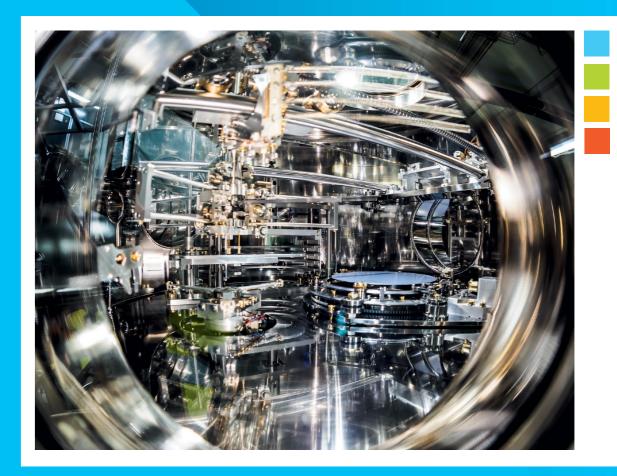


HZB STRATEGY PAPER

Abridgment



NOTES TO THE READER

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A result of the HZB strategy process with participation by heads of the organisational units, the Science and Technology Board, as well as in accordance with the strategic parameters and directives of the Management Board

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Chapters are color coded to ease orientation of the reader:



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HZB 2020+: STRATEGY AND FIRST IMPLEMENTATION STEPS

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1. OUTLINE

The Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB) was founded in 2009 by the merger of the former Hahn-Meitner Institute GmbH (HMI), a member of the Helmholtz Association of German Research Centres e.V. (a registered association) the previous Berliner and Gesellschaft für Elektronenspeicherring Synchrotronstrahlung (BESSY), a member of the Wissenschaftsgemeinschaft Gottfried Wilhelm Leibniz e. V. (Leibniz Association).

The mission of Helmholtz-Zentrum Berlin für Materialien und Energie is to research complex systems of materials for Germany's energy transition, energy storage, and energy efficiency; to operate the BER II neutron source until the end of 2019¹; and to operate the BESSY II photon source in the energy regions of VUV and soft X-ray radiation for the national, European, and international user communities. The research of the HZB takes place within the "Energy" and "Matter" Research Divisions of the Helmholtz Association of German Research Centres (a registered association).

The HZB carries out its mission in an adaptive and forward-looking manner in the evolving socioeconomic and scientific environment. The strategy for its scientific profile and portfolio in the coming years and beyond 2020 has evolved from this directive. It is the result of an intense development process involving all of the scientific organisational units, panels, and committees and has lasted several months. The process has been characterised by the effective merging of pioneering scientific and technical concepts with overall strategic parameters and directives.

Building on the history of the HZB and its antecedents, on the results of the second period of Programme-Oriented Funding (POF II), and on the current positioning of the HZB in POF III, the vision and mission of the HZB for the next 15-20 years

¹ Operation of the BER II neutron source will cease on December 31, 2019 in accordance with the resolution of the Supervisory Board passed June 25, 2013. The HZB will no longer conduct any neutron research thereafter nor operate any neutron instruments at other sources.

has been worked out both at the macro-level and at greater resolution.

Taking the pressing problems of society as its starting point with special attention to the research fields involved in Germany's energy transition, the HZB has identified and parameterised the objectives and areas for action that offer the potential for applying its existing, internationally recognized expertise and unique features to new, scientifically challenging tasks.

Research with and for new materials in energyrelated systems, as well as the on-going operation and continued development of the BESSY II photon source into a next-generation light source are at the core of the HZB strategy. These objectives are intimately bound up with one another. Special weight will be accorded to the interdisciplinary topic of "Theory and Simulation". Additional important topics include questions of the integration and involvement of the HZB in the international research landscape, collaboration with general and technical universities, as well as the transfer of knowledge to the economy and society.

The HZB has authored white papers on its future strategic directions together with a summary executive paper that have been coordinated with and approved by its advisory committees. The Supervisory Board of the HZB has taken note of the papers with approval in its meeting of June 3, 2015.

The Shareholders of the HZB, which are the German federal government and the State Government of Berlin, requested for а Perspectives Commission (PC)² in order to assess the development of the HZB since its founding through the fusion of its antecedents along with its future strategic orientation within the research policy and scientific environment, as well as to formulate recommendations. Members of the PC included representatives of the Shareholders, directors of Max Planck Society (MPS) and large research institutions in Switzerland and Great Britain, the chair of a large German industrial concern, as well as a representative of the German national metrology institute (PhysikalischTechnische Bundesanstalt/PTB)³ as one of the strategic partners of the HZB.

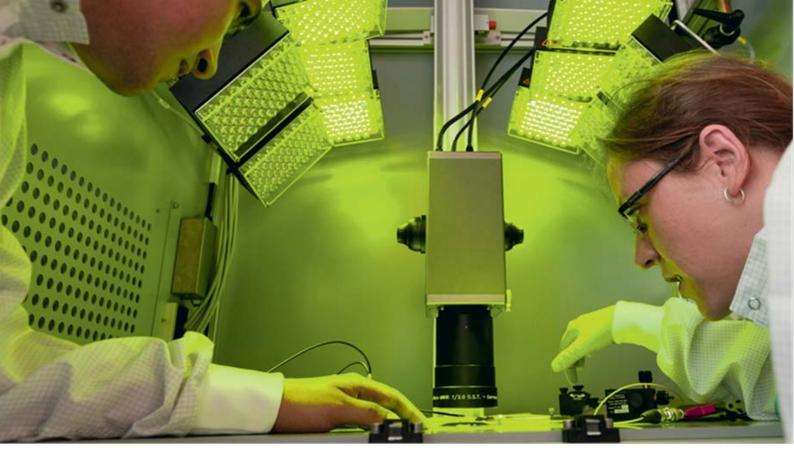
The PC informed itself about the HZB beginning with the strategy papers, through the management board of the HZB, as well as through scientists in management positions and those at earlier points in their careers. The Perspectives Commission also heard from representatives of important collaborating partners of the HZB and the coordinators of the "Energy" and "Matter" Research Divisions of the Helmholtz Association.

The final assessment by the PC on the development of the HZB following its founding and for its future strategic orientation was forwarded to the HZB from the Shareholders on Nov. 19, 2015. The PC indicated it was very impressed with the development of the HZB during the six years since its founding. It shares the views of the HZB on its future strategic orientation. The focus of the HZB on its in-house research and development of energy materials was persuasive to the PC. They articulated their recommendations regarding the materials portfolio, technology transfer, the continued development of the major scientific facilities, as well as the decommissioning of BER II. The linkage of energy materials research with the current capabilities and future potential of the BESSY II photon source was deemed a unique feature of the HZB. The realisation of BESSY-VSR as an upgrade to BESSY II was viewed as a significant development for the future of BESSY II and storage rings worldwide. The PC was also very impressed with the young scientists of the HZB and viewed the measures put in place by the HZB for compatibility of career and family as exemplary.

With the approval provided by the Perspectives Commission, the HZB has also been called upon to make a brief presentation and outline of the intended steps for implementing its strategy available to the Senate of the Helmholtz Association. That is the genesis of this paper. It has been coordinated with and approved by internal and external committees of the HZB, the partnering institutions of the HZB, as well as the Helmholtz Association.

² The employment of the Perspectives Commission was agreed upon as part of the fusion process (or merger of HMI GmbH and BESSY m.b.H.).

³ PTB: Physikalisch-Technische Bundesanstalt. The PTB utilises BESSY II as the European radiation standard. It uses specialised beamlines at BESSY II and the PTB's own source, named the Metrology Light Source, for research and contracts from industry. The Metrology Light Source was built by the HZB and is operated by the HZB.



2. INITIAL STATE OF THE ORGANISATION

Energy materials research; photon and accelerator research; operation of BESSY II and BER II

The HZB pursues the mission of the Helmholtz Association⁴ and the principle of leading with its strengths.

The HZB contributes to the "Energy" Research Division programmes in POF III (2015-2019) under Performance Category I (LK I)⁵ of the strategic programmes of the Helmholtz research Association.

- RE: "Renewable Energy" (topics: Photovoltaics, Solar Fuels),
- EMR: "Energy-efficient Material Resources" (topic: Methods and Designs for Materials Development),
- FIT: "Future Information Technologies" (topics: Controlling Spin-based Phenomena, Controlling Collective States), and

⁴ "We contribute to solving grand challenges which face society, science and industry by performing top-rate research in strategic programmes in the fields of Aeronautics, Space and Transport, Earth and Environment, Energy, Health, Matter as well as Key Technologies.

We research systems of great complexity with our large-scale facilities and scientific infrastructure, cooperating closely with national and international partners.

We contribute to shaping our future by combining research and technology development with perspectives for innovative applications and provisions for tomorrow's world.'

[[]https://www.helmholtz.de/en/about_us/the_association/missio

⁵ The Helmholtz Centres focus their research and development activities within the programme and work on their own scientific problems. These activities are designated as inhouse research and are classified as Performance Category I (LK I). In contrast, the operation of large-scale scientific facilities represents a separate and independent Performance Category, LK II. BER II as well as BESSY II count as Performance Category II.

 SCI: "Storage and Cross-linked Infrastructures" (topics: Electrochemical Storage).

In the Research Division of "Matter", it contributes to the following programmes:

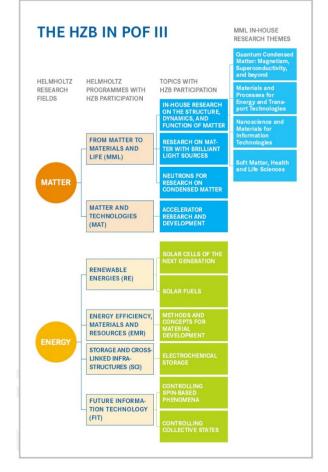
- MML: "From Matter to Materials and Life" (topics: in-house research on the structure, dynamics, and function of matter),
- as well as MaT: "Matter and Technologies (topic ARD: Accelerator Research and Development).

In accordance with the mission of the Helmholtz Association, the HZB also operates large, complex infrastructure for the national and international user communities (Performance Category LK II). During POF III, these are the BESSY II photon source and the BER II neutron source. Approx. 1800 instrument-days on average are available annually at the BER II medium-flux neutron source for users; 10 instruments are operated. BER II was utilised by about 240 individual researchers in 2014. The HZB is specialised in extreme sample environments; this includes a unique high-field magnet with a maximum field strength of about 26 Tesla. The BESSY II photon source for VUV / soft X-ray radiation is a "world-class soft X-ray facility" 6. About 5600 instrument-days on average are available to users; it was utilised by about 840 individual researchers in 2014; the HZB operates 46 beamlines (25 simultaneously).

The HZB has entered into thematic contractual collaborations with universities and non-university research institutions. These collaborations also form an effective network for the future development of the HZB.

The HZB concentrates on energy materials research, methods and development of instruments for conducting research with soft X-ray radiation, as well as accelerator research and development.

The strengths in these areas are the basis for future strategy and will be described in greater detail below.



The HZB contributes to a total of six prorgrammes in the Research Divisions of "Energy" and "Matter" under POF III.

⁶ Vote of the reviewers from the POF III evaluation.

2.1 HZB 2015: ORIENTATION TOWARD ENERGY MATERIALS RESEARCH

The HZB possesses the following key expertise in energy materials research:

- fabrication and analysis of thin-film systems for energy technology applications,
- employment of a broad portfolio of materials for customised systems and modules,
- development and application of unique insitu and operando methods of characterising materials by means of X-ray radiation.

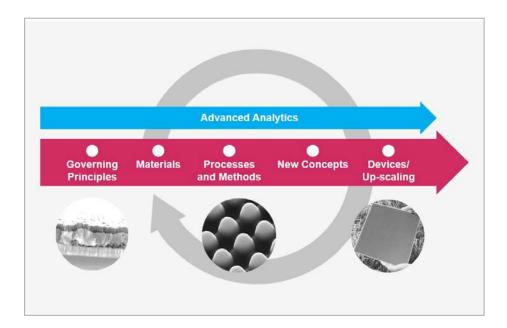
This key expertise individually and combined represents a unique feature of the Centre.

Focus on thin-film systems for energy materials. Synergies with research using soft X-ray radiation

2.2 HZB 2015: LEADING IN EUROPEAN MATERIALS RESEARCH FOR PHOTOVOLTAICS

The HZB occupies 3rd place worldwide and 1st place in Europe in the Elsevier ranking of publications in its Alternative Energy Research Leadership Study⁷. The HZB received highest ratings in the POF II and POF III reviews for the topic of photovoltaics jointly addressed with Forschungszentrum Jülich (FZJ). The materials and processes portfolio of the HZB comprise all of the important inorganic thin-film materials and was expanded to include hybrid inorganic/organic materials in POF III.

The HZB has a complete chain of expertise, from basic research, to fabrication of materials, to fabrication process lines for scaling up to prototypes⁸. Companies that produce equipment and modules for photovoltaics, as well as manufacturers of other complex functional thin-film systems (for instance for thermal insulation) are examples of collaborating partners and customers for joint development projects. These include many German and European companies involved in facility construction in particular.



HZB 2015: Focus on energy materials, broad material portfolio, unique in-situ and inoperando analytical capabilities, and synergies with research using soft X-ray radiation.

⁷ https://www.elsevier.com/about/pressreleases/corporate/elsevier-releases-results-of-alternativeenergy-research-leadership-study-identifying-top-25institutions-worldwide. ⁸ In the Photovoltaics Competence Centre PVComB, an institute of the HZB.

The HZB and FZJ have created a joint research programme for POF III that takes advantage of the complementary strengths of both partners and was evaluated by the reviewers as outstanding.⁹ The HZB is connected with the Fraunhofer Institute for Solar Energy Systems (ISE) through many collaborative projects. The HZB is stronger in basic research while direct cooperation with industry and contract research is ISE's forte.

2.3 HZB 2015: INTERNATIONALLY **RECOGNISED RESEARCH ON PHOTO-**ELECTROCHEMICAL GENERATION OF SOLAR FUELS

The HZB has already achieved an international profile for its new research area of solar fuels¹⁰ thanks to its expertise in the design and fabrication of complex multinary oxides and custom-tailored interfaces, analysis of catalytic processes, as well as in PV technologies. The HZB has outstanding partners in Berlin in the field of catalysis, including the Fritz Haber Institute (FHI) of the MPG as well as the Einstein Center for Catalysis. The HZB participates there with projects and with one of its departmental heads as principal investigator. The HZB, together with its partners (including FHI of the MPG and the Leibniz Institute of Surface Modification IOM/Leipzig¹¹), has created several specialised and unique means of characterising systems and subsystems relevant to the generation of solar fuels both in-situ and inoperando.

The HZB coordinates the "Solar Fuels" research topic within the Helmholtz Association. It is pursuing strategies with its photo-electrochemical approaches that are complementary to the thermochemical approaches of the German Aerospace Centre (DLR) and artificial photosynthesis of the Helmholtz Centre for Environmental Research (UFZ).

2.4 HZB 2015: SOFT X-RAY RADIATION. A **KEY TO ENERGY MATERIALS RESEARCH**

Important processes for energy conversion and storage take place at surfaces and interfaces. VUV and soft X-ray radiation uniquely offer the necessary atomic specificity and chemical selectivity for characterising these processes. The HZB through its BESSY II infrastructure provides a dedicated portfolio of instruments and spectroscopic methods for this.

The HZB meets the special challenge of investigating the systems under realistic conditions during fabrication and reaction (in situ and in operando) through having set up dedicated and sometimes unique instruments at BESSY II. These instruments facilitate studies that include fluids and solid-fluid interfaces relevant to catalytic processes for generating solar fuels.

Functionality is always coupled to length scales. The HZB possesses the expertise to fabricate and characterise energy materials from the atomic level, to molecular systems, to interfaces, multiple layers, and modules. One of the challenges is the integration of in-situ and in-operando methods for the characterisation of suitable specimen sizes and handling of the systems (mostly under high vacuum). The HZB has set up a unique infrastructure with its Energy Materials in-situ Laboratory (EMIL) at BESSY II.

The characterisation and control of dynamic processes in systems for energy conversion and storage as well as in systems for energy-efficient information technology (IT) ¹² require methods having temporal resolution in the picosecond to femtosecond range. The HZB has set up the FEMTOSPEX experimental stations at BESSY II especially for measuring these kinds of ultrafast processes¹³.

The HZB and its strategic partners have expanded the beamlines and experimental stations at BESSY Il effectively (see Chap. 2.7). This, and the opportunity to use the Centre's own complementary labbased methods, have continually increased the

⁹ Meeting of the Helmholtz Senate Commission Research Field "Energy" in Berlin on September 10, 2014 and Meeting of the Helmholtz Senate Research Field "Energy" in Berlin on October 17, 2014.

¹⁰ Solar fuels are artificially manufactured chemical energy media produced through utilisation of sunlight.

¹¹ Leibniz Institute of Surface Modification (IOM).

¹² For example, the motion of charge carriers, the progress of chemical reactions, or switching processes in storage materials.

The electron beam pulse structure in the storage ring at BESSY II is modulated for this purpose by interaction with a short-pulse laser and employed for investigating ultrafast switching processes and ordering phenomena in complex materials. The shortest pulses for European ring sources were realised at BESSY II in this way.

proportion of energy research experiments of the user community¹⁴.

2.5 HZB 2015: TECHNOLOGY AND INNOVATION FOR RESEARCH WITH SOFT X-RAY RADIATION

All of the experimental stations at BESSY II are optimised – from the source of the soft X-ray radiation (storage ring and undulators), to the beamline (optics), and the sample position (methods and sample environment). The HZB has developed unique and internationally recognised features in these fields:

SOURCE

The HZB has invested continuously in developing the BESSY II storage ring since the merger¹⁵ so that BESSY II is state-of-the-art. The associated development of the operating team has ensured that the operation of BESSY II is at an international level of quality and reliability. One unique feature of BESSY II is the successful implementation of new fill patterns and innovative processes for pulse separation (MHz chopper, pulse picking by resonant excitation, and island buckets) that make the short pulses at the beamlines and measurement stations usable for all the experimenters.

UNDULATOR DEVELOPMENT

The HZB develops and builds new undulators. These include the APPLE II undulators that allow complete polarisation control of the photons. To tap the tender X-ray region (2 - 8 keV) with high photon flux, new cryogenic vacuum undulators are currently being developed that are cooled down to the temperature of liquid nitrogen¹⁶.

OPTICAL COMPONENTS AND BEAMLINES

The basis of all beamlines at BESSY II is a modular set up of largely standardised precision mechanical components (mirror chambers, monochromators, and optical splitters).

The HZB develops systems and technologies for manufacturing optical gratings at very high line densities for monochromators and delivers these gratings to synchrotron radiation sources worldwide.

DEVELOPMENT OF METHODS AND INSTRUMENTS

With its new beamlines and measurement stations for resonant inelastic X-ray scattering (RIXS) and coherent X-ray scattering (CXS), the HZB has created unique means of investigating the time and energy domains of complex materials. Through its LIXedrom instrument, the HZB has successfully moved spectroscopy of liquids into user service (including analysis of catalytic processes). The HZB leads the world in X-ray microscopy that is using integrated absorption spectromicroscopy.

2.6 HZB 2015: LARGE-SCALE INFRASTRUCTURE FOR THE INTERNATIONAL USER COMMUNITY

In the operation of its **BESSY II** and **BER II** largescale research infrastructure the HZB takes into account the interests and needs of the user community constantly and steadily. The HZB advises users during more than 3000 visits to its facilities per year. Users receive beam time allocated by a peer review procedure in which the external international evaluators select the best proposals.

All the HZB organisational units that operate beamlines and measurements stations at BESSY II and BER II use them as well for their own research and in this way incorporate their scientific expertise in advising users.

Complementary, technically complex laboratory infrastructure supplements this service. External scientists can use the synthesis and characterisation labs of the HZB. Laboratories for sample preparation and complementary measurement techniques, referred to as LabClusters, are available in connection with proposals for beam time at BESSY II and BER II.

¹⁴ The proportion of energy research amounted to about 30 %, key technologies to about 25 %, and life sciences to about 25 % in 2014.

¹⁵ Including a new linear accelerator (LINAC), replacement of

the HF transmitter, and cavities.

¹⁶ These will be used in EMIL for the first time.

2.7 HZB 2015: WELL-CONNECTED – REGIONALLY, NATIONALLY, AND INTERNATIONALLY

Since its inception, the HZB has closely associated itself institutionally with the universities, technical universities, and non-university research institutions in the Berlin / Brandenburg region (FHI / CEC of the MPG, PTB, and the German Federal Institute for Materials Research and Testing/BAM).

Strategic partnerships with Freie Universität Berlin and the Humboldt Universität zu Berlin have developed under the Excellence Initiatives. Policy instruments for cooperation with the institutions of higher learning include joint appointments, Joint Research Teams, and graduate schools.

The HZB has established a new model of partnership with universities and non-university

institutions through the Berlin Joint Labs. The foundation for a Joint Lab is the common research interest of the partners, the joint operation of infrastructure (either large-scale facilities or in complex laboratories), and common support programmes for junior researchers¹⁷.

The HZB makes its BESSY II and BER II largescale facilities available to the international user community. It collaborates at the international level with 23 partner institutions from 17 countries in research, technological development, and the exchange of scientific and technical personnel. The collaborations with partners from the European research sphere as well as with universities and non-university partners from the USA are particularly strong.



The annual HZB User Community meeting supports exchanges between international User Groups and with the HZB

Institute for Molecular Pharmacology (FMP). The state of functional materials can be investigated at the lowest possible doses of X-rays in UBjL. Additional methods allow detailed grasp of the electronic structure of energy materials.

¹⁷ Examples include the Uppsala Berlin Joint Laboratory (UBjL), and the Joint Macromolecular Crystallography Lab (MX-Lab) with Humboldt Universität zu Berlin (HU), Freie Universität Berlin (FU), the Max Delbrück Center for Molecular Medicine in the Helmholtz Association (MDC), and the Leibniz



3. HZB 2020+

Strategy and initial implementation steps

As part of the strategic process, the HZB has formulated the following as its mission:

- We perform use and user inspired energy materials research for a sustainable, economic and secure energy system. Our approach encompasses basic principles, guided design, synthesis and analysis of materials using dedicated infrastructures, as well as the transfer to application. We make our infrastructures available to our users and collaboration partners. We therewith provide know-why and knowhow for the society.
- We design, develop and operate worldclass large-scale infrastructures for photon-based and energy materials research. We provide these infrastructures

for the needs of the national and international scientific communities. We stand for expert user service based on our leading research activities within the framework of our participation in the programs of the Helmholtz-Association.

 We conduct top-level accelerator research and development, from theoretical concepts to operating machines. We collaborate with universities and nonuniversity research institutes. We are an active partner in the regional, national and international research communities. We make our knowledge and our results available to others through pro-active transfer to industry and society as well as education and promotion of young scientists and professionals.

3.1 GOALS FOR 2020+

In the 2020+ period, the HZB will be dedicated to energy materials research, the operation of the BESSY II / BESSY VSR photon source for the national and international user communities, research with soft X-ray radiation, as well as to accelerator research.

The chief challenges are:

- Maintenance and expansion of internationally competitive energy materials research, adaptation of the materials portfolio, and technological, scientific, and economic advancements
- Advanced development of BESSY II as a leading VUV / soft X-ray source for the national and international user communities
- Best possible transfer to the economy and society for increasing growth and the standard of living
- Support for mobility of staff to new areas of endeavour

The HZB has defined the following Centrewide goals for 2020+:

HZB is a world-class research centre for energy materials research, thus contributing to knowledge-based solutions to great societal challenges.

HZB provides world-class large-scale research infrastructure for the national and international scientific communities and industry.

HZB exploits synergies by integrating excellent research with the operation of dedicated infrastructures, thus creating a unique research environment

The HZB has defined specific goals derived from the above (Sections 3.2 - 3.6).

3.2 HZB 2020+: LIGHTHOUSE OF ENERGY MATERIALS RESEARCH

New materials and processes are the foundation for new products. The HZB is focussed on research for energy materials that promise innovations for efficient energy conversion and usage, for energy storage, and energy-efficient IT, thereby contributing significantly to Germany's energy transition.

In contrast to the activities of other Helmholtz Centres in the energy research field, the HZB concentrates on energy materials research and functional materials that take the form of thin-film systems. Important future applications of thin-film systems consist of the generation of fuels and energy-efficient data storage based on spintronics, for example. The HZB is working closely with partners like Forschungszentrum Jülich (FZJ), the Karlsruhe Institute of Technology (KIT), and the German Aerospace Centre (DLR) mostly at the level of fundamental research, and collaborates as well with additional Helmholtz Centres for synergies in energy materials research.

The goals of the HZB for energy materials research are:

- Goal EM-1: Discover governing principles for novel functionalities in Energy Materials
- Goal EM-2: Tailor materials and processes for energy-relevant devices
- Goal EM-3: Develop materials, processes, and prototypes relevant to industry

And predominantly

Goal EM-4: Create synergetic effects and uniqueness by (large scale) unique infrastructures operated for national and international users, characterise on all relevant length and time scales and link experiments and simulations (model-based material design)

To achieve these goals, the HZB has formulated the following measures for energy materials research in the 2020+ period.

MEASURE A

Continual advancement of research topics that are congruent with the core expertise and strengths of the HZB. On-going critical review and evaluation of research topics and modification of the priorities and tasks of topics as needed.

Implementation: Research results will he presented during Scientific Retreats each year and critically considered also with respect to the achievement of the POF goals. To continually adapt the research portfolios to the challenges and opportunities in energy materials research, the HZB will subject the on-going activities to a task critique and carry out "Foresight" processes every two years. In the short term, photovoltaic research will be subjected to a critical analysis with respect to its scientific potential and medium-term market importance. Key topics for the future include tandem and triple devices. The HZB will maintain and utilize its leading role in thin-film photovoltaics and in the application of soft X-ray radiation to further expand research on fabrication of solar fuels in a rapid and internationally competitive manner. To this end, dedicated instruments will be created under the "Berlin Lab Joint for Electrochemical Interfaces (BEIChem)" with partners from the MPG and universities 18 at BESSY II and BESSY VSR. Topics that the HZB addresses include the characterisation and improvement of defect structures in material systems for photo-electrochemical fuel production (appointments in progress) as well as the simulation of processes at the system level and system integration.

MEASURE B

Establishment of new research topics. The HZB has defined topic clusters for this purpose that build on core expertise in thin-film technology, synthesis

and characterisation, as well as on the synergies with research using soft X-ray radiation.

Implementation: The HZB is augmenting its modelling and simulation capabilities, for example knowledge-based materials bv synthesis particularly for fuel production. In accordance with the recommendations of the Perspectives Commission, the HZB is studying chemical energy storage (not battery research) as a new research area and banks on synergies from research with soft X-ray radiation and the complementarity to the existing activities in the Helmholtz Association.

MEASURE C

Design and expansion of dedicated, often unique research infrastructure for energy materials research. This infrastructure will be operated for the national and international user communities.

Implementation: The HZB will further develop its complex laboratory infrastructure for energy materials research based on the needs of the user community and will open it to external users. In doing so, the HZB will build upon its expertise in operating large-scale infrastructure acquired through BESSY II and BER II. The HZB will focus and expand expertise in materials synthesis within Helmholtz Energy Materials the Foundry (HEMF) ¹⁹. Α corresponding facility for characterisation will be established by the Helmholtz Energy Materials Characterisation Platform (HEMCP). Unique potential for in-situ and in-operando materials synthesis and characterisation at BESSY II and BESSY VSR will be developed by the Energy Materials In-situ Lab (EMIL). For research on nanostructuring of energy materials, the HZB is opening the Zeiss lab@location with state-of-the-art instruments and methods for the user community (see also Section 3.4).

¹⁸ Joint Labs: see Section 2.7

¹⁹ The HZB is in charge of the strategic development investment as the foundation for this infrastructure within the Helmholtz Association.

Overarching Goal 4 Synergy, Infrastructures and Simulations		
Goal 1	Goal 2	Goal 3
Governing principles	Tailoring materials	Develop processes and prototypes
Measure A: Portfolio evaluation	1	Pa
Measure B: New research ther	nes	
Measure C: Dedicated infrastru	ctures for Energy Materials Research	
Measure D: BESSY-VSR and I	BESSY III for Energy Materials Researc	h 🧿

Goals and accompanying measures for energy materials research of the HZB.

MEASURE D

Advanced development of BESSY II to BESSY VSR and the preparation of a next-generation light source for soft X-ray radiation beginning 2028+.

Implementation: BESSY VSR will create unique new potential for energy materials research with soft X-ray radiation. The HZB has submitted a scientific case and a technical design study (TDS) for BESSY VSR as well as applied for strategic development investment from the Helmholtz Association. These efforts were all assessed as excellent in evaluations. The Perspectives Commission views the realisation of BESSY VSR as central to the strategy of the HZB and expressly supports this. The HZB will work toward concrete financing approval as the next step (see Chapter 3.3). With regard to a next-generation light source, the HZB is attentively following accelerator technology for light sources and actively communicating with its user community in order to take the next steps for identifying the different phases in the life cycle of such infrastructure²⁰ as

a preliminary project in accordance with the definition by the German Council of Science and Humanities.

HORIZON 2030

From today's perspective, the questions raised about progress on the technical and economic efficiency of energy conversion and storage as well as energy-efficient information technology are of great relevance. Based on its core expertise in thinfilm technology, in energy materials research for the field of renewable energy, solar power, solar fuel production, and chemical energy storage, the HZB wants to have assumed a leading role globally in 2030. At the same time, the HZB will also maintain sufficient flexibility in the future through its generic research topics and its expertise throughout the value-added chain - from materials design to components - in order to address new social challenges as necessary. It is conceivable, for example, that guestions about the life cycle and sustainability of energy materials, components,

German Council of Science and Humanities, 2013, German accounting standards/DRS 2841-13_engl

²⁰ Report on the Science-driven Evaluation of Large Research Infrastructure Projects for the National Roadmap (Pilot Phase),

and systems might become priorities.

3.3 HZB 2020+: BESSY VSR - THE BEST INFRASTRUCTURE WORLDWIDE FOR ENERGY MATERIALS RESEARCH USING SOFT **X-RAY RADIATION**

The HZB is constantly developing BESSY II in all areas. These areas are the storage ring, the beamlines, and the measurement stations. The strategic objective is to maintain the unique features of BESSY II in energy materials research that have already been achieved, add on new features, and thereby make the best possible means for the user community to conduct their research.

The goals of the HZB for the advanced development of BESSY II as a leading VUV / soft X-ray source for the national and international user communities are:

- Goal SR-1: Make BESSY II a world leader BESSY through VSR and modernisation of the instruments
- Goal SR-2: User service at BESSY II / BESSY VSR recognised as outstanding worldwide
- Goal SR-3: Preparation for the next-generation light source (see Chapter 4)

The most	
important	"The close coupling of
component	energy research and
for the mid-	large-scale facilities offers
term	0
strategy of BESSY II is	unique opportunities for
its upgrade	research and is expressly
through	supported by the PC.

Statement of the Perspectives Commission on the importance and involvement of BESSY II

midterm of ll is grade rough realisation of the unique **BESSY VSR** design ²¹. This design

builds on the years of experience at the HZB in beam dynamics of short pulses in storage rings and the expertise in the area of continuous wave (CW) superconducting accelerators. BESSY VSR will enable materials - particularly energy materials to be studied with high photon fluxes and information about supplementary dynamic processes to be simultaneously obtained using short pulses. This will allow access to the systems dynamics using X-rays on time scales of a few picoseconds down to a few hundreds of femtoseconds - which are otherwise hardly accessible with storage rings. The HZB is thus advancing its strategy of facilitating maximal flexibility for its users in relation to pulse lengths and temporal structure for soft X-ray radiation at every beamline. BESSY VSR will extend the high average brilliance of the existing BESSY II multiuser light source to the shortest pulses at high repetition rates. BESSY VSR thus creates the link between the extremely high brilliance of the diffraction-limited storage rings (DLSR with long pulses such as MAX IV and PETRA III) and the free electron lasers (such as FLASH and XFEL for example).

BESSY VSR will be the international high-profile photon source for researching materials used for magnetic, electrical, and optical switches, for catalysis, photovoltaics, and the production of solar fuels.

Superior accelerator research is indispensable for realising these kinds of developments. The HZB will develop and operate a new experimental accelerator in 2020+ called the Berlin Energy Recovery Linear Accelerator Prototype (bERLinPro) that will be unique in this energy and performance range.

FIRST MEASURES:

- The HZB has successfully placed BESSY-VSR on the Helmholtz Roadmap for largescale infrastructure and introduced the project into the selection procedure for strategic development investments of the Helmholtz Association.
- Strengthening its own contribution to BESSY VSR: A total of 7 million Euros will be expended from investment funding

²¹ The combination of two superconducting cavities driven at different frequencies has permitted for the first time the simultaneous storage both of conventional long electron bunches as well as of additional very short electron bunches in

the ring. The latter create short light pulses of only a picosecond. Users can choose between long and short pulses for all experiments in the storage ring by using "pulse-picking" methods that have already been tested.

repaid from the Helmholtz Association (for investments of < 2.5 million Euros) and utilised for BESSY-VSR during the 2018-2020 period. The HZB has appropriately adjusted its medium-term finance planning and is examining opportunities to tap additional financial sources.

- Increased operational flexibility of BESSY: BESSY II can also provide "dual track" operation. In this mode, individual bunches of electrons circulate on another orbit in the storage ring than the majority of the electron bunches. This is a significant prerequisite for additional adaptability of BESSY VSR operations also, in that individualised selection of short and long pulses at every beamline becomes possible.
- Development of technology: Diagnostic methods and superconducting highfrequency cavities in R&D projects under the ARD topic ²² that will probably be beneficial for the realisation of BESSY VSR. The initial prototypes are already

under construction.

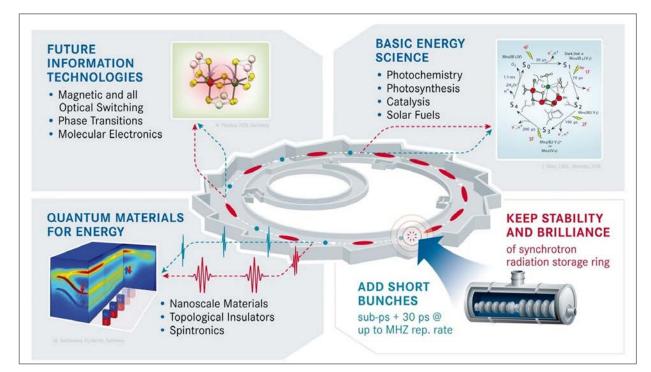
The HZB will also continue to expand services for the user community of BESSY II and BESSY VSR as one of its core

responsibilities, as with all of its infrastructure. This also comprises an extended range of services for new user groups that have little to no experience in carrying out experiments at storage rings. Theory and simulation will represent

"In particular, the means and potential for making temporally resolved measurements ... are of great interest for energy research."

Statement of the Perspectives Commission on BESSY VSR.

additional building blocks for this extensive user service. The HZB will primarily involve theoretical support by means of collaborations in order to carry out evaluation and interpretation of empirical data on the one hand, and on the other to facilitate the development of new methods or the setup of



Superconducting cavities in the storage ring simultaneously generate both long and short light pulses in BESSY VSR.

²² ARD: Accelerator Research and Development, topic of the Matter and Technologies (MaT) programme.

scientific experiments. To support staff in advising users, the HZB will promote staff mobility and continually obtain additional expertise from the BER II neutron source environment for this purpose, particularly after 2020.

3.4 HZB 2020+: STRATEGIC PARTNER FOR INDUSTRY

The development of new materials and device architectures is an important foundation for future energy production and storage at high efficiencies. Results from these areas are then incorporated into developments important for industry via collaborative relationships.

The goal of the HZB as a strategic partner for industry is:

To make best possible usage of scientific knowledge for increasing growth and the standard of living.

MEASURE 1

Facilitate the increase of innovation through basic research

Implementation: The HZB will expand and augment its contact with the economy through its large-scale research infrastructure and the associated user service. The HZB has introduced organisational changes in order to anchor Technology Transfer in the scientific departments of leading scientists with industrial experience. Short-term supplementary resources will be made available for Technology Transfer. Besides direct Technology Transfer, companies can expect consulting services, integration in externally funded projects, and education of specialised staff by HZB.

MEASURE 2

Transfer of new developments to the economy and society

Implementation: The HZB is already wellpositioned for transferring new developments to the economy and society (for example through infrastructures like the Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin (PVcomB)²³). The generic process capabilities for lithography and the integral thin-film technology will be augmented by the HZB through PVcomB 2020+ for the area of solar fuels. In this instance, the HZB will offer the entire process chain, from theory, to basic research, to applications-oriented research, upscaling for industry through to Technology Transfer for mass production.

MEASURE 3

Strengthen direct collaboration with industrial companies.

Implementation: The HZB will establish an Industry Advisory Council that will explicitly bolster activities with industry. With the help of this new committee, the HZB will assess the industrial applicability of its energy materials and devices and prioritise those projects offering promise for future applications.

The Zeiss lab@location, which will be fully established in 2020+, is exemplary for direct collaboration with companies. This laboratory infrastructure will be equipped with the newest microscopy systems from ZEISS. lab@location will make available state-of-the-art imaging and process engineering of three-dimensional nanoarchitectures for energy conversion. HZB experts and specialists from ZEISS will jointly support academic and industrial collaborative partners. The ZEISS lab@location at the HZB will be integrated into HEMF.

3.5 HZB 2020+: SHUTDOWN OF BER II AND PREPARATION FOR DECOMMISSIONING

The Supervisory Board of the HZB decided on June 25, 2013 to carry out permanent shutdown of the BER II neutron source as of December 31, 2019. It determined that the HZB will not operate any instruments at other neutron sources beyond the end of 2019. The financing of the decommissioning is no longer the responsibility of the HZB. That fraction of funding resources that becomes available after the shutdown and remains in the Centre will be invested by HZB in advanced developments of BESSY II and new tasks in energy materials research²⁴.

²³ Thin-film photovoltaic technologies and products are jointly developed with industry at the Competence Centre Thin-Filmand Nanotechnology for Photovoltaics Berlin (PVcomB). Technology and knowledge transfer takes place through

research projects with industrial partners as well as through education of highly qualified specialists.

²⁴ The German Federal Ministry of Education and Research (BMBF) and the HZB have agreed that the HZB will no longer receive a proportion of the previously earmarked operating

The goals of the HZB for operating BER II until 2020 and the decommissioning of BER II presumably beginning in 2023 are:

- **Goal NE-1:** To operate BER II until December 31, 2019 and to optimally use of the High-Field Magnet
- **Goal NE-2:** To begin decommissioning BER II as quickly as possible

The HZB will operate BER II with the ten most competitive instruments (in accordance with the assessment of external experts and involving the Science Advisory Board of the HZB) for the international user community. The High-Field Magnet (HFM) will have special priority during this period; the HFM provides a continuous magnetic field of up to 26 Tesla that can be combined with temperatures down to 0.6 Kelvin. Experiments with neutrons are currently being conducted. The sample position is accessible for other measurement methods as well though. The HZB has developed the scientific case for its utilisation with neutrons as well as with other types of probes and is jointly studying with its external committee possible future prospects for the HFM as well as for the instruments being operated at BER II. The HZB will continue with the "Preparation for Decommissioning" project begun in 2014 in order carry out the decommissioning of BER II as quickly as possible (probably beginning 2023 at the earliest) following removal and transport of the combustion elements. The "Preparation for Decommissioning" project (with subprojects such the documentation and as compiling communications, for example) will be carried out according to the obligatory project management rules of the HZB.

3.6 HZB 2020+: FLEXIBLE ORGANISATION CREATES PROSPECTS FOR STAFF MEMBERS

The HZB adapts its organisational structure, personnel planning, and investment planning continuously to its responsibilities in the sense of "Change Management". For this purpose, the HZB has set the following goals:

Goal OR-1: Periodic adaptation of the organisational structure to the tasks of research and the responsibilities for developing and operating the largescale infrastructures

- Goal OR-2: The HZB is attractive for staff worldwide
- Goal OR-3: Support of mobility of staff into new areas of endeavour

The task critique of the organisational units takes place in a three-year cycle. Particular attention has been given to the mapping of the POF programmes onto the organisational structure. With the termination of neutron source operations at the end of 2019 and the new POF period beginning in the 2020's, the HZB will critically re-examine its organisational structure again and adapt.

The HZB is embedded in a network of foreign institutions through its large-scale research infrastructures and collaborative relationships in energy materials research. It plans to further expand its international collaborations strategically and concomitantly increase the number of international staff recruited.

The HZB enables its staff members to develop their technical and interpersonal skills and prepare themselves for new tasks and responsibilities under its programme of personnel development. Measures in the coming years and in the 2020's in this area address particularly those staff members who have been active in the research environment of the BER II neutron source and are re-orienting themselves in energy materials research or the operation of the BESSY II photon source.

The HZB has set itself ambitious goals regarding equal opportunity and the diversity. For example, the proportion of female professors among the senior scientists should amount to 30 per cent in 2020. The Perspectives Commission viewed the efforts of the HZB to facilitate good compatibility of family and career for its staff as exemplary.

The HZB intends to further develop its – successful – structured project management (PM) for its large projects such as the "Preparation for Decommissioning" of BER II, the BESSY VSR project, and HEMF, as well as for medium-sized projects and those of higher complexity. In 2020, the HZB will have a fully developed process management for its administration as as well as for its science management at its disposal.

funds following shutdown of BER II. In exchange, the remaining portion of these funds will facilitate re-orienting the HZB toward other topics important for the future. (letter from

State Secretary Dr. G. Schütte to Prof. Dr.-Ing. A. Kaysser-Pyzalla, Prof. J. Treusch and Mr. T. Frederking of February 18, 2014).



4. HZB 2030

Energy Materials Research and Soft X-Ray Radiation – Innovative Solutions for Future Challenges

In the medium term, the User community of VUV / soft X-ray radiation requires a next-generation light source. The DALI source planned at HZDR for the Terahertz and infrared regions, BESSY III in the VUV / soft X-ray region, and PETRA IV at the German Electron Synchrotron (DESY) in the hard X-ray region complement one another well with regard to photon energy and the established experimental methods at the facilities.

To meet the challenges of a light source for the coming generation, especially with respect to energy materials research and user orientation, the HZB is carrying out the following measures:

Analysis of the demand side

The initial basis for the future development is the analysis of the demand side from the User community regarding the priority of photon energies, the requirements for quality of the light source, the experimental methods, as well as specialised sample environments. The HZB is establishing a network of listening posts for exploring these parameters. The initial approaches for this consist of a systematic evaluation of the beam time applications and periodically carrying out Foresight Workshops focussed on various topics.

Focussing on the User Community

The successful concept of focussing on requirements of users, as already established at BESSY II and BER II, will be continued for a successor light source more intensively. Energy materials research is an important priority.

Next-generation light source for VUV / soft Xray radiation

Over the course of the next years, reliable results will become available on how suitable state-of-theart light source technologies (ERL, VSR, DLSR²⁵, and FEL - currently in their initial phases) actually are for routine daily utilisation. The HZB will critically review these technologies and designate the most suitable technology for a next-generation XUV / soft X-ray light source to serve energy materials research based upon this accumulated knowledge. Scenarios will be formulated and subjected to an unbiased cost-benefit analysis. An emittance upgrade based on new multi-bend achromats (MAX IV design / ESRF upgrade concept) is currently under consideration at BESSY II for comparison with constructing a new light source. The amalgamation of the VSR design with the DLSR design is being examined for both variants in order to facilitate maximum flexibility for the future User Community in relation to matching the beam parameters for each of the experiments or beamlines.

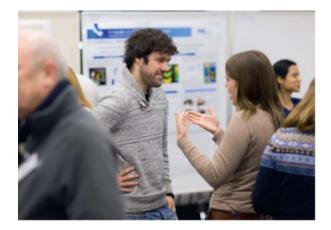
The requirements on soil physics and stiffness of the foundation will be even more ambitious when operating diffraction-limited storage rings than for third-generation light sources. The HZB intends to clarify this aspect early on, in particular regarding the costs.

FIRST MEASURES

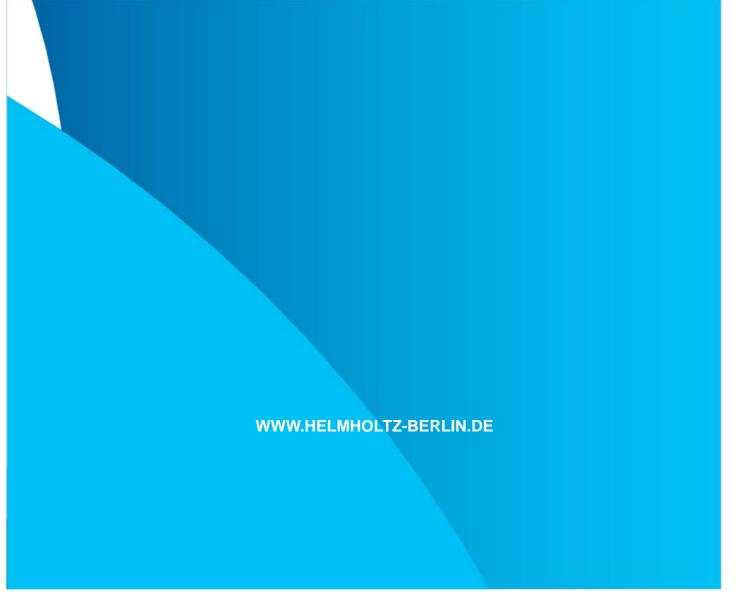
- The HZB has successfully introduced a next-generation light source into the Helmholtz Roadmap for large infrastructures.
- The HZB has decided to introduce the next-generation light source as a suggestion in the next Invitation For Bid (IFB) of the National Roadmap of the German Federal Ministry of Education and Research (BMBF).
- Foresight Workshops: the User Community will be involved in defining the BESSY III project through topical workshops. Five workshops have been completed in this series so far with overwhelmingly positive participation:
 - BESSY II: Tender X-ray Workshop
 - BESSY II: From PICO to FEMTO, Time-resolved studies at BESSY II
 - BESSY II: Imaging Workshop
 - THz to Soft X-ray Foresight Workshop
 - Tender X-Rays in MX Workshop

The series will be continued with two to four topical workshops annually.

International Foresight Workshops are an integral component for involving the User Community in defining the "BESSY III" project



²⁵ diffraction-limited storage ring (DLSR



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