology (Zeiss SMT) either in R&D cooperation or licensing of patents. HZB also advises companies and provides them with know-how, e.g. through licensing agreements with Research Instruments GmbH (RI) and Vacuumschmelze GmbH & Co. KG, together with SEAlab and Supralab as test-beds for advanced superconducting RF components. During the years 2010 to 2020, user research and development at BESSY II resulted in 281 patents granted to BESSY II scientists and technicians and 420 BESSY-related publications which are cited in 1059 patents.

Approach: HZB is currently intensifying the cooperation with local and national and international industrial companies for the development of components and equipment for the new facility. In joint development partnerships HZB will drive forward emerging technologies, e.g. additive manufacturing of vacuum chambers, development of state-of-the-art undulators, or implementation of sustainable and energy efficient permanent magnets for bending and focusing the electron beam.

As a vital part of its innovation strategy, HZB is expanding long-term strategic partnerships with selected industry partners already at an early stage of research and development, in particular in the currently emerging fields of energy storage and quantum materials. As part of the integrated research facility approach, a dedicated “Innovation Center for Sustainable Technologies” will enable new possibilities for cooperating on-site within “companies on campus” models in a dynamic science-entrepreneurship ecosystem. Fast and flexible facility access is guaranteed by assigning a certain number of shifts at relevant experiment endstations to the industry cooperation. Standardization and ↘#automation of experiments and fast data analysis tools will enable ↘#high throughput and short experimentation cycles.

Recently initiated strategic collaborative projects CatLab and Care-O-Sene in the area of catalysis will serve as blueprints for accelerating innovation in joint user consortia. BASF is the prime strategic partner within CatLab for the development of novel thin-film catalytic systems. Care-O-Sene is a high priority project in collaboration with the internationally leading company in Fischer-Tropsch process, Sasol Ltd., on novel catalysts for the production of sustainable aviation fuel. Flexible access to the facility, swift characterization of potential catalytic materials and unique ↘#*operando* and *in-situ* capabilities in a tailored lab environment including staff assistance are key for successful collaboration in a public-private partnership. In close feedback loops with the involved companies, these blueprints will guide the developmental phase for **BESSY III**. At BESSY II we have already started new initiatives and developments in terms of industry-ready services and entrepreneurship as a career. These new developments are anticipated to mature within BESSY II to become part of daily life at **BESSY III.**

In addition, PTB and BAM already intensively serving industrial partners will double their activities at **BESSY III** leveraging the impact of the new facility for industry or industry-related research. Both PTB and BAM are in part acting as intermediary service provider, who establish standard procedures for industrial users. Intermediary service companies can act as a link between facility and industrial customer and offer all services that industrial users need.

Impact: The opportunity for the successful development of technologies and components and their proven performance and usability will allow the involved local and national industry to achieve worldwide visibility and to become a global market leader. Technology development in additive manufacturing for instance can have a major impact on production of devices suitable for UHV applications, which is highly relevant not only for the SR community, but also for applications in other fields of research and industrial applications like chip manufacturing. A mature additive manufacturing of UHV components demonstrated in the **BESSY III** context certainly will position the company to gain leadership in this market.

Through our design of an integrated research campus (see ↘Chapter 6), we will expand strategic partnerships with industry through new formats of cooperation on the Science and Technology Park Adlershof and create an innovation culture that deeply integrates science and entrepreneurship. This will massively accelerate technology transfer to develop new sustainable technologies for green energy solutions and stimulate start-ups and spin-offs in an innovation ecosystem. The establishment of industry-ready services and the embedded entrepreneurial culture at **BESSY III** will generate a constant stream of transfer results, incl. spin-offs and cooperations with industrial partners.

8. Cost Framework

To realize the requirements for the source and the scientific-technical infrastructures outlined in ↘Chapter 6, the HZB has drawn up the cost framework for the construction of **BESSY III** (basis: cost levels IV/2021). Starting point for the developmentof the cost framework was a thorough cost estimate for the accelerator complex, insertion devices, beamlines and experimental infrastructures and a detailed analyses of the personnel and lab space requirements for **BESSY III.** The analysis was also compared with the existing experience at BESSY II and data available from other facilities in operation, construction, or planning. Based on this analysis the space needs beyond the large-scale facility have been forecasted. The used characteristic values correspond to those which are usual in the research sector. The following key points were assumed:

- **The footprint of the planned facility is feasible on the available construction site in Berlin-Adlershof.**
- **The entire staff for the operation of the BESSY III facility will be accommodated in the new building complex.**
- **BESSY III will provide significantly more laboratory space for BESSY III-related research (integrated research approach).**
- **The space development within the framework of BESSY III is taken into account in the cross-site structural HZB campus development and possible synergies and space savings will be identified at an early stage.**

Building and technical building infrastructure (C1)

The available construction site in Berlin-Adlershof has a gross area of 44,500 m^2, thereof a footprint of 29,300 m^2 will be used for construction (66 % occupancy). This includes storage ring building (21,700 m^2) as well as adjacent office and laboratory buildings (7,600 m^2). The office and laboratory space are planned to be realized as three-storey buildings. In the personnel planning for **BESSY III** it is currently assumed that 480 people will be located on site to operate the research facility at full capacity. This assumption includes the requirements of the strategic partners PTB and BAM (75 researchers) and spaces for users. Together with the storage ring building approx. 48,300 m^2 of gross floor space can be realized consisting of:

- **17,600 m^2 for large equipment/ring**
- **29,700 m^2 for office, laboratory, storage buildings (thereof 6,400 m^2 offices)**
- **1,000 m^2 for supply engineering buildings**

The required assembly area (6,500 m^2) is not intended to be part of the facility on the new site. This assembly and storage building will need to be erected on the HZB campus before the start of the **BESSY III** construction.

Accelerator complex (C2)

The accelerator complex includes the electron source with injector LINAC, the 1 Hz low emittance combined function booster synchrotron (to be installed within the same tunnel as the storage ring), the storage ring itself and all the related infrastructures for the operation of the accelerator complex, including control system environment. The interface to the beamlines is defined to be the last valve of the front-end systems, as they are part of the storage ring vacuum system. So, cost wise the front-ends are included here. The investment costs for all technical infrastructures for air- and water-cooling systems, supply of electrical power, gases, cryo cooling, etc. are not covered here, as they are accounted for in the costs for building and technical infrastructures (C1). The cost framework for the machine is based on the current assumptions that HZB will pursue a rather conservative approach for the chosen technologies of the accelerator complex, relying largely on already existing or presently developed technologies and concepts, see ↘Section 6.1.1. For the accelerator complex some detailed analyses of the sub-system costs have been done. These estimates are partly based on our own experience, e.g. for the fundamental and harmonic RF-systems or the NEG coated vacuum systems, where we could rely on our experience with the bERLinPro / SEAlab, or on cost overviews made available from other labs and scaled to the size of our facility. Wherever necessary, costs have been adjusted to the IV/2021 price base.

Experimental infrastructure (C3)

For the start of **BESSY III** operation, a 60% (24 of max. 42) utilization of the potentially available experimental facilities at the storage ring is assumed, including the requirements of the strategic partners PTB and BAM. This will guarantee a competitive user operation already during the first year of operation. The remaining free capacity will ensure that the research facility **BESSY III** has sufficient potential for further development and the integration of the needs of future partners or industrial consortia. The shown cost framework considers 8 new insertion devices (ID), 16 ID beamlines, 8 dipole beamlines, and 24 experimental endstations each. Also here, the costing relies on HZB experience with recently planned and realized projects in this field and estimations based on data provided by other labs.

Scientific computing, automation, and laboratory equipment (C4)

To maximize the efficiency of the facility, **BESSY III** will provide on-site experimental infrastructure and laboratories for basic material synthesis and characterization techniques as well as highly advanced laboratory-based analytic methods. This is interweaved with reliable automated, remote and autonomous experimentation, advanced real-time data analysis and decision making, and calibrated data sources. Emphasis on quality will initially lead to higher costs for hardware and installations, even if curation, storage and accessibility of the FAIR data and published results is in large parts covered by federated infrastructures (NFDI). Eventually the extra effort will pay off in sustainable, efficient operation and guarantee the necessary data integrity for the scientific community.

Property, replacement areas, development (C5)

The ground reference value of the available construction site in Berlin-Adlershof has been taken into account (BORIS, cost level IV/2021). Since the area is a green recreation area and partly in use, costs for replacement areas are required. Further costs result from the development of the property (fresh water and wastewater, electricity, heating, ...)

Sustainability (C6)

With **BESSY III,** HZB aims to rigorously pursue the path of a sustainable, future-oriented research infrastructure. Resource-efficient building materials with the lowest possible carbon footprint are already used in construction and can also be reused where possible. Energy- and resource-efficient accelerator components contribute to sustainable scientific expansion. The building itself should produce energy that is then used in the facility. Waste heat generated in the experiments and the infrastructure will be reused on the campus. Implementation increases the initial investment costs for the new facility. However, these costs are amortized several times over the life cycle. The cost projection assumes a 15 % surcharge for the building (C1) and machine (C2).

Operating costs

As first classical estimate it can be assumed that the expected operation costs can be estimated to be ca. 10 % of the construction costs (C1 – C4). This estimate also includes operation costs to be covered by PTB and BAM who will be likely to use 15 % of the **BESSY III** operation capacity. It is nevertheless inevitable to reduce the energy consumption to a maximum tolerable limit and to include local energy sources such as PV or thermal heat (C6).

9. Life Cycle Analysis

Life Cycle of BESSY III

The life cycle of the **BESSY III** facility and the building infrastructure must be viewed in different phases (↘see ↘Figure 9.1).

After planning (phase 0) the first phase covers construction from 2029 on. Approaching phase 2 the facility comes to real life with commissioning of the machine, beamlines and endstations (planned for 2035) at a capacity of 60 %. In the following years, expansion of the capacity towards full operation in phase 2 will take place. After about 15 years in phase 2, a ”major upgrade” of the facility is envisioned. This will allow for another at least 15 years in phase 3. During the predicted approximately 35 years of operation, continuous investments will be made in the modernization of the facility, the experimental stations, and the laboratory infrastructure, with a volume of up to about 3 % of the replacement asset value (RAV) per year. At the end of operation, large parts of the technical infrastructure will be dismantled. As we will follow a concept of concentrating beam losses to a small number of localized and individually shielded collimators, we do not expect in general any issues with the re-usage or disposal of the main fraction of the accelerator components. Following dismantling of the accelerator complex and beamlines, the building infrastructure can be used alternatively for another 25 years. At the end of the cycle, the building will be dismantled and the area renaturalized. The full building life cycle in this case covers 80 years, of which the building is in operation for 60 years.

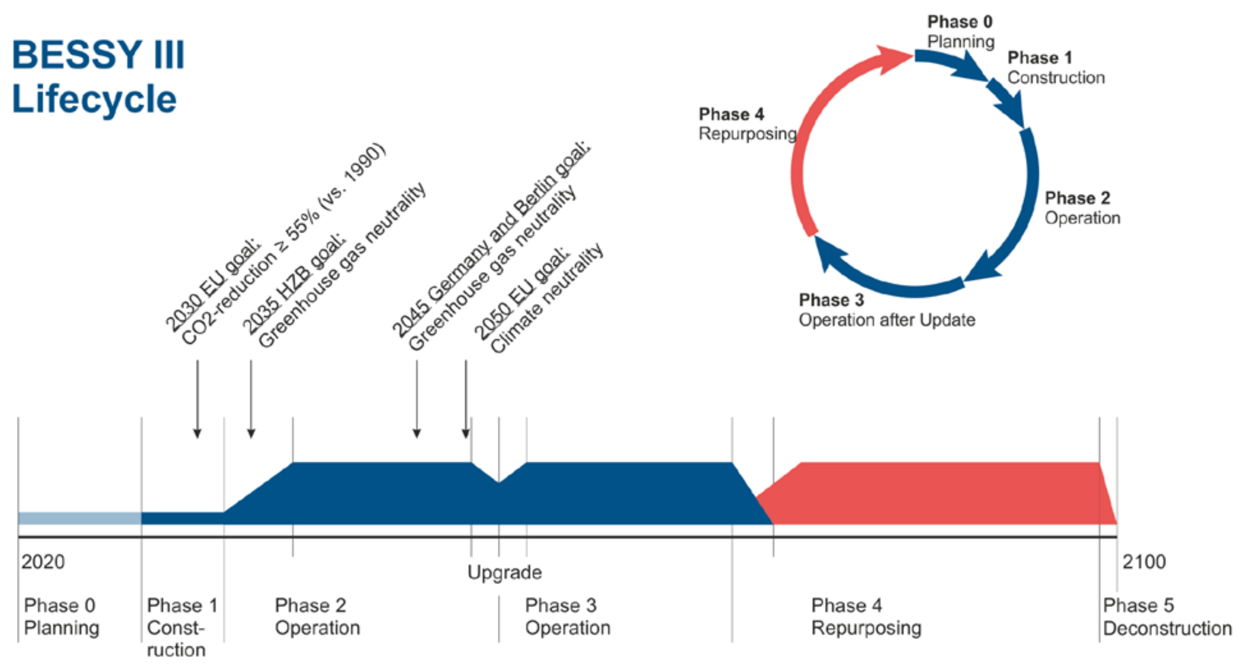


Figure 9.1: Illustration of the **BESSY III** lifecycle with HZB’s, German and EU climate targets marked by arrows.

Sustainable building, sustainable operation

Taking into account the EU target of reducing CO_2 emissions by at least 55 % compared to 1990 levels by 2030 and climate neutrality by 2050, as well as the HZB's goal of greenhouse gas-neutral research by 2035 and Germany's national goal of greenhouse gas neutrality by 2045 (see ↘Figure 9.1), the current planning results in corresponding requirements for the building. With **BESSY III,** HZB is aiming at the highest possible standards of sustainable buildings as defined by the DGNB and BNB (the federal government's portal to the sustainable construction rating system). Both, the DGNB and the BNB evaluation scheme considers the overall performance of a building based on the criteria: environmental and economic quality as well as sociocultural-, functional-, technical-, process-, and site quality.

Determining land requirements in line with realistic needs forms the basis for the economical use of subsoil. During construction of the facility, the focus is particularly on the use of resource-conserving building materials, the construction and operation of a resource-saving and climate-adapted building shell. Energy-efficient building technology and accelerator components in addition to the integration of renewable energies and recycling and reuse of excess heat as well as innovative air conditioning, are intended to make the energy intensive research operation sustainable as depicted in ↘Figure 9.2. Within the accelerator complex we will use permanent magnets for accelerator bending magnets and hybrid magnets for most of the quadrupoles. In addition, in a system approach, we will be an on-site source of renewable energy from e.g. PV and geothermal cooling / heating capacities. A first estimate suggests that the facility can produce an energy equivalent of at least 3 GWh / a. The facility is expected to consume 0 GWh/a of thermal energy through the use of the facilities' waste heat; instead, the surplus heat will be used to supply the entire HZB campus. Possible cooling by geothermal energy is being analyzed and will be verified in the further course of planning. In this way, the **BESSY III** facility will become part of the campus energy system when in operation.

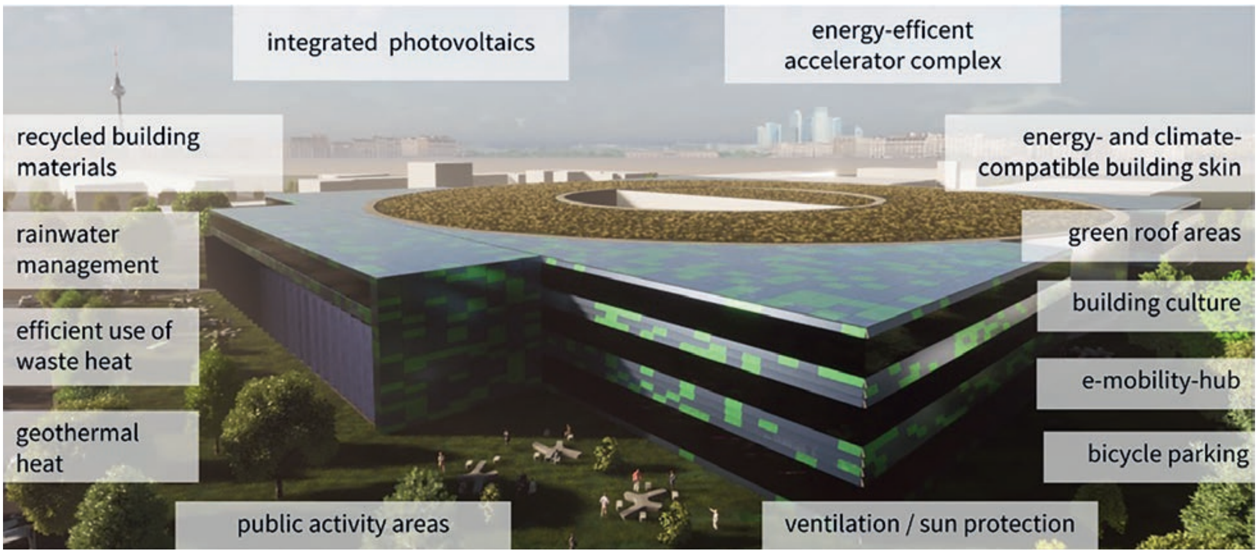


Figure 9.2: BESSY III – a sustainable research infrastructure.

Options for the BESSY II building infrastructure

HZB is planning to expand the site as a logical consequence of the relocation of research activities from the Wannsee campus (LMC) following the decommissioning of the BER II research reactor. At the same time, areas as LMC that become available are to be opened up for scientific activities by and with third parties. The expansion of HZB's Adlershof campus (WCRC) will build on the existing network at the Science and Technology Park Adlershof. The relocation offers the opportunity for better HZB-internal cooperation and the promotion of informal contacts and exchange.

The space at the existing BESSY II campus that will be freed up by the construction of **BESSY III** will be adapted to the new use but can largely continue to be used in its existing form. With the commissioning of **BESSY III,** about 3,700 m^2 of office space and 1,700 m^2 of laboratory space will become available in the existing BESSY II building complex in walking distance to **BESSY III**. In addition, the BESSY II storage ring hall comprises about 8,600 m^2 and can be converted into a combined laboratory and office complex with a capacity up to 16,000 m^2 net floor space according to current projections. These free room and space capacities will be used by HZB as part of the concentration/consolidation of the HZB research activities on the WCRC in Adlershof.

The BESSY II building is ideal to host very sensitive research equipment and lab technology like cryo electron microscopy, e-beam-writing, zone plate and grating production, at wavelength surface finishing of X-ray mirrors, X-ray optics coating technology and even quantum computers. The ring-shaped 0.6 m thick slab of 112 m outer diameter and specific road reinforcements of the Ernst-Ruska-Ufer nearby have been designed for BESSY II to efficiently damp away vibrations from civil noise and traffic.

10. Community

The user community is addressed in various ways, e.g. through the involvement of the German Committee for Research with Synchrotron Radiation (KFS), in regular project updates at the BESSY II User Committee, and on the occasions of the BESSY Users Meeting. The Scientific Motivation was developed on the basis of 15 international expert workshops and foresight workshops that addressed strategically relevant topics for **BESSY III,** e.g. Magnetization Dynamics and X-ray Microscopy, Heterogeneous Catalysis and Chemistry on Surfaces, Correlated Materials and Antiferromagnets, Life Science Research, Materials Design/High-throughput Experimentation, Materials Metrology, Energy storage and Batteries, Energy conversion and harvesting, Information Technology. More than 150 participants contributed their expertise (↘see below).

Scientific Expert Workshop Series, HZB 2020 – 2022 Contributors

The Scientific Motivation was developed on the basis of 15 international expert workshops that addressed strategically relevant topics for **BESSY III.** In addition to the authors and contributors listed in the imprint, more than 150 participants contributed their expertise.

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PTB

Annex

Glossary

AFM Atomic Force Microscopy [23]

AI Artificial Intelligence [17, 19, 29, 42, 43, 47, 54]

ALBA Sunrise in Spanish, ALBA SR facility, Barcelona, Spain [36]

ALS Advanced Light Source, LBNL [32, 36]

APPLE Advanced Polarized Photon Light Emitter [39, 40, 41]

ARPES Angle-Resolved Photo-Emission Spectroscopy [15, 22, 23, 28, 46]

ARPES 13 and 12 BESSY II photoemission stations, ultra high resolution X-ray excitation, electron energy analyser, sample temperature, short: 1meV x 1meV x 1K = 13 and 1meV x 1meV = 12 [45, 46]

ASML Advanced Semiconductor Materials Lithography – https://www.asml.com/en/company [55, 56]

BAM Bundesanstalt für Materialforschung und -prüfung, Berlin [8, 11, 27, 28, 29, 30, 35, 41, 46, 49, 50, 56, 58, 59, 60]

BASF Badische Anilin- und Sodafabrik [56]

BElChem Berlin Joint Lab for Electrochemical Interfaces [30, 45, 48]

bERLinPro The Superconducting Energy-Recovery LINAC Project at HZB [59]

BESTEC Bestec GmbH Berlin [51, 55]

BMBF Bundesministerium für Bildung und Forschung, German Federal Ministry of Education and Research [14, 15]

BNB Bewertungssystem für nachhaltiges Bauen [12, 62]

BORIS Bodenrichtwert Informationssysstem [59]

Care-O-Sene Catalyst Research for Sustainable Kerosene – https://care-o-sene. com/en/ [48, 56]

CatLab Catalysis Laboratory MPG/HZB [8, 20, 22, 48, 49, 50, 56]

CCMS Correlative Microscopy and Spectroscopy CoreLab [49]

CDI Coherent Diffractive Imaging [16, 46]

CDR Conceptual Design Report [36, 38, 41]

CERN Conseil Européen pour la Recherche Nucléaire, European Organization for Nuclear Research, Switzerland [46]

CF Combined Function [37]

CoreLab Complementary Labs at HZB in user operation [48]

cPGM collimated Plane Grating Monochromator [42, 43, 44, 46]

CPMU Cryogenic Permanent Magnet Undulator [32, 33, 39, 40, 41]

cw continuous wave [35]

DALI Upgrade Proposal DALI, HZDR, Dresden [28, 29]

DAPHNE DAta from PHoton and Neutron Experiments [11]

DAPHNE4NFDI consortium consists of experts of the photons and neutrons communities, it interacts with users and scientists at large scale infrastructures as well as with other NFDI-consortia. [53]

DCM Double Crystal Monochromator [42, 43]

DDL Helmholtz Distributed Detector Lab [46]

DECTRIS – DECTRIS Detector company, Switzerland [26, 46, 55]

DESY Deutsches Elektronen-Synchrotron, Hamburg [28, 36, 42, 46]

DGNB German Sustainable Building Council [12, 62]

DLR Deutsches Zentrum für Luft- und Raumfahrt [51]

DOPU Double Period Undulator [33, 41]

EELS Electron Energy Loss Spectroscopy [49]

EGI – EGI Federation, Advanced computing for research, https://www.egi.eu [53]

EM Electron Microscopy [45]

EMIL Energy Materials *In-situ* Laboratory, HZB, Berlin [30, 36, 39, 41, 43, 45, 46]

EOSC European Open Science Cloud [11]

EPICS Experimental Physics and Industrial Control System. EPICS provides a software infrastructure for use in building distributed control systems to operate devices such as Particle Accelerators, Large Experiments, major Telescopes, etc. [52]

ErUM – Data action plan, from Big Data to Smart Data: Digitization in the basic research in the natural sciences [11, 53]

ESA European Space Agency [26, 46]

ESRF European Synchrotron Radiation Facility, Grenoble, France [14]

ESRF-EBS ESRF – Extreme Brilliant Source upgrade, Grenoble, France [8, 10, 14]

ESS European Spallation Source, Lund, Sweden [52]

EU European Union [34, 62]

EUV Extreme Ultraviolet [26, 28, 55, 56]

EUXFEL European X-ray free-electron laser, Hamburg [29]

ExPaNDS European Open Science Cloud (EOSC) Photon and Neutron Data Service [11, 53]

FAIR Findable, Accessible, Interoperable, Reusable (or Repurposable) [11, 17, 27, 34, 41, 52, 53, 54, 59]

FAIRmat FAIR data infrastructure for condensed-matter physics and the chemical physics of solids [11]

FBH Ferdinand Braun Institut für Hochfrequenztechnik, Berlin [50]

FEL Free-Electron Lasers [16]

FHI Fritz-Haber-Institut – Max-Planck-Gesellschaft, Berlin

FIB Focused Ion Beam [16, 46]

FMB Feinwerk und Messtechnik GmbH Berlin [51, 55]

FUB Freie Universität Berlin [45]

FWHM Full Width at Half Maximum [35]

GDP Gross domestic product [20]

GI Grazing Incidence [26, 27]

HDF5 Hierarchical Data Format, a set of file formats designed to store and organize large amounts of data. [48]

HHC Higher Harmonic Cavity [36]

HOA Higher Order Achromat [37]

HOM Higher Order Modes [34, 36]

HPC High Performance Computing [54]

HUB Humboldt-Universität zu Berlin [45, 50, 51]

ICS Industrial Control System [53]

ID Insertion Device [36, 39, 40, 43, 59]

IKZ Institut für Kristallzüchtung Berlin [50]

IR Infrared [26]

ITER International Thermonuclear Experimental Reactor, Cadarache, France [52]

IVUE In-Vacuum undulator, Elliptical polarization [33, 40, 41]

IVUE32 In-Vacuum undulator, Elliptical polarization, with a period length of 32 mm [39]

KFS Committee for Synchrotron Radiation – the body elected by the user community to represent user interests [14, 64]

KIT Karlsruher Institut für Technologie, Karlsruhe [46]

LCLS LINAC Coherent Light Source, SLAC, USA [52]

LEAPS League of European Accelerator-based Photon Sources [9, 28, 36, 45, 46, 48, 53]

LINAC Linear Accelerator [36, 58]

LMC Lise-Meitner Campus of the HZB in Berlin-Wannsee [50, 51, 63]

MAX IV the MAX IV facility, Lund, Sweden [32, 35]

MAXYMUS MAgnetic X-raY Microscope with UHV Spectroscopy [45, 46]

MBA Multi Bend Achromat [22, 29, 31, 35, 36, 37, 38, 41]

MBI Max-Born-Institut, Berlin [50]

MDC Max-Delbrück Zentrum für Molekulare Medizin in der Helmholtz-Gemeinschaft [25]

MEMS Micro-Electro-Mechanical Systems [48]

Micro CT Micro Computed Tomography [27]

ML Machine Learning [43, 51, 52]

MLS Metrology Light Source, PTB [26, 29, 34, 35, 50, 52]

MPG Max-Planck-Gesellschaft [20, 49]

MX Macro-molecular Crystallography [11, 25, 44, 49]

MYSTIIC Microscope for X-ray Scanning Transmission *In-situ* Imaging of Catalysts [46]

NASA National Aeronautics and Space Administration [46]

NEG Non-Evaporable Getter [37, 59]

NEXAFS Near Edge X-ray Absorption Spectroscopy [17, 19]

NeXus NeXus is a common data format for neutron, x-ray, and muon science. It is being developed as an international standard by scientists and programmers representing major scientific facilities in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data. [48]

NFDI Nationale Forschungs Daten Initiative [11, 53, 59]

NMR Nuclear Magnetic Resonance [37]

PEEM Photo Electron Emission Microscopy [45, 46]

PerMaLIC Permanent Magnet LEAPS Internal Collaboration [36]

PETRA III / IV Synchrotron Radiation Facility PETRA III and its planned upgrade PETRA IV, Hamburg [5, 10, 14, 28, 29]

PTB Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin [5, 8, 9, 10, 11, 16, 17, 26, 27, 28, 29, 30, 31, 35, 38, 41, 46, 49, 50, 56, 59, 60, 66]

PV Photovoltaics [60, 62]

R&D Research and Development [50, 55, 56]

RAV Replacement Asset Value [61]

RDA Research Data Alliance [11]

RF Radio Frequency [35, 36, 59]

RI RI Research Instruments, Bergisch Gladbach [34, 35, 56]

RIXS Resonant Inelastic X-Ray Scattering [16, 22, 23, 46]

rms Root Mean Square [35, 36]

RXS Resonant X-Ray Scattering [46]

RZP Reflection Zone Plates [46]

Sasol Sasol – A global chemicals and energy company, https://www.sasol.com [56]

SAXS Small Angle X-Ray Scattering [26]

SEAlab Superconducting rf Electron Accelerator laboratory [35, 50, 56, 59]

SEM Scanning Electron Microscopy [21]

SF Separated Function [37]

SI International System of Units [11, 49]

SIL Safety Integrity Level, see IEC 61508, Functional safety of electrical/electronic/programmable electronic safety related systems, IEC 61511, Safety instrumented systems for the process industry sector, IEC 62061 safety of machinery [53]

SIRIUS the SIRIUS SR facility, Campinas, Brazil [35]

SME Small and Medium-sized Enterprises [55]

SNOM Scanning Near-field Optical Microscopy [26]

SoC System on Chip [52]

SOLEIL Source Optimiśee de Lumìere d'Energie Interḿediaire du LURE (Laboratoire d'Utilisation du Rayonnement Electro-magńetique), the national synchrotron radiation facility in France [32]

SPECS Surface Nano Analysis GmbH [55]

SPM Scanning Probe Microscopy [49]

SR Synchrotron Radiation 10, 11, 15, 17, 18, 19, 20, 21, 25, 26, 27, 29, 31, 32, 34, 45, 46, 48, 49, 50, 56]

SSMB Steady-State Micro-Bunching [35]

STM Scanning Tunnelling Microscopy [23]

STXM Scanning Transmission X-Ray Microscopy [16, 45, 46]

Supralab Superconducting Radiofrequency Laboratory at HZB [35, 50, 56]

SXM Scanning X-ray Microscopy [46]

TDR Technical Design Report [36, 41]

TEM Transmission Electron Microscopy [21, 25]

THz Tera Hertz [26, 28, 45]

TRIBs Transverse Resonance Island Buckets [16, 35, 37, 39]

TUB Technische Universität Berlin [45]

TXM Transmission X-Ray Microscopy [45, 46]

UE Undulator, Elliptical polarization [41]

UHV Ultra High Vacuum [20, 21, 33, 45, 56, 57]

VSR Variable pulse length Storage Ring [35]

VUV Vacuum Ultraviolet [28, 29, 30, 32, 41]

WCRC Wilhelm-Conrad-Röntgen Campus Adlershof [11, 13, 20, 32, 50, 51, 63]

WISTA Wissenschaftsstandort Adlershof [33, 51]

WLS WaveLength Shifter, in its simplest form, a wiggler that contains three magnets [41]

XAS X-ray Adsorption Spectroscopy [28, 49]

XFEL X-Ray Free Electron Laser [25, 29]

XMCD X-Ray Circular Dichroism [35]

XPS X-ray Photoelectron Spectroscopy [49]

XRF X-Ray Fluorescence [27]

XRR X-Ray Reflectometry [26]

XUV Extreme Ultraviolet [30]

Zeiss SMT Zeiss Semiconductor Manufacturing Technology– https://www.zeiss.de/smt [55, 56]

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