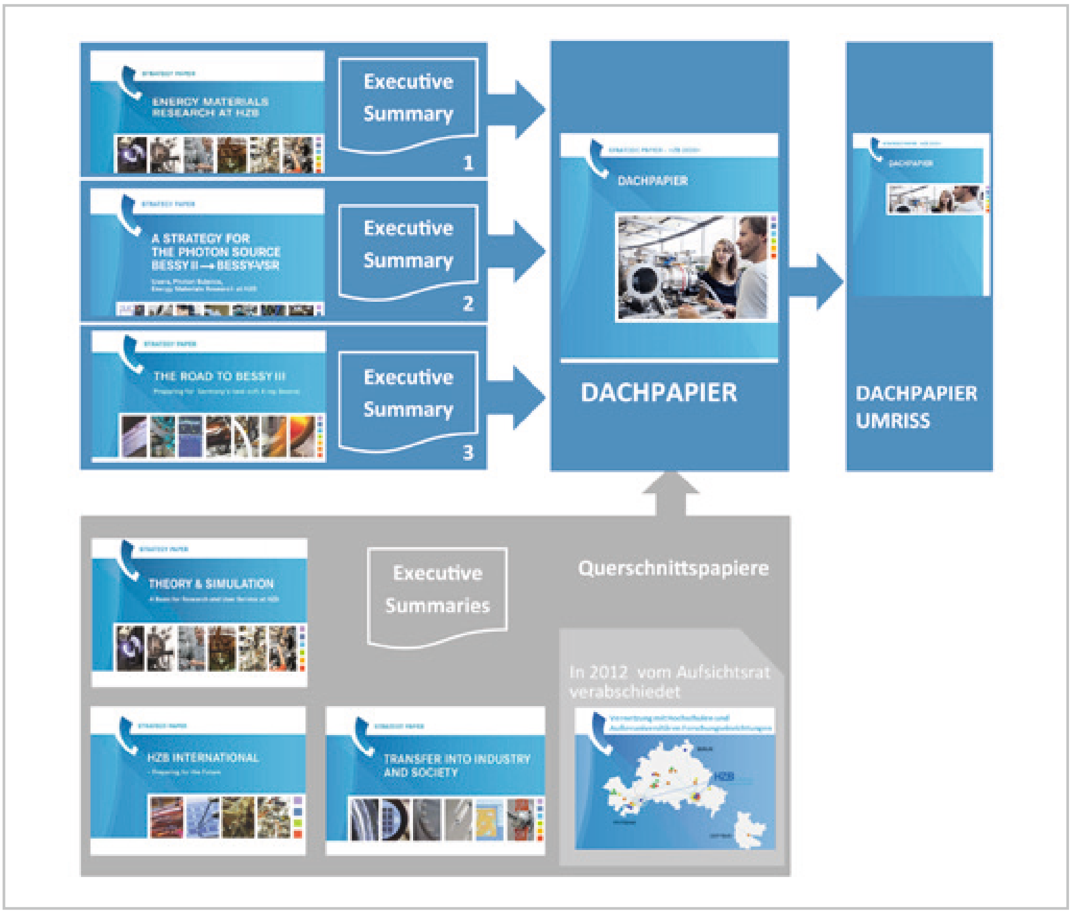
HZB Helmholtz Zentrum Berlin

STRATEGY PAPER – HZB 2020+

COMPILATION OF EXECUTIVE SUMMARIES



Strategy Papers of HZB. The Executive Summaries of the individual papers can be found in this brochure. The "Dachpapier" and its "Umriss" are compiled in an additional brochure.

NOTE TO THE READER:

The documents in this brochure have been approved by the HZB Scientific Advisory Committee in May 2015. This document is confidential and shall not be distributed without a formal consent by the HZB.

Berlin in May 2015

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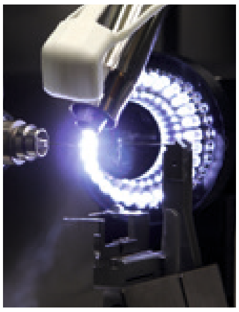
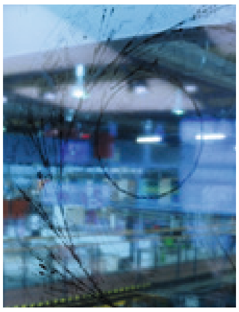
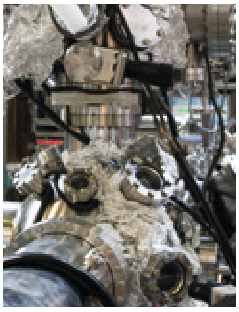
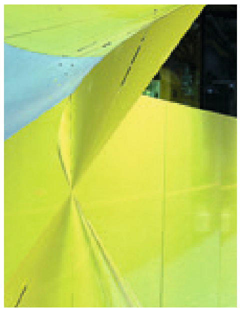
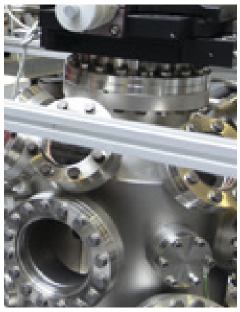

EXECUTIVE SUMMARY

HZB’S ENERGY MATERIALS RESEARCH IN 2015

Energy research at HZB has expertise in thin-film based systems for energy conversion for more than 25 years which has been top-ranked internationally. **Fundamental materials** research at HZB means decades of top-flight research experience in understanding and controlling electronic properties of quantum materials, and in developing soft matter / colloidal systems using soft X-rays at BESSY II and neutrons at BER II. Decades of know-how in the **operation of large scale infrastructures** like BESSY II enables outstanding science performed by the international scientific community.

Energy materials research at HZB is the synthesis of expertise in energy and materials research to provide the strategic thrust for the next decades.

HZB is convinced to be the right place for fundamental energy materials research and photon-related infrastructures for materials and energy (cf. Figure ES 1).

STRATEGY PROCESS

By enhancing its expertise in energy materials research through new research appointments and the re-orientation of existing organisational units, HZB has broadened its scope. It has been successful as strong partner in the Helmholtz-Association’s POF review of the research field “Energy”. Based on the POF III review results and a multi-stage process, HZB has systematically developed a thorough strategy for energy materials research. HZB’s scientists have identified the organisation’s specific strengths and utilised these for the proposed energy research activities. The scientists rated the benefits of the available infrastructures, expertise and capabilities for their own research as well as for the scientific communities and have

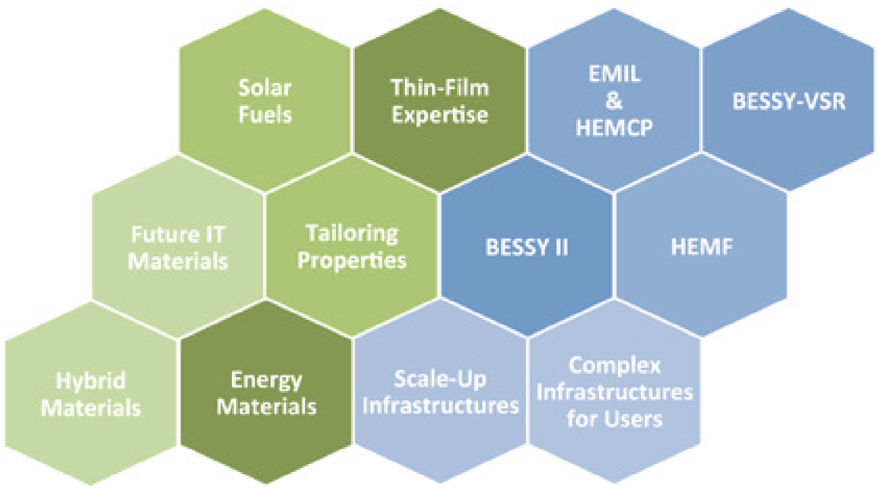

Figure ES 1: Scientific value constellation of energy materials research at HZB taken into account the activities of the most relevant competitors.[1] HZB has consulted its Scientific Advisory Council, its user community at BESSY II, in particular regarding the science case for the BESSY-VSR (the variable pulse length synchrotron source), and other external experts in energy materials science.

CHALLENGES

The primary aim of HZB is to maximise the impact of its photon-based capabilities and expertise on the achievement of the goals of energy materials research (↘ A Strategy for the Photon Source BESSY II – Section 4.1). HZB has identified relevant future trends in order to develop a sustainable and robust growth strategy. Carrying out an analysis of the political and scientific environment has allowed the main challenges to be identified and understood. To maintain its success over the long term, HZB will take measures to

- position itself as a focal point for energy materials research in the Helmholtz Association within the German research environment
- position itself in energy materials research both in the portfolio of the Helmholtz Association and internationally
- operate and offer state-of-the art large-scale facilities
- support the implementation of the Energy Transition through its research in general
- apply its expertise in photovoltaic technologies to pioneer new research topics related to energy materials
- pursue knowledge-based designs of processes and materials
- continue building on its successful and suitably focussed networking activities

VISION

HZB can make a significant difference to research progress on materials and devices for sustainable energy systems through its BESSY II photon source by carrying out its development into a unique variable pulse-length storage ring (BESSY-VSR) and applying its expertise to investigate the underlying principles that govern materials. The **vision of HZB** is:

- 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 community and industry.
- HZB exploits synergies by integrating excellent research with the operation of dedicated infrastructures, thus creating a unique research environment.

MISSION

HZB's mission related to energy materials research is:

"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 infrastructure, as well as the transfer to application. We make our infrastructure available to our users and collaboration partners. We therewith provide know-why and know-how for the society."

HZB'S ENERGY MATERIALS RESEARCH IN 2020+

HZB's **unique scientific palette** in 2020+ in the field of energy materials research will include:

- **New research themes:** HZB will take decisions on promising new research themes to be added (e. g. **combinatorial materials research** for new solar-fuel catalysts, new thin-film **materials for future energy-efficient IT,** new materials for **CO_2 capture, and chemical engineering of colloidal systems),** and on re-orientation or termination of on-going activities if necessary.

1 For details on competitors and collaboration partners see Section 2.7 and for established research themes as well as new research themes and infrastructures Chapter 6 of the strategy paper ENERGY MATERIALS RESEARCH.

- Retention of its **leading position in basic research for thin-film photovoltaics** in Europe; this is **also the basis for other complex thin-film systems,** e. g. in future energy-efficient IT materials, and thermoelectric materials.
- **Dedicated** beamlines, experiments and unique sample environments enabling **in-situ, ambient, and operando conditions for research on energy materials** (cf. Figure ES 2); these will be available at BESSY II / BESSY-VSR (↘ A Strategy for the Photon Source BESSY II – Section 4.1).
- The **BESSY-VSR scheme for simultaneously available long and short pulses** offers new opportunities for time-resolved experiments on energy-related processes and materials (↘ A Strategy for the Photon Source BESSY II – Section 4.3). The **picosecond short pulses** of BESSY-VSR will open access to few picosecond pulses needed to investigate **electronic processes in photosynthesis** (thanks to lower radiation damage and higher signal-to-noise ratios), **catalysis** (identification of reaction paths), **solar fuels** (carrier lifetimes of transition metal-oxides, water oxidation), and switching processes in energy-efficient devices for future IT.[2]
- **Provision of user access to complex facilities for energy materials synthesis and analysis;** experimental infrastructures requiring BESSY II or being complementary to BESSY II (laser photons) will be offered similar to the "Molecular Foundry" at LBNL (USA).
- **Scale-up infrastructure: from lab samples to prototypes;** this has already been successfully carried out for photovoltaic devices

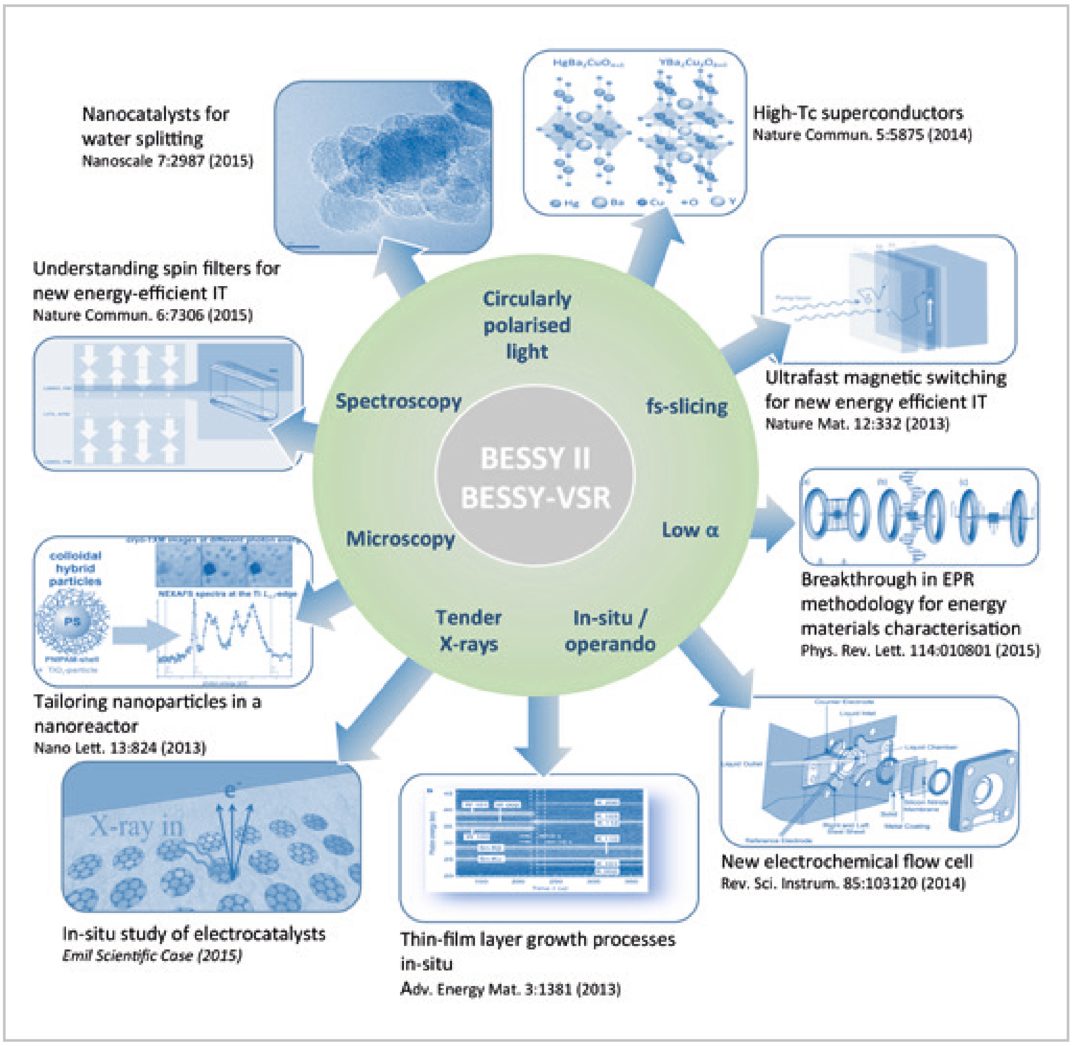

Figure ES 2: Unique scientific features and benefits from BESSY II for energy materials research

2 Details on the benefit of BESSY-VSR for energy research are given in the Scientific Case of BESSY-VSR.

(PVcomB). HZB’s experience and capability will be applied for upscaling solar fuel devices and processes in the near future (↘ Transfer to Industry and Society – Section 4.1).

- **Theory and simulation:** HZB is embedded in the scientific landscape of Berlin and Brandenburg, with Humboldt Universität zu Berlin, Freie Universität Berlin, Research Center Matheon, and the Fritz Haber Institute (Max Planck Society) being the key partners. The regional clusters of expertise allow for particularly close linkage between theory and simulation for the **design of experiments and interpretation of experimental data in energy materials science.** The scientific community will benefit from concerted multi-scale modelling of structure-function relationships in materials (e. g. for modelling of transport processes in electrochemical cells) and from the theory of quantum materials in developing efficient thermoelectric materials and new catalysts for solar energy conversion (↘ Theory and Simulation – Section 4.3 and 5.3).

GOALS FOR HZB’S ENERGY RESEARCH

Within this framework, HZB has formulated its three general goals for energy materials research (cf. Figure ES 3):

1. Discover governing principles for novel functionalities in energy materials
2. Tailor materials and processes for energy-relevant devices
3. Develop materials, processes and prototypes relevant to industry

By pursuing these goals, HZB will strengthen its position in the scientific landscape, and contribute to the future energy system and to solutions for the grand challenges of the society. HZB has clearly focussed its activities on energy materials research using photons and has defined an

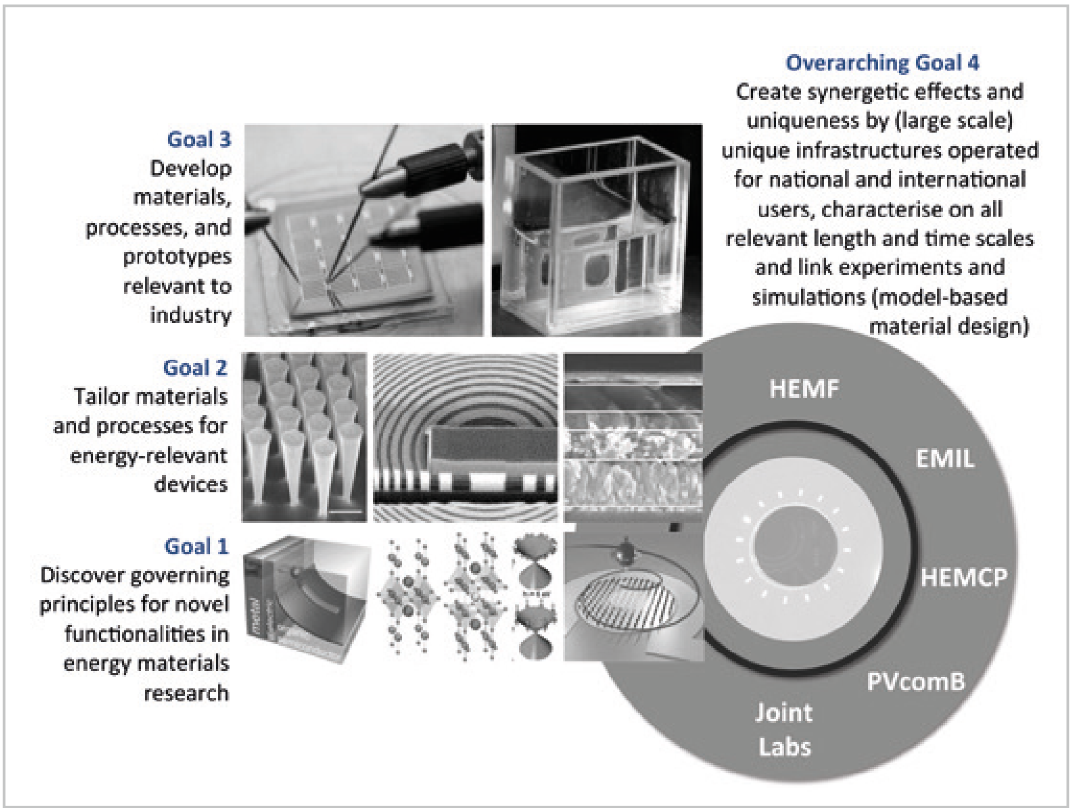

Figure ES 3: Examples from HZB’s energy materials research exemplifying the strategic goals.

Overarching Goal:

Create synergetic effects and uniqueness by (large scale) infrastructures operated for national and international users, to characterize on all relevant length and time scales and to link experiment and simulations.

HZB’s activities will encompass a wide range of energy materials research. HZB will continuously survey and adapt its portfolio based on its mission and is also open to apply its results of energy materials research to other fields such as e. g. optics or control systems.

Goal 1 – Discover governing principles for novel functionalities in energy materials

The discovery of governing principles for novel functionalities (Goal 1) is seen by HZB as the **fundamental, knowledge-based approach** to materials relevant for energy conversion and storage. **With its dedicated and in some cases unique infrastructures and experimental stations, BESSY II** makes HZB the right place to investigate interfaces of multi-layer systems of inorganic materials and hybrids of inorganic/ organic materials, for example. Understanding and controlling novel quantum phenomena are essential to developing and deploying energy-saving functionalities of materials relevant to future IT, for example switching magnetization by electric potential (cf. Figure ES 3). New capabilities that become available with BESSY-VSR will further accelerate energy materials research by providing access to the picosecond time-regime. **BESSY-VSR** (Goal 4) will address challenges in photochemistry, photosynthesis, photovoltaics, catalysis, and the basic reaction steps underlying solar fuels on picosecond timescales.

Goal 2: Tailor materials and processes for energy-relevant devices

For tailoring materials and processes for energy-relevant devices (Goal 2), it is crucial to understand the chemical and electronic properties of materials. The next step is to apply this knowledge to gain control over materials with optimized functionality and their synthesis. This goal is particular relevant in the area of solar fuel research. The challenge here is to tailor the stability and catalytic efficiency of materials for the generation of fuels from solar energy, e.g. by using 3-dimensional nano-architectures and controlling morphology and composition of the catalyst (cf. Figure ES 3). With its dedicated research infrastructure for energy materials research in particular for thin-film systems, HZB will provide complex and often unique possibilities to optimise the controlled growth of thin layers in-situ by using synchrotron radiation (Goal 4).

Goal 3: Develop materials, processes, and prototypes relevant to industry

Industry-relevant materials, processes, and prototypes (Goal 3) often follow from knowledge-based approaches and tailor-made materials. HZB is well suited to transfer process know-how and technology by virtue of its PVcomB infrastructure. Originally initiated as a competence center for thin-film photovoltaics, the generic knowledge and process capabilities will allow PVcomB in the future to move into upscaling and transfer of processes and devices for other fields, in particular relevant to solar fuels (cf. Figure ES 3) as well as other thin-film based processes and prototypes for other applications (Goal 4).

MEASURES

In order to attain its strategic goals, HZB will implement measures that can be grouped into “research themes” and “infrastructures” (cf. Figure ES 4).[3]

Measures A and B: Research themes

Research activities based on strengths and core expertise will continuously be developed further (Measure A). This includes the discontinuation of activities that are no longer competitive and the focussing on promising activities – scientific excellence and industrial need being the decision criteria.

New research themes (Measure B) will be established with the above-mentioned challenges and goals in mind. HZB intends to extend its research portfolio step-by-step starting with four new theme clusters centering on important new research themes (cf. Figure ES 5).

Cluster I

Solar fuels

The new research themes on device design, modeling, and advanced operando characterization techniques will expand HZB’s solar fuels portfolio and consolidate its role as one of the internationally leading centers for solar fuels research. Within Cluster I HZB aims at achieving its goals of i) demonstrating module-sized solar fuels generators, and ii) establishing an internationally unique solar fuels research infrastructure that is a “one-stop shop” for both internal and external users. Urgent major scientific questions concern e.g. the model-based experimental design of optimal electrode structures that combine short ion diffusion distances with easy separation of the reaction products which is crucial for upscaling of devices.

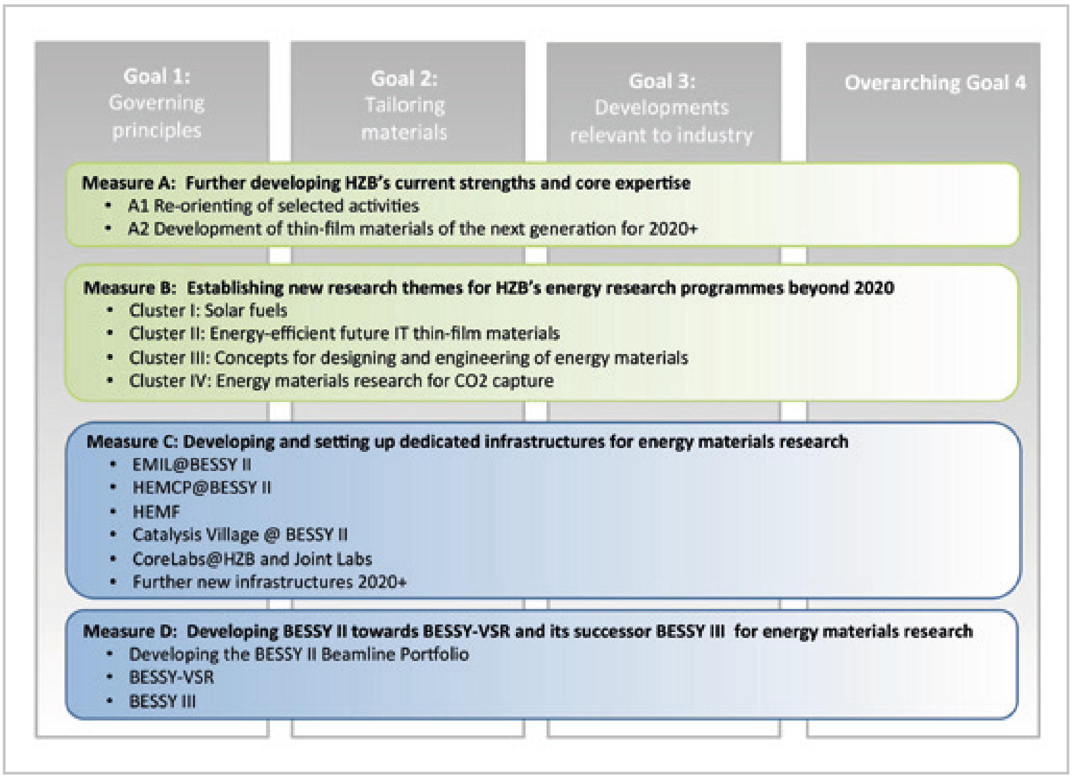

Figure ES 4: Measures for implementing the energy materials strategy of HZB. Research themes are indicated in green and infrastructures in blue, respectively.

3 For details on the measures taken to achieve the goals and on the particular strengths and unique features of HZB see strategy paper ↘ Energy Materials research Chapter 5 and Chapter 6.

Cluster II

Energy-efficient future IT thin-film materials

HZB’s unique combination of ab-initio calculations, single crystal synthesis and their thin-film production along with in-situ characterization at BESSY II will provide the full suite of research tools from the theoretical conception and tailoring of new materials to their functionalization. Closing the loop between thin-film and 2D materials synthesis, and the investigation of multi-scale electronic, spin and dynamic properties will enable breakthrough results. Scientific questions in this field concern tuning of coherence times in qubits in order to reduce limiting information loss, for example. Within Cluster II, HZB will contribute to spin-orbit torque-based magnetic random access memory (MRAM), spin transistors, topologically protected interconnects, and high-Tc-superconducting wires in prototype energy-efficient devices.

Cluster III

Concepts for designing and engineering of energy materials

The design of new functional materials is at the heart of HZB’s energy research activities. By establishing new facilities for high-throughput combinatorial discovery and optimization of functional thin films as well as the synthesis, characterization and processing of functional colloidal systems, HZB will bridge the gap between basic research and applications and offer a new value proposition for industrial partners. Scientific questions on the one hand concern the deposition and screening of truly continuous composition gradients of e.g. metal oxides, metal nitrides and metal sulfides which are highly relevant to solar fuels, thermoelectric materials, and electrochemical energy storage applications. On the other hand the model-based engineering of (concentrated) colloidal systems gives access to cost-effective large scale production of e. g. cathodic materials for electrochemical storage.

Cluster IV

Energy materials research for CO_2 capture

This activity will build upon HZB’s expertise in crystallographic analysis and fill a gap in the programmes of the Helmholtz research field ENERGY. HZB’s work on future carbon-capture materials will contribute to reducing the costs of efficient CO_2 sorbents. Material development including synthesis of compounds for CO_2 sorbents requires in-situ analysis during the selective uptake and release of CO_2. Scientific questions concern the model-based design of sorbents with high binding constants of more than 10,000 $M^{-1}s^{-1}$ but relatively low dissociation enthalpies 40–80 kJ / mol.

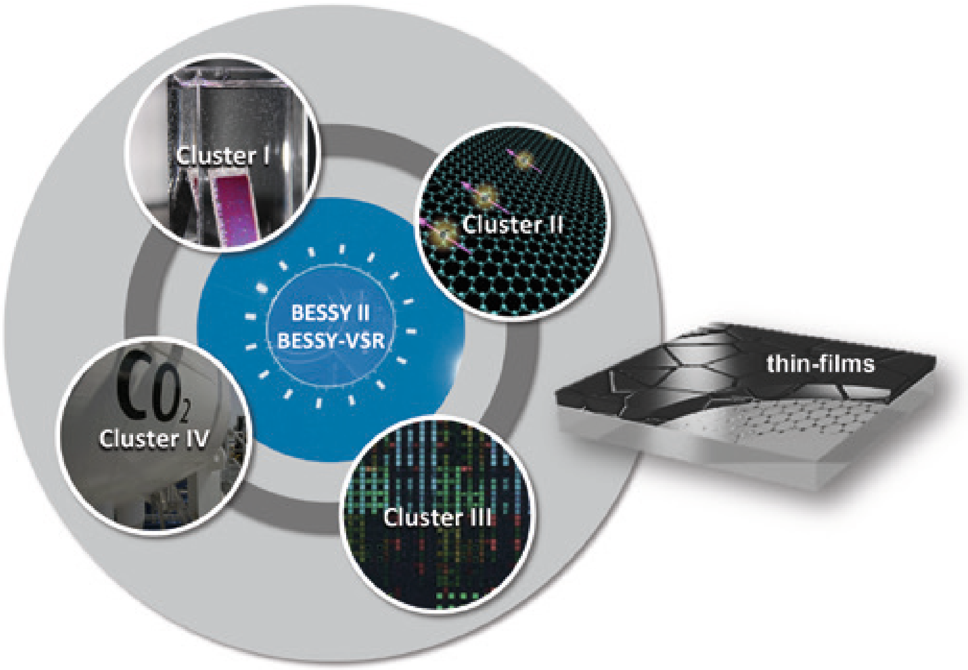

Figure ES 5: All new research themes in the Clusters I-IV build upon current HZB's strengths and are closely connected to BESSY II and HZB's dedicated infrastructure for energy materials research.
Cluster I: Solar fuels;
Cluster II: Energy-efficient future IT thin-film materials;
Cluster III: Concepts for designing and engineering of energy materials;
Cluster IV: Energy materials research for CO_2 capture.

Measures C and D: Infrastructures

Unique new infrastructure for research will be set up and opened for external users. This includes complex infrastructure, large-scale infrastructure and up-scaling infrastructure. HZB considers itself as the right place for realisation of research infrastructure if one or more of the following conditions apply: the infrastructure fits specific research themes of HZB, the infrastructure requires the use of BESSY II or BESSY-VSR **(Measure D),** it requires a significant amount of permanent and technical personnel resources to operate highly complex systems, the infrastructure involves high costs both in construction and operation, or the infrastructure will be used by a significant share of external, short-term users. Examples of these types of infrastructures are EMIL@BESSY II (Energy Materials in-situ Laboratory), HEMF (Helmholtz Energy Materials Foundry), and Joint Labs. In addition to the large-scale BESSY II and BESSY-VSR (in 2020) infrastructures, HZB will bundle its capabilities for analytics and synthesis, which can be modularly expanded (cf. Figure ES 6, **Measure C).**

Measures to be implemented with high priority in 2016+

In general, the implementation of measures has to take into account the aspects of time, strategic relevance and resources. For the process implementation of Core Labs at HZB, the X-Lab and EMIL@BESSY II have been identified already. In the following, measures will be given to be implemented with high priority for HZB starting in 2016.

Measure A

Current critical evaluation of on-going HZB activities and measures regarding their further development or, if necessary, termination; deposition technologies for semiconducting compounds for example will be coupled with existing research activities at the institute PVcomB or discontinued. HZB has already reallocated resources towards strengthening the theory support for quantum magnetism by founding a new organisational unit (EM-BerQUAM).

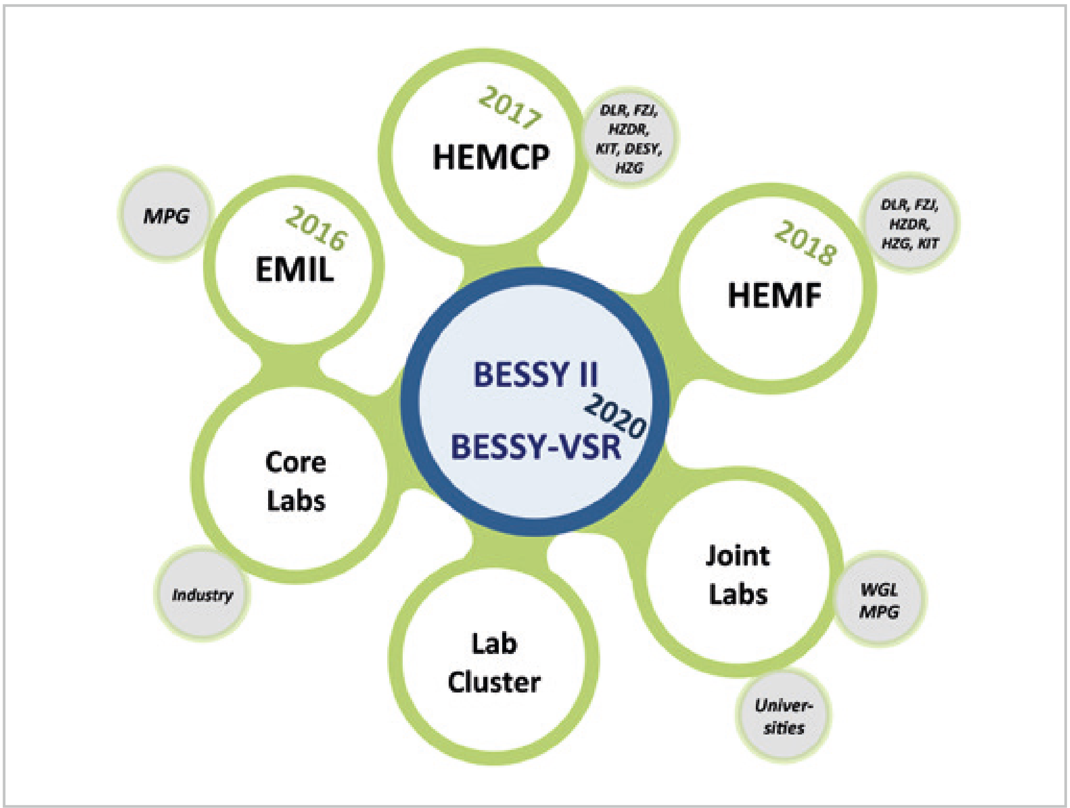

Figure ES 6: In addition to BESSY II and BESSY-VSR (blue), HZB will bundle its dedicated infrastructure for energy materials research as a “one-stop shop” (green) which is open to kinds of collaboration models.

Measure B

Control of photons, electrons, and ions (protons) in the liquid phase plays an essential role in developing efficient and stable building blocks for solar fuel systems. HZB will give priority to establishing a Young Investigator Group for fundamental research on functional materials and electrochemical processes in liquids and at interfaces using synchrotron radiation. HZB also intends to found a new institute (by re-channelling resources from photovoltaics) dedicated to solar fuels device design and covering the issues of smart chemical engineering solutions, advanced multi-scale multi-physics modelling, as well as detailed process simulations. Since these activities mutually depend on each other, they need to be executed and coordinated in parallel in order to make the overall approach as effective as possible. This will reinforce HZB’s leadership in solar fuels research.

Measure C

To strengthen its material synthesis capabilities for new materials, devices, and systems, HZB will immediately begin implementation of the HEMF project (assuming a positive funding decision). HZB will also open its infrastructure for energy material science to the user community. In the medium term, HZB will represent a unique access point to all these infrastructures.

Measure D

The unique “Energy Materials in-Situ Laboratory” EMIL@BESSY II will become operational shortly. HZB will further develop the dedicated beamlines for energy materials research at BESSY II, in particular the METRIXS beamline and the Berlin Joint Lab for Electrochemical Interfaces (BEIChem). HZB has completed its technical design study for the BESSY-VSR upgrade for BESSY II and will now submit a funding proposal to the Helmholtz Association. BESSY-VSR will provide picosecond pulses at high repetition rates for investigating fundamental processes of photosynthesis, catalysis, solar-fuels, and switching processes in energy-efficient devices for future IT for example. The follow-on step for development during the 2020s will be the planning and realisation of BESSY III.

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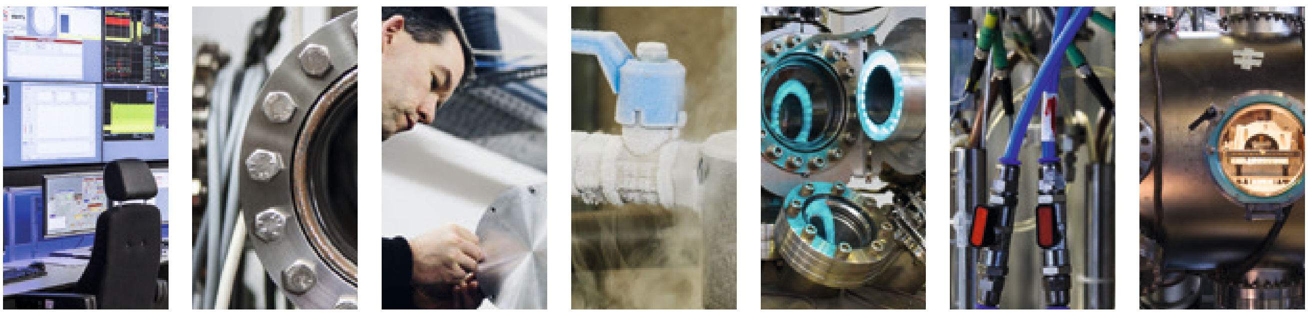
STRATEGY PAPER – EXECUTIVE SUMMARY

A STRATEGY FOR THE PHOTON SOURCE BESSY II → BESSY-VSR

Users, Photon Science, Energy Materials Research at HZB



PEOPLE

- Scientists
- Engineering Experts
- Support Personnel
- Administration
- Students
- Young Investigators

COMPETENCES

- Scattering
- Dynamics
- in-situ methods
- Optics
- Accelerator R&D
- Undulators
- Imaging
- Spectroscopy

FIELDS OF ACTION

- Scientific Drivers
- Photons for Users
- Science and Technology
- Education and Career

Fig. 1: HZB’s fields of action for the photon science. To achieve the goals, HZB relies on the strengths of its competences and people.

EXECUTIVE SUMMARY

Building on its strengths in in-house science, user service and accelerator technology, HZB has developed a strategic plan, which will sustain BESSY II at the forefront of synchrotron radiation facilities and make the source the prime choice for external users and HZB staff in the field of energy and materials research. BESSY-VSR is a major upgrade project of BESSY II, which will allow the user to choose from a variety of pulse lengths and which will fill the gap in time resolution and repetition rate of Diffraction Limited Storage Rings (DLSR) and FEL sources. bERLinPro is central to developing accelerator technology. Projects like BESSY-VSR and bERLinPro are paving the way for a future successor source in the mid-2020s.

The purpose of this paper is to present the future development of HZB's photon source BESSY II. Besides being a paper of strategic guidelines for internal action plans, this paper will be presented to the committee on perspectives (↘ Dachpapier). The committee will evaluate the strategy proposed by HZB and consequently pave the way for HZB's orientation towards materials and energy research as well as for the political decision on a future light source.

The BESSY II synchrotron radiation source of HZB is a 1.7 GeV 3rd-generation storage ring of high average brilliance optimized for the soft X-ray photon range. It is operated to generate synchrotron light for the scientific community. Each year HZB registers about 2,800 user visits. BESSY II operation covers a multitude of operating modes from multi-bunch and multi-bunch hybrid as standard modes for most user groups to single bunch, low-α operation and fs-slicing for time-resolved experiments in the ps to fs regime. Top up has been introduced as standard for both multi-bunch and single bunch operation. The source is characterized by its outstanding stability, high reliability and reproducibility.

At BESSY II, instrumentation development is science driven, as illustrated, amongst others, by the 10 nm resolution X-Ray microscope, the femtosecond pulse facility FEMTOSPEX (fs-slicing source), the micro-spot X-Ray photoelectron spectroscopy end station LiXEdrom and the highly automated macro-molecular crystallography laboratory (MX-Lab). The major competitors are ALS, ELETTRA and the new Soleil facility. In order to stay competitive the BESSY II storage ring itself and its instrumentation have to be continuously upgraded.

In Germany, researchers, politicians, businesses, and society are facing the challenge of the century: implementing the Energiewende, or energy turnaround, that has been adopted by the federal government and which constitutes a paradigm shift in energy technology in Germany. The Helmholtz Association, of which HZB is a member, explicitly supports the goals of the Energiewende. Substantial efforts in research on energy-relevant materials and processes will be necessary to meet the challenges of providing a stable and affordable supply of renewable energy. HZB is committed to contributing to solving these challenges: by 2020, research in HZB's organizational units will focus on materials and energy research, with BESSY II and its associated lab infrastructure being a cornerstone.

The BESSY II photon source has been operational since 1998 and is roughly midway through the operation period usually ascribed to synchrotron radiation sources. Due to ongoing, large international investment projects, financial resources for building a successor to BESSY II will only become available when these projects come to an end, presumably in the mid-2020s. The resulting challenge is twofold: to keep BESSY II at the forefront of synchrotron radiation sources until the mid-2020s and beyond, and to establish both a scientific and a political process for the development of a successor source for BESSY II.

In constructive discussions with its scientists, its boards and advisory bodies as well as its cooperation partners, HZB has identified four fields of action corresponding to four strategic goals, which are of equal importance for meeting the aforementioned challenges, and are mutually interdependent. The four fields are “Scientific Drivers”, “Photons for Users”, “Science and Technology” and “Education”. HZB is able to realize the strategy for each of these fields because of the competences and people on board (see Fig. 1).

Science- and curiosity-driven research seeks to understand and control the properties of materials. On the one hand, these activities generate scientific publications and technical applications (scientific output), on the other they drive the development of instrumentation and technology within the scope of BESSY II (science driven instrumentation). The goal for the field of action **Scientific Drivers** is:

Goal 1

To be a large-scale facility recognized globally for the excellence of its scientific output and its relevance for energy research

To achieve this goal, HZB has to ensure that BESSY II is the top address for soft X-ray users and users concentrating on energy research particularly with regard to renewable energy system. Activities at BESSY II have to focus on the research topics which best exploit the specific characteristics of the source. Energy and energy materials research are key drivers for research at BESSY II. The goals of HZB’s strategy on energy materials research are substantial drivers being addressed by the capabilities of the photon source BESSY II: the expertise in science and methods at BESSY II is used to discover the governing principles of novel functionalities in energy materials, to tailor materials for energy relevant devices and to develop materials relevant to industry. (↘ Energy Materials Research at HZB – Section 5.4)

HZB’s activities in the field of energy and materials research of the programs for the research field Energy (Helmholtz program oriented funding, POF), will be strengthened by the infrastructure EMIL – built and operated with Max-Planck-Gesellschaft (MPG) at BESSY II - and the planned infrastructure HEMF (↘ Energy Materials Research at HZB - Section 3.3.4.2). Research concentrates on the governing principles of materials for future information technology with the aim of increasing the energy efficiency of modern devices, and on solutions for sustainable energy supply. This includes materials for energy conversion and storage, such as photovoltaic, photocatalytical and photochemical systems and devices. Success will rely on the availability of in-situ, in-operando and time resolved characterization techniques, and will benefit from access to the “tender” X-ray range between 2 keV and 10 keV of photon energy. To pursue the goal for this field of action, HZB is taking advantage of the scientific landscape of Berlin and its surroundings by building strong networks with the universities and research facilities.

These activities have to be supplemented by laboratories for sample synthesis and characterization. In order to support this strategic approach HZB can use the experience gained during the last decades in the field of renewable energy research using synchrotron radiation methods. Expertise is on board in the field of science of solar energy converting systems and in the field of experimental methods for analytics.

Photons for Users is the field of action that covers all aspects of user service. It also initiates scientific activities at HZB as well as the corresponding development of instrumentation (science-driven instrumentation). The associated goal is:

Goal 2

To be recognized as one of the most user-supportive and science-enabling synchrotron radiation facilities worldwide

To achieve this goal, HZB has to offer excellent support by providing adequate staffing, regular training and secure knowledge transfer, and to ensure the quality of user support by employing appropriate guidelines and controls. A balance has to be found between beamlines that serve a large number of disciplines and specialized beamlines for energy science or exploiting BESSY II to its highest capabilities. The provision of unique sample environments for photon science is a field in which HZB has the potential to excel.

The increasing number of inexperienced users and the continuing diversification of the user community, together with the growing complexity of the experiments at BESSY II, demand more intensive user support (↘ Transfer to Industry and Society - Section 4.2). This means organizing user support more efficiently, including regular, mandatory training for instrument support staff and an increase in the number of instrument staff. The establishment of structured Quality Management for User Support with well-defined procedures creates a basis for monitoring, reporting on and controlling the quality of the user service. Together with regular foresight workshops fostering the special needs of emerging communities, continuous beamline evaluation is the foundation for state-of-the-art instrumentation and a balanced beamline and instrument portfolio.

BESSY II is equipped with beamlines and instrumentation covering the VUV and hard X-ray energy range. On the one hand, request for experimental time at VUV instruments might decrease in the future not least because laser-based lab sources have become available increasingly. On the other hand, experiments using both VUV (below 100 eV) and soft X-ray radiation are important for complementary investigation of e. g. topological insulators or energy conversion systems.

Building on the competences of the existing Sample Environment Group at the neutron source BER II, the establishment of a dedicated Sample Environment Group at BESSY II will create a strategic advantage for the BESSY II synchrotron over its competitors. Furthermore, providing dedicated theory support for experiments as part of the complete user service package can generate significant added value for user service (↘ Theory and Simulation - Section 5.2).

The development of accelerator technology and photon instrumentation is driven by the requirements of the scientific question being addressed (scientific drivers, photons for users) and, in return, enables novel scientific experiments. The goal related to the field of action **Science and Technology** is:

Goal 3

To be a scientific hub for designing soft X-ray instruments and accelerator technologies for next generation sources; to prepare for a future successor to BESSY II

To achieve this goal, HZB has to be a point of reference for other facilities designing and constructing instruments in the soft X-ray range; it is essential that the BESSY variable storage ring (BESSY-VSR) is implemented, in order to safeguard BESSY II’s competitiveness into the mid-2020s; HZB considers BESSY-VSR as the decisive upgrade of BESSY II that will allow for an extended lifetime of the photon source with a unique proposition against other light sources. Future light source concepts like Diffraction Limited Storage Rings (DLSR) will push imaging capabilities by increase in coherence and brilliance, while BESSY-VSR will fill the gap of high repetition rate, short pulse, flexible fill pattern storage rings (see Fig. 2). The implementation of BESSY-VSR will not require modifying the complete lattice structure of the storage ring, hence, reducing downtime of the photon source.

Furthermore, HZB has to ensure that its competence in accelerator design and construction is commensurate with preparing a successor for BESSY II. Last but not least, in-house expertise in project management has to be developed ahead of constructing a large-scale facility.

HZB capabilities in beamline and instrument design rely on its proven expertise in ray tracing and optics design and fabrication; here, innovative new concepts like 2D and 3D optics enable novel, more performant instrumentation. HZB’s competence in undulator design and construction constitute a pillar for accessing the tender X-ray range. Its expertise in superconducting RF (SRF) technology and short pulse, high current accelerator sources will be further boosted

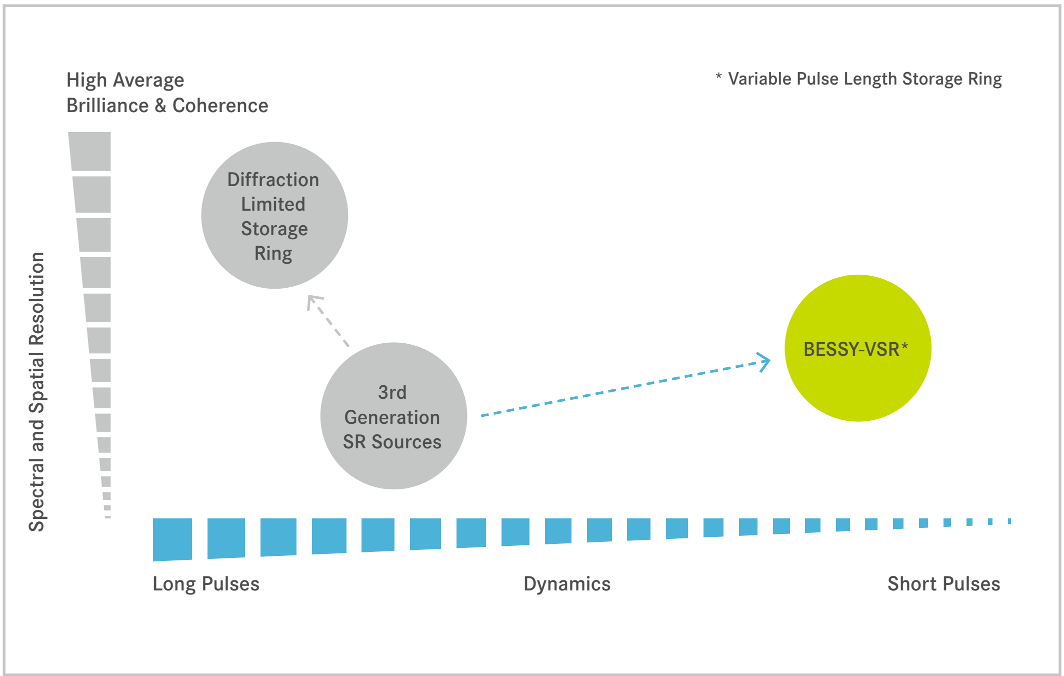


Fig. 2: In a parameter space spanned by pulse lengths and brilliance, BESSY II will develop towards shorter soft X-ray pulses while keeping the average brilliance of today's storage rings.

under the POF program, "Matter and technologies", in the research field Matter, thus laying the ground for the development of BESSY II and other accelerator-based applications. The first results from the bERLinPro project have already proven to be crucial for developing the required CW SRF technology for the BESSY-VSR concept for BESSY II. On the experimental side, the implementation of bunch separation schemes, together with the new ARTOF electron spectrometers, provide dedicated experimental capabilities for MHz repetition rate picosecond time-resolved experiments at BESSY II, and are crucial for the success of BESSY-VSR. This development will also benefit from access to simulation for electron accelerators (↘ Theory and Simulation – Section 5.1). With accelerator projects like bERLinPro and BESSY-VSR, the groundwork has been laid for a successor source to BESSY II beyond 2028. HZB has introduced a well-defined, structured project management framework, thus ensuring that the project of constructing a successor will be conducted appropriately and efficiently. The establishment of both a scientific and a political process for the development of a successor is addressed in more detail in a separate paper (↘ The Road to BESSY III).

Intricately woven into all of the aforementioned fields of action and their related goals is HZB's commitment to offering excellent education and training to next generation of scientists and to foster the careers of experts, technicians and staff. The goal related to the field of action **Education and Career** is, therefore:

Goal 4

To be an educational resource in synchrotron radiation science, technology and innovation and foster the careers of scientific and technical staff as well as users

To achieve this goal, HZB has to ensure that experiments with soft X-rays are included in university curricula. It has to map out career paths within and beyond HZB and continue increasing staff mobility, also within and beyond HZB. The composition of the staff also has to become more diverse.

The implementation of graduate and summer schools related to BESSY II is a key issue (↘ HZB international – Section 2.3). A structured program for PhD students and PostDocs providing these groups with opportunities for networking, further education (including soft skills), mentoring and career guidance will be implemented. Lighthouse projects like bERLinPro will be used to attract senior experts, young scientists and students from all over the world to work at BESSY II, and to open up career options for the scientists and engineering staff affected by the shutdown of the neutron source. Here, staff mobility will be fostered by special training and preferential access to vacancies. According to a binding cascade model, HZB will increase the proportion of women in scientific and engineering positions working at BESSY II.

Relying on the successes of the last years as well as its strengths in in-house science, user service and accelerator technology on one hand, and the expertise of its entire scientific, technical and administrative staff on the other, HZB has developed a strategic plan, which will sustain BESSY II at the top of synchrotron radiation facilities and make it the prime choice for the scientific community in the field of energy and materials research. Ultimately, it paves the way for a future successor source in the mid-2020s.

HZB is part of a regional, national and international network of partners. The Max Planck Society (MPG), the national metrology institute Physikalisch-Technische Bundesanstalt (PTB) and the Federal Institute for Materials Research and Testing (BAM) are the most important national partners, being involved in the operation of the photon source BESSY II by driving beamlines and instruments. Universities like e. g. Humboldt-Universität Berlin (HUB), Freie Universität Berlin (FUB) and Technische Universität Berlin (TUB) operate their own beamlines and instruments at BESSY II mainly in terms of Joint Laboratories.

BESSY-VSR

The upgrade of BESSY II keeps it at the top of synchrotron radiation facilities. Along with dedicated infrastructures BESSY-VSR will be the scientist's prime choice for research, in particular on energy materials.

Key projects supporting the strategy for the next years are:

bERLinPro
the prototype study for a continuous wave energy recovery LINAC based on superconducting radio-frequency (SRF) technology.

BESSY-VSR
the combined quasi-continuous and short-pulse high repetition rate synchrotron source allowing users to choose freely the appropriate time and length scales for their research.

EMIL
the in-situ soft- and hard-X-ray spectroscopy lab specialized on solar energy converting device and catalytic systems.

A JOINT LAB ON ELECTROCHEMICAL INTERFACES
the joint HZB - Max-Planck-Society lab pushing the understanding of phenomena at liquid / gas, liquid / liquid and solid / liquid interfaces.

METRIXS
the momentum and energy transfer spectroscopy instrument specialized on electronic properties and catalytic activity of energy materials.

PEAXIS
the high resolution spectroscopy instrument specialized on energy converting and generating materials.

ENERGIZE
the x-ray spectroscopy beamline for inorganic-organic hybrid materials for energy conversion devices.

The strategy paper is an evolving document which has been adapted continuously while having been prepared. Details of the strategy will be developed further and adapted to emerging requirements but the major strategic lines are drawn: materials and energy research, science driven instrumentation, technology enabling scientific output and education and careers. Further strategic topics of relevance to HZB are energy materials research, networking with universities, internationalization, theory support, and last but not least the future photon source BESSY III. These topics have been elaborated in additional strategy papers.

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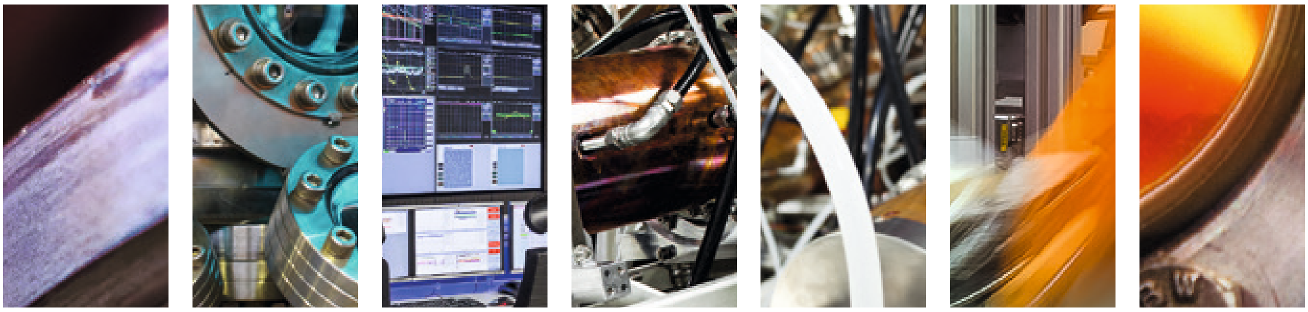
STRATEGY PAPER – EXECUTIVE SUMMARY

THE ROAD TO BESSY III

Preparing for Germany's next soft X-ray Source



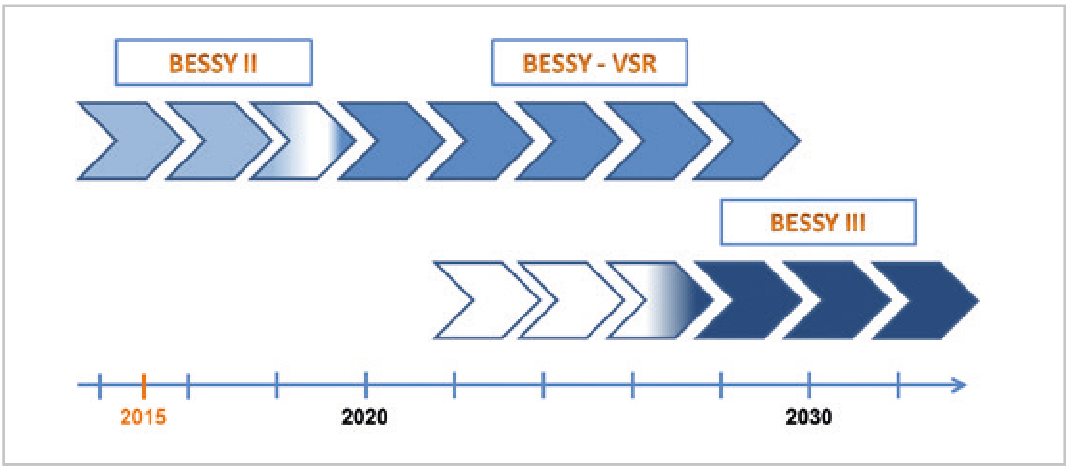
EXECUTIVE SUMMARY

VUV / SOFT TO TENDER X-RAYS, NOW AND IN THE FUTURE

High-flux, high-brightness, and increasingly high-coherence X-ray beams with well-defined energy and polarization have become an indispensable tool in the exploration of matter. Especially in the VUV and soft X-ray range, spectroscopy is commonly used to determine the elemental composition, chemical state, and physical properties of both inorganic and organic materials, and also biological systems. Element-specific images containing information on a nanometer scale can be obtained by combining microscopic and spectroscopic methods, and using tunable soft X-ray beams. This establishes the link of a material's or system's structure to its function.

Key future development areas of soft X-ray spectroscopic and microscopic techniques include their extension to the multi-dimensional phase space with length scales down to nanometers, time scales down to femtoseconds, and energy scales to tens of micro-eV. For energy materials research, success will rely on the availability of in-situ, operando and time resolved characterization techniques, and providing access to the tender X-ray range (↘ Energy Materials Research at HZB – Section 5.5). **Fulfilling these needs will require new sources with unprecedented beam characteristics.**

BESSY II – Germany's VUV and soft X-ray source operating at the highest international standards [1]
HZB's BESSY II synchrotron radiation source is Germany's VUV and soft X-ray source. BESSY II has been operating since 1998 and has been continuously enhanced and upgraded (↘ A Strategy for the Photon Source BESSY II – Section 2.2, 2.3). The BESSY-VSR upgrade will keep BESSY II at the forefront of synchrotron radiation sources until 2030 (see figure below and ↘ A Strategy for the Photon Source BESSY II – Section 4.3). The process leading to the BESSY III successor source in the mid-2020s will first need to establish the future scientific and technological challenges that the user community using VUV to soft X-rays will face. The most appropriate source type and its instrumentation will then need to be determined.



Timeline for photon source projects at HZB. Until mid-2019: operation of BESSY II; mid-2019: upgrade of BESSY II to BESSY-VSR; start of BESSY-VSR operation in 2020 until 2030; in parallel: from 2023 on, construction of BESSY III, start of operation in 2028, lifetime at least 30 years.

1 "BESSY II is a world-class soft X-ray facility", report on the review of the research facility (LK II) in: Reports on the Reviews of the Large-scale Research Infrastructures (LK II), Review Report of the POF Program "From Matter to Materials and Life (MML)".

VUV / SOFT TO TENDER X-RAY SCIENCE DRIVERS

Most developed societies worldwide face a common set of major challenges. These include health, secure, clean, and efficient energy; smart, green, and integrated transport; resource efficiency and raw materials. **Solutions to these challenges rely on the application of knowledge to control phenomena and create new functionality by developing new, tailored materials and systems.**[2] **Key challenges for developing such materials include observing how desired materials form, determining their nanoscale structure, and tracking the functions and the dynamics of their structural, magnetic, and electronic changes on all relevant time scales.** Developing a capability to observe material synthesis, material functions, degradation, as well as multi-material systems in-situ and operando (i.e. at actual pressures, temperatures, and other conditions relevant to the processing or in-service conditions) is essential for understanding and optimizing a device or process under working conditions.

Energy and materials research as scientific anchor of the BESSY III future photon source

Advanced systems for the sustainable conversion, storage, and utilization of energy, such as photovoltaic cells, thermoelectrica, batteries, light-emitting diodes, and fuel cells, along with new catalysts, depend critically on the development of new materials that can meet demanding performance and economic requirements. This requires an optimization of material composition, materials processing, interface and surface design as well the integration of materials into a device. An example is the development of high-efficiency solar cells using nanostructures for charge generation and separation. More generally speaking, optimizing the structure and function of nano–structures and particles requires the observation of their electronic and atomic structure in three dimensions with nm resolution while operando. The comprehensive understanding of complex and emergent electronic materials is one of the still outstanding great scientific challenges in Future Information Technology (↘ Energy Materials Research at HZB – Section 4.2, 5.5). The understanding and modeling of materials is essential for making the transition from an empirical and observational understanding of materials to targeted design, synthesis, and control of materials from the atomic scale to the everyday world (↘ Theory and Simulation – Section 1). Quantum effects in particular promise to have a revolutionary impact. For example, controlling magnetic states of matter is crucial for understanding the underlying fundamental physical phenomena and engineering the next-generation magnetic devices that combine ultrafast data processing with ultrahigh-density data storage. In order to generate, manipulate, and eventually control such magnetic states of matter, we need to understand the dynamical behavior of these key parameters at their characteristic time, i. e. from femtoseconds to nanoseconds, and their length scales from local spin moments to extended nanostructures.

The BESSY III user facility will be anchored by HZB’s strong and growing expertise in energy and materials research, thus serving the expanding user community in this field, and also service the strong user demand from biological and life sciences.

Biological and life sciences

Biological function is profoundly influenced by changes in molecular conformation that span several orders of magnitude in time, from picoseconds to milliseconds. These dynamics are central to the function of biological systems and macromolecular machines, ranging from the enzymes responsible for DNA repair and replication, to ribosomes responsible for protein synthesis, to dynamic membrane protein channels and signaling complexes, to organelles and the hierarchical structures of the cell – the fundamental unit of life. An enhanced understanding of the role of dynamics in biological function has both fundamental and practical importance, ranging from understanding how cells work to the design of improved therapeutic treatment. The challenge here is to develop and apply new methods for imaging biomolecules in native environments (in solution rather than crystalline form), capturing the dynamics of molecules during their functional cycles, and imaging cellular components in their native context. **The ability to dynamically image cellular events at 1 – 5 nanometer resolution with temporal resolution covering the range of**

2 These materials and systems and related processes have to rely on earth-abundant elements and secure supply chains.

interest in biology (femtoseconds to seconds), would revolutionize our understanding of complex biological systems and their interaction with substances such as pharmaceutical ingredients, for example. This is especially relevant if dynamical imaging with soft to tender X-rays will be combined with atomic resolution, information from crystallography, and other complementary methods.

OPPORTUNITIES FOR NEW SOURCES

Shaping the characteristics of pulsed light such as brightness, coherence, flux, repetition rate and pulse duration and structure in the X-ray spectral regime is the goal of novel accelerator designs for X-ray light sources. Here recent advances include low-emittance electron guns, normal and superconducting linear accelerators as well as highly integrated storage ring electron optics. Since the breadth of scientific applications requires control over brightness, coherence, pulse length and repetition rate, optimization of these light sources attempts to strike a balance within this parameter space.

Multi-user storage rings provide highly stable average flux and brightness with rather low peak flux and brightness at very high pulse-repetition rates (typically hundreds of MHz) in a tunable photon energy range from the far-IR to hard X-rays. These facilities serve a broad and diverse user community with several tens of beamlines at each one. Increasing the average brightness of storage ring technology beyond the highly successful 3rd-generation synchrotron radiation sources has led to the novel electron optics of the Multi-Bend Achromat (MBA), where smallest electron beam sizes are realized accompanied by elongated electron bunches. This technology was pioneered at the MAX IV facility in Sweden, extending the diffraction limit for high-energy storage rings into the X-ray regime. This concept of the diffraction-limited storage ring (DLSR) is currently being pursued as an upgrade option at various facilities internationally. Their coherent radiation will allow new classes of experiments.

Free-electron lasers (FELs) based on normal or superconducting accelerator technology provide X-ray pulses down to tens of fs with unprecedented peak brightness through a coherent amplification process, so far at limited repetition rates. Up to now, FELs serve a rather small number of users simultaneously. With the development of continuous wave (CW) superconducting accelerator technology, new operating modes come within reach of FELs, Energy Recovery Linacs (ERLs)[3] and even storage rings, driving the bERLinPro project and the BESSY-VSR upgrade at HZB. The promise of ERLs is to combine linac technology with the repetition rate of a ring-type source. At FELs, CW operation seeks to provide higher and evenly spaced repetition rates on the order of tens of kHz up to MHz. CW operation will improve the duty cycle of time-resolved experiments. The implementation of a CW superconducting accelerator is the basis of the modified LCLS-II[4] upgrade proposal that has been favorably reviewed. A possible upgrade to CW operation is also of highest priority for the European XFEL in Hamburg.

BESSY III seeks to provide a unique multi-user light source that fulfills the science-driven requirements for control of light pulse average and peak brightness as well as coherence, flux, repetition rate and pulse duration and structure. In particular, limitations in current DLSR designs of intrinsically long electron pulses as compared to 3rd-generation storage rings need to be overcome. The fluctuations and restricted pulse patterns of current FELs also require thorough improvements to suit a true multi-user facility such as BESSY III. HZB is pushing to resolve these seemingly contradictory requirements, combining innovative electron optics, CW operation, and superconducting technologies. A first step here is the upgrade of BESSY II to the BESSY-VSR variable pulse length storage ring. **In this way BESSY III will provide unique opportunities not being offered by any other facility being operative within the next 15 years.**

MAJOR ACTORS AND ROADMAP PROCESSES

International User Community and HZB's Strategic Partners

HZB's leading scientists are embedded in their respective scientific communities. In addition, HZB works closely with the users of BESSY II / BESSY-VSR and the national and international scientific community to stay abreast of emerging science areas and user needs to expand the breadth and depth of its experimental capabilities.

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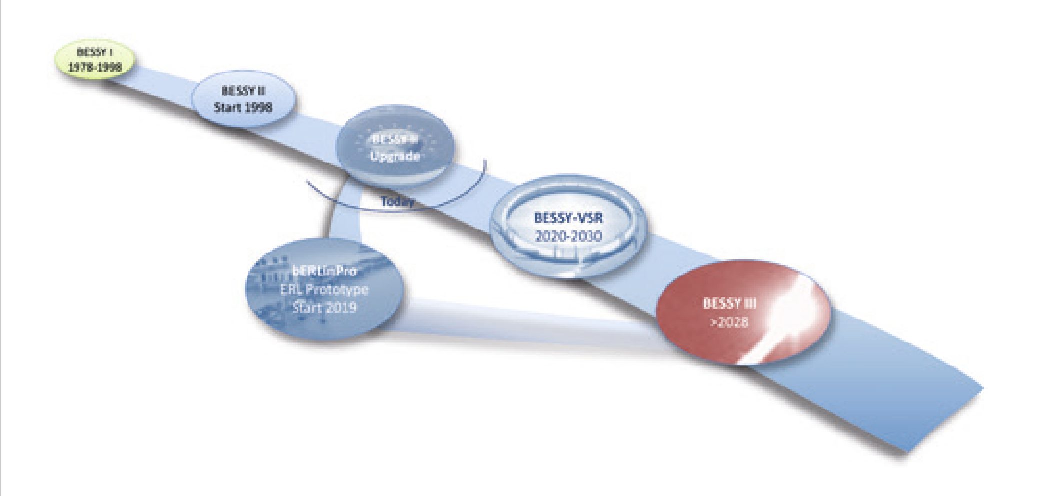
3 In an ERL-type X-ray source, synchrotron radiation is generated in a ring-type beam. However, each electron bunch is only used once (performing one single turn) and then dumped. The energy stored in the bunch is recovered at near-perfect efficiency in the linear accelerator (linac) of the ERL and "recycled" to accelerate the next electron bunch. In the Berlin Energy Recovery Linac Project bERLinPro, HZB will build a high-current ERL test facility that can put all subsystems relevant to large-scale ERLs to the test and perform a rigorous comparison of theory with the real world.

4 LCLS-II is a proposed upgrade of the Linac Coherent Light Source (LCLS) FEL at Stanford, USA.



The Road to BESSY III.

Further intensifying its dialogue with its current and future users from universities, research institutes, and industry, HZB has started a series of foresight workshops to establish a discussion forum for future projects and research activities. The aim of this dialogue is to identify future scientific fields and expectations, needs, and requirements for cutting-edge science with VUV / soft to tender X-ray synchrotron radiation. Besides giving valuable input for the on-going upgrades of BESSY II, including BESSY-VSR and BESSY II instrumentation, the results of the workshops will yield input for the BESSY III science case. The needs and requirements of the scientific communities (including possible new, emergent communities) identified as science drivers will be collected in a structured process. These drivers will have to be thoroughly assessed, analyzed, and taken into account for the decision on the type of the new source and its characteristics. This process will be organized and guided by HZB’s organizational units, building on HZB’s scientific expertise and experience in user service.

HZB has strong connections to many universities thanks to its user community. **Most of HZB’s leading scientists are jointly appointed with nearby universities and even more HZB staff is involved in teaching at the universities in Berlin and Brandenburg. HZB’s foremost partners among non-university scientific organizations in Germany are the Physikalisch-Technische Bundesanstalt (PTB, Germany’s national metrology institute), the Bundesanstalt für Materialforschung und -prüfung (BAM, Germany’s national institute for materials research and testing), and Institutes of the Max Planck Society (Max-Plank-Gesellschaft, MPG).** In order for HZB to get full support for the successor to BESSY II, HZB’s long-term strategic partners need to be closely involved in the process of defining the source characteristics and its instrumentation. In particular, metrology purposes have to be discussed well ahead of time with the PTB and taken into account in the decision on the BESSY III source.

HZB is being advised by its Scientific Advisory Council and its Board of Governors on BESSY III. HZB’s Scientific Advisory Council is composed of national and international experts from many different disciplines and meets twice per year to provide high-level advice on scientific and technological issues of basic importance for HZB’s future development. Intermediate results of the structured process towards BESSY III are being discussed with SAC regularly. HZB’s Board of Governors includes major actors from the BMBF and the State of Berlin.

Helmholtz Association

The BESSY II photon source covers the VUV to soft X-ray range within the Helmholtz Associations’ portfolio of storage ring sources, the hard X-ray range being covered by PETRA III at DESY. **BESSY III will keep the VUV to soft X-ray focus,**

with an extension to the tender X-ray range. The possible choice of an FEL source would have to be extremely well justified due to the obvious competition with DESY's existing FLASH facility and its on-going upgrades. In any case, BESSY III will be competing with other large-scale research infrastructure projects both within the Helmholtz research field “Matter” and the Helmholtz Association as a whole. Therefore, positioning the project in the forthcoming Strategy Paper on Photon Research and Sources of the research field “Matter” as well as within the roadmap process of the Helmholtz Association will be of utmost importance. Work on the Strategy paper for the Helmholtz research field “Matter” has just started; the paper is expected to be finalized in 2016. The Helmholtz Roadmap for Research Infrastructure is currently being updated; its finalization is planned for June 2015. The Helmholtz Roadmap is one of the documents constituting the basis of the Federal Ministry of Education and Research (BMBF) “National Roadmap on Research Infrastructures” that is currently being updated. [5]

Federal Ministry of Education and Research (BMBF)
BMBF is the relevant national funding body for the construction of and, indirectly, later operation of large-scale research infrastructures (RIS). [6] Proposals for new infrastructures must be submitted to the National Roadmap Process, in which an in-depth strategic, scientific, technical, and organizational review takes place. In addition to a successful review, the decision for the construction of an infrastructure also requires a commitment from all partners of a proposed RIS to cover its operating costs. Due to the current construction and operation of new international large-scale infrastructures for research with neutrons and synchrotron radiation, **the opportunity for constructing a new large-scale photon source will presumably be coming up in the mid-2020s. This implies that plans for a new facility as a successor to BESSY II need to be more detailed and presented to the BMBF by the end of the POF III period (i. e. end 2019) at the latest** in order to allow for in-depth reviewing. BESSY III will have to be positioned on BMBF's update of the “National Roadmap on Research Infrastructures”. Proposals for inclusion on the Roadmap have to provide details on construction and operation costs, time schedules, and resource plans that will then be assessed by external experts.

HZB is following closely and, with bERLinPro and BESSY-VSR, also actively contributing to rapid developments in the field of accelerator-based light sources and the scientific opportunities they will provide. Therefore, the strategic decision on the type of source and its specific characteristics will be taken towards the end of the POF III period. Anticipating a 4 – 5 year cycle for the updates of the National Roadmap, HZB will therefore focus on inclusion of BESSY III in an update in 2019 / 2020.

HZB'S EXPERTISE FOR DESIGNING AND BUILDING A NEW SOURCE

In order to fully exploit any future light source, the complete technology chain from source to detector must be developed. This requires expertise in such different fields as accelerator physics, undulators, beamlines, optics design, instrumentation, and timing and synchronization. In addition, user support must be appropriate and complementary laboratory infrastructure available. Furthermore, broad project management skills are required during the planning and construction phase.

HZB's units working in theoretical and experimental accelerator physics have maintained and even enhanced their worldwide reputation. The combination of the ability to calculate and simulate accelerators together with the means to perform accelerator experiments is a strong asset for accelerator physics at HZB (↘ Theory and Simulation – Section 2). The accelerator expertise developed over the last decades is the foundation for bERLinPro, a project of international significance, and the BESSY-VSR upgrade of BESSY II.

HZB has longstanding experience in the design and development of undulators, optical concepts and components, as well as cutting-edge instrumentation. These developments are driven by the needs of the scientific community, including the in-house research program at HZB. Synchronization and timing issues are addressed within the femto-slicing instrument, and on a much larger scale, within BESSY-VSR.

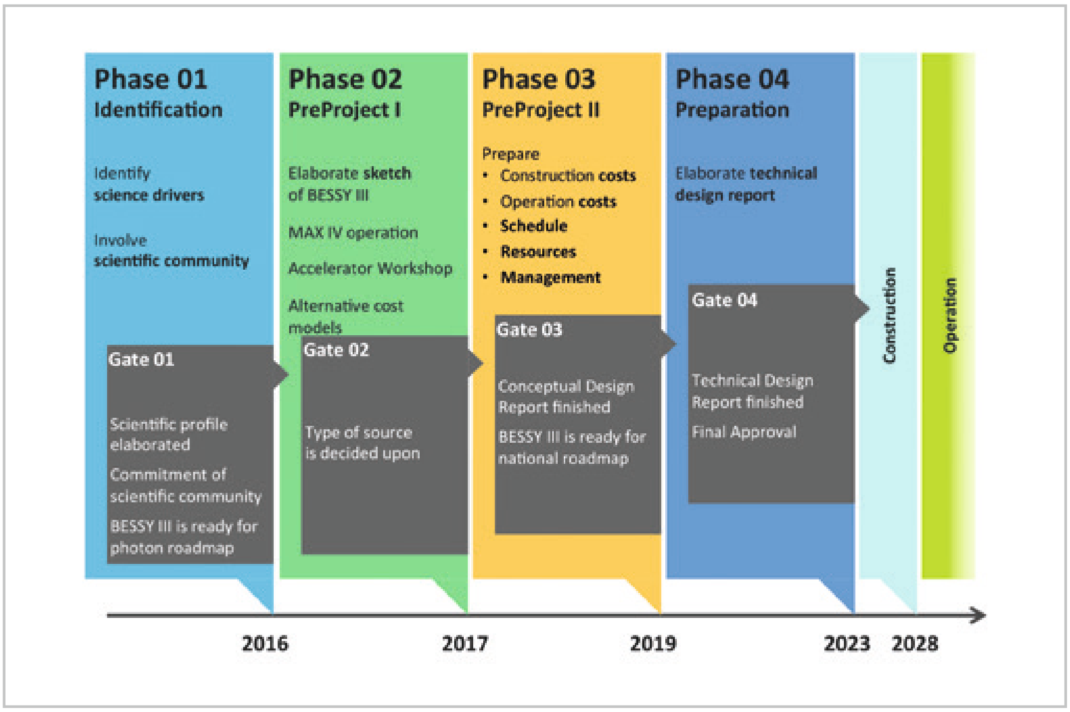
5 The update of the German National Roadmap is closely linked to the update of the Roadmap of the European Strategy Forum on Research Infrastructures (ESFRI) that gathers projects of scientific and technological excellence having a pan-European impact. HZB is open to any European partner interested in contributing to the BESSY III project, and to a possible joint application for inclusion on the ESFRI roadmap.
6 The operating costs for RIS operated by the centers of the Helmholtz Association have to be covered by the respective center or centers; however, BMBF covers 90 % of the Helmholtz Association's budget.

All scientific units of HZB are already involved today in photon science and operate at least one instrument at BESSY II. Theses research activities have led and will continue to lead to development of unique sample environments and associated laboratory infrastructures at BESSY II, together with improved in-house support for user research. Resources have already been and will continue to be reallocated from neutron to photon research. By 2020, research in HZB's scientific units will focus completely on energy and materials research, with the BESSY II/ BESSY–VSR photon source, its upgrades, and its associated lab infrastructure being the cornerstone.

HZB has introduced a well-defined, structured project management framework in early 2014; bERLinPro has already been implemented under this framework, and BESSY-VSR will be as well. The framework relies on the experience gained within the successful High-Field Magnet (HFM) project, which is now close to completion, both on time and under budget. **Applying this framework to BESSY III will ensure that the project will be carried out appropriately and efficiently.**

PRE-PROJECT PHASES

The successful BESSY III project will rely on thoroughly conducted pre-project phases defining the parameter space covered by the source, its type, its location etc. Relying on HZB's well-established project management expertise, and in line with the different phases in the life cycle of a research infrastructure identified by the German Council of Sciences and Humanities (Wissenschaftsrat) in the framework of the Pilot Phase for a National Roadmap on Research Infrastructures, HZB has defined a stage-gate approach to handle the BESSY III project efficiently and successfully (see figure below). A draft structure for the identification phase, i. e. the first phase of the pre-project phases has been defined. Besides establishing the scientific profile of the new facility, the structure and governance of the subsequent pre-project phases will be defined. In addition, the requirements concerning financial and especially human resources in the fields of accelerator physics, technical infrastructure, planning and construction, and controlling will be addressed. Work package leaders for the identification phase are currently being identified and will be appointed by mid-2015, as will be an experienced project coordinator.



HZB has defined a stage-gate approach to handle the BESSY III project efficiently and successfully over all the different project phases.

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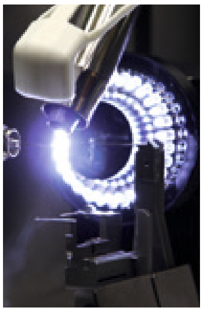
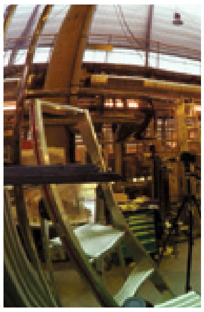
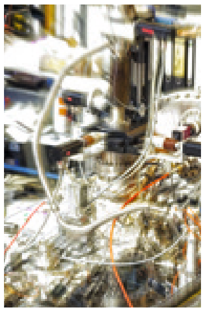
STRATEGY PAPER – EXECUTIVE SUMMARY

THEORY & SIMULATION

A Basis for Research and User Service at HZB




CROSS-SECTIONAL ACTIVITY AT HZB

EXECUTIVE SUMMARY

AIM OF THE PAPER AND PRIMARY ADDRESSEE

Advancing the theoretical foundations and the means to implement them through the computational power now available provide new paths in material and systems development. Numerical methods and simulations open up opportunities in particular for taking a computational approach in material development in order to start guiding the synthesis of new materials up to the threshold of an industrial application. Thus theory and simulation will become one of the four cornerstones – Theory Synthesis, Characterisation, Application – for materials development. The new opportunities offered by theory and simulations for new materials and systems in energy conversion, energy storage and efficient energy utilisation will enhance HZB's contribution to Germany's national energy transition strategy.

HZB operates the large-scale facilities BESSY II and BER II for an international user community. Here, theory and simulations play a growing role in the design of experiments, the evaluation of their results, and the understanding of phenomena. Increasing capacity for theory and simulations in this field would strongly benefit both HZB's user community and HZB staff scientists. As both experiments and data analysis become increasingly complex and the amount of data taken steadily rises, HZB sees the need for strengthening its user support by providing expertise in theory, simulation, and data analysis. (↘ A Strategy for the Photon Source BESSY II – Section 4.2)

The upgrading of the existing photon source BESSY II into BESSY-VSR as well as the development of a future photon source BESSY III will need a strong basis in simulation-based accelerator and storage ring design, beamline design, and optics development. (↘ The Road to BESSY III – Section 4.1 / 4.3)

Despite being convinced that excellent science needs theoretical insight, HZB will not be able to cover all fields of its current and future research portfolio with in-house theory and simulation expertise. HZB will thus explore the options for partnerships with universities and non-university research institutes for providing access to expertise and support in the theoretical realm.

The aim of the strategy paper "Theory and Simulation: A Basis for Research and User Service at HZB" is to identify ways and options on how targeted and demand-based access to theory and simulation can be realised to support the research activities and the user services at HZB.

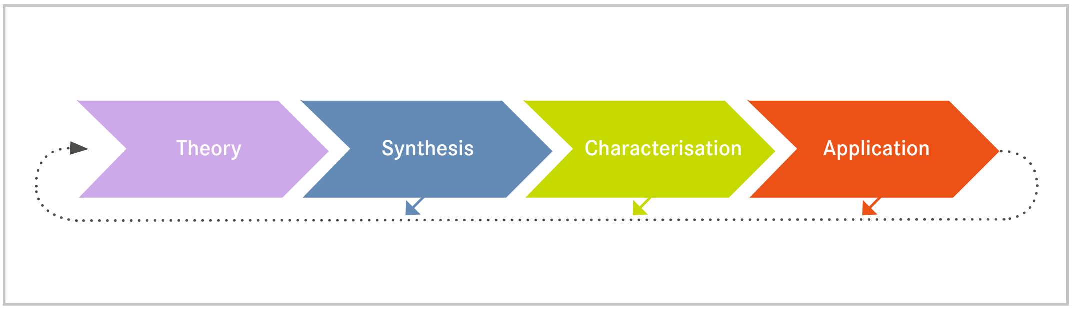


Fig. 1: Four cornerstones for material development

It is primarily intended for the “Perspective Commission” that has been appointed to accompany the long-term development of the HZB. (↘ Dachpapier)

GENESIS OF THE PAPER

The necessity of developing a strategy for theory and simulation originated from a strategy workshop on energy materials research at HZB. It has been recognised that the benefits of this strategy go beyond energy materials research and should extend to accelerator developments and user service.

HZB has appointed a “Theory” working group that has elaborated the structure and the content of the paper in two workshops and in various bi- and multilateral discussions. The group members also discussed relevant issues with external partners and brought in their experience with collaboration partners and universities. The outline of the paper was presented and discussed by the HZB Science and Technology Board in October 2014 and was presented to the Scientific Advisory Council in November 2014. The draft of the paper was discussed in a Workshop of the Scientific Advisory Council in March 2015.

ACTION FIELDS FOR THEORY AND SIMULATION AT HZB

From the outlined HZB mission, the goals defined in the POF III programmes and most importantly the three strategy papers on “A Strategy for the Photon Source BESSY II”, “Energy Materials Research at HZB”, and “The Road to BESSY III”, HZB identified three major action fields and related overarching objectives, in which theory and simulation play a crucial role for the Centre to be successful in the near and long term.

1 **Photon Sources and Instrumentation: HZB will maintain and expand its own expertise in building new generation photon sources and developing state-of the-art instrumentation for new and existing sources.**
This expertise requires access to simulation for both electron accelerators and photon management in beamlines and instruments.

2 **User Support: HZB will complement user service at its experimental research infrastructures through support and guidance in theory, modelling, and simulation as well as data analysis.**
Establishing dedicated theory-based guidance and support for experiments as part of the user service beyond interpretation of the collected experimental data will generate significant added value for users at BESSY II and BER II.

3 **Material Design and Devices: Expertise at HZB and its partners will cover the entire value chain, from theoretical foundations of material systems to prototype devices, facilitating predictions of material and device properties.**
Theoretical and simulation approaches need to span the atomic to macro scales, cover material design, fundamentals of synthesis, material characterisation, and optimisation as well as growth processes and device simulation. This will be crucial for HZB to maintain its leading role in solar energy research, and to develop expertise for acquiring leading positions in new research fields, and will also be beneficial for user support.

STATUS QUO

HZB today has theory activities in carefully selected areas, such as the theory groups for soft and organic matter, on quantum magnetism, on electronic structure calculations. These groups participate to the POF Programmes in the Helmholtz Research Field “Energy” to which HZB contributes and to the HZB in-house energy research. The theory groups on high brightness photon beams and on ERL-Design simulation are actively involved in the POF Programme “Matter and Technology”.

At BESSY II and BER II, users for most experiments are provided with data handling and tools for data interpretation/evaluation areas a standard service at the individual beamline or instrument. A full support on sophisticated theory and data interpretation within the regular user service currently takes place only at a few beamlines and instruments at BER II and BESSY II. Additional theory support mostly for HZB staff is provided through collaborators from universities and non-university partners on selected topics.

For HZB's key tasks such as the development of the acceleration system and the instrumentation at BESSY II and BER II and for the development of energy converting devices HZB develops own software and program codes. These are strongly based on the available theoretical background in connection with an excellent experimental expertise.

Device modelling is performed by staff researchers at HZB with state-of-the-art one-dimensional modelling. Further efforts cover multi-dimensional modelling of light absorption as well as electrical performance of solar cell devices.

On the hardware side, HZB operates a scalable *dirac* high-performance computing cluster and has access to external computational infrastructures, e.g. at Konrad-Zuse-Zentrum für Informationstechnik Berlin or at Freie Universität Berlin.

MAJOR ACTORS AND FUTURE TRENDS

Research Policy:
The funding bodies have outlined their expectations of the science system in the "Pact for Research and Innovation". Accordingly, the commitment of German research institutions to develop, build, and operate unique research infrastructures should be expanded in order to further strengthen Germany's international competitiveness and its science sector. The funding bodies will monitor the implementation of POF recommendations such as strengthening theory in selected programmes. Interaction of academia with industry and society is expected to be intensified. The objective of close cooperation between the sciences and business is specifically to bridge the gap between research (both pure and applied) and the commercial marketplace for their mutual benefit by more rapidly transforming new scientific discoveries and knowledge into value-added chains, sustainable high-skill jobs, and innovative products[1].

The Helmholtz Centres are expected to take a leading role in research and development to help facilitate the successful transition of the German energy system and to meet further grand challenges of our society.

HZB has identified the following key strategic drivers, in which theory and simulation play an important role:

- To maintain the HZB research infrastructures at the highest level and develop future research infrastructures (BESSY III, for example), HZB needs to conceive new concepts and to assess those by simulations.
- In order to contribute to the success of Germany's national energy transition policy, HZB needs to be able to develop new material concepts having a sound theoretical basis.
- Reaching the goals formulated in the proposals for Programme-Oriented Funding (POF), in particular in the FIT-programme, necessitates close collaboration of scientists at HZB performing experiments with scientists excelling in theory and simulation.
- In order to enable technology and knowledge transfer to industry, HZB needs to cover the entire value chain, from theoretical foundations of material systems to a prototype device, and requires awareness of commercial applications in other research fields (simulation and design of compact accelerators for semiconductor industry or medical applications, for example).

HZB Research and Scientific Community:
As innovation at HZB is almost exclusively based on its scientific output, substantial science-related drivers exist:

- Individual scientists wish to refine their theories and experiments with the objective of being the scientific leader in their respective

1 Pakt für Forschung und Innovation – Fortschreibung 2016 – 2020:
http://www.gwk-bonn.de/fileadmin/Papers/PFI-III-2016-2020.pdf (only German)

field by, for example, being the first to discover a novel material class with improved properties for certain applications. Major breakthroughs and scientific discoveries are increasingly possible only when combining theory and simulation with experiments.
- Scientific output is more and more measured mainly by high-quality publications in leading scientific journals that often need to be based on both theory and experiment.
- New fields of science become accessible due to technological improvement of either the hardware for experiments (new accelerator designs, for example) or the theory for discovering new phenomena (aided by continuous increases in computer power, for example).

The user community of BESSY II will presumably further diversify, resulting in fewer users with a general interest in synchrotron-based research and more users with specific questions from various research fields. This is true in particular for users from industry. This results in an increased demand for “service packages” covering measurements and data interpretation in relation to simulations, to support in the theoretical aspects of the experiment or sample. (↘ A Strategy for the Photon Source BESSY II – Section 4.2)

Most materials science centres have strong established theory departments and with direct on-site access to High-Performance Computing. Those centres are already in the forefront of inverse material design (i.e. from a desired property to the structure of a material) at least in selected research fields and HZB faces strong competition in several research fields.

Strategic drivers by the user community are:

- In order to stay competitive and attractive with respect to its research infrastructures (BESSY II / BESSY-VSR / BESSY III), HZB needs to provide service that also covers theory and simulation for data interpretation, in particular for non-specialist users and users from industry.
- In order to develop new measurement and evaluation methods for specialised problems, a theoretical comprehension using simulations is needed to prepare feasibility studies.
- To keep research and innovation at HZB on a high level, HZB needs to intensify its collaborations with theoreticians outside HZB and establish in-house theory expertise in selected fields.
- In order to face the worldwide competition in materials and energy research, HZB needs to either develop its own theory groups or to establish new strategic partnerships with theory centres in universities or non-university institutes.

Collaboration and Partners:
Collaboration and Partners: The excellent networking with universities and non-university institutions in the Berlin–Brandenburg metropolitan region elevates the degree of recognition of the institutions and the region. HZB finds important connections and partners for theory and simulation in the universities, in particular in theoretical physics and chemistry at the FU Berlin and the HU Berlin and through them in institutions like the Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB) or the Matheon-Verbund and in non-university institutions, such as Fritz-Haber-Institute (FHI). This offers opportunities for the research region to position itself as a beacon worldwide in several fields through joint funding applications and attract excellent scientists.

- To optimise the use of resources of its partners and its resources, HZB needs to collaborate with external groups who can bring in a high level of complementary expertise. Those groups and the HZB should share scientific interest in energy and materials research and the development of tools, synchrotron radiation methods, or the development of accelerators.
- If HZB and the universities in the Berlin-Brandenburg region that have developed strong theory groups and hired excellent scientists want to succeed in attracting substantial funding, HZB needs to foster collaborations between scientists working on theory and simulation at the partner institutions and HZB staff.

From HZB’s status quo and the future trends related to the major actors, HZB identified the following challenges for the three aforementioned Action Fields:

CHALLENGES

The Key Challenges in the Action Field "Photon Sources and Instrumentation" are:

- Ensure competencies to perform the simulations necessary for accelerator design and operation, in particular for BESSY-VSR and BESSY III. (↘ The Road to BESSY III – Section 4.1 / 4.3)
- Access to High-Performance Computing (HPC) infrastructures to allow start-to-end parallel simulation of future light sources and support adaptation of simulation software to local and external HPC sites.
- Assume responsibility and leadership within the synchrotron community for upgrading the existing HZB source codes for modelling and simulation of future beamlines and BESSY II / BESSY-VSR / BESSY III and x-ray optical systems.

The Key Challenges in the Action Field "User Support" are:

- Offer a dedicated theory guidance and support for experiments as part of the complete user service package. (↘ A Strategy for the Photon Source BESSY II – Section 4.2)
- Provide adequate support in data interpretation and theory for non-specialist users and industry. (↘ Transfer to Industry and Society – Section 4.4)
- Provide adequate theoretical support for users in selected scientific fields that are not covered by HZB's in-house research staff.
- Identify instruments, experimental methods, and research fields where theoretical support is most promising for broadening the user community.

The Key Challenges in the Action Field "Material Design and Devices" are:

- Generate a critical and visible mass of theory resources at HZB. Implement an exchange and possibly coordination between theory groups at HZB.
- Establish expertise in the theory of electronic structure and excited-state dynamics.
- Facilitate concerted multi-scale modelling efforts for structure-function relationships and theory-guided experimental design and synthesis of materials.
- Facilitate modelling up to macro-scale devices and integrated functional elements.

In the strategy paper "Energy Materials Research at HZB, sections 5 and 6", additional expertise in theory, simulation, and modeling has been identified as an essential ingredient to achieve the envisaged breakthroughs in the development of e. g. efficient thermoelectric materials, new light absorbers and catalysts for solar energy conversion, and new reactor and device designs for solar fuel applications.

GOALS AND MEASURES

In order to meet the key challenges in the three Action Fields, HZB has defined the following six major goals and optional measures. Several optional measures are associated with each goal. The measures are listed according to the relevance perceived.

1 **HZB will provide the best possible user theory-support in at least three research fields which are linked to several instruments and methods at BESSY II (2017).**
HZB will intensify collaboration with existing and new strategic partners, such as universities in the field of theory and experiment, and will establish at least one senior scientist position to bridge theory and experiment with electronic structure expertise. The person to fill this position is expected to contribute to user service at BESSY II together with an annual workshop series to train in-house researchers and users in simulating spectra.

2 **HZB will strengthen collaboration and exchange between experiment and theory in the FIT programme and theory support for material sciences as recommended by the POF review panels (2015 – 2020).**
HZB will intensify collaboration with strategic partners in the field of theory and experiment, will recruit professors (W1 / W2) in selected theory fields, and will nominate an additional SAC Member with applicable theoretical expertise.

3

HZB will contribute expertise through its theory groups in at least one coordinated research programme of the DFG or the EU together with Berlin-Brandenburg university partners (2018).
HZB will become more actively involved in networks on theory and experiment and will intensify collaborations with strategic partners in the field of theory and experiment. HZB and its partners will explore funding opportunities for a graduate school focussing on the combination of theory and experiments related to basic phenomena for energy-efficient future IT.

4

HZB will establish a HZB theory network to enhance internal and external visibility and to create a more attractive working environment for theoreticians (2017).
HZB will establish an annual workshop series with collaboration partners to train HZB staff and users in simulating spectra and the simulation of images and various signals originating from electron probes and will establish a summer school on the linkage between theory and experiments conducted with BESSY II in the materials and energy sciences. Also, HZB will launch a HZB internal “virtual theoretical research group” to foster scientific exchange among its theoreticians.

5

HZB will enable and provide support for access to internal and external High-Performance Computing infrastructures (2017).
HZB will establish a team to support maintenance and adaptation of simulation software to local and external High-Performance Computing infrastructures and will provide the infrastructure for updating, upgrading and flexible access to in-house High-Performance Computing.

6

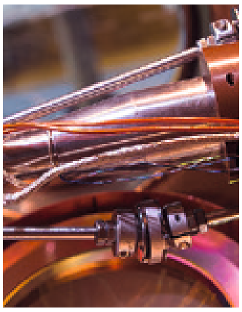
Theory at HZB is visible at the advent of the next funding period (2020).
HZB will recruit professors (W1 / W2) for joint labs in selected theoretical fields and will become more actively involved in networks on theory and experiment. HZB will launch a HZB internal “virtual theoretical research group” to foster scientific exchange among its theoreticians and will establish a summer school on the linkage between theory and experiments conducted and an annual workshop series to train in-house researchers and users in simulating spectra and the simulation of images and various signals originating from electron probes (cf. Goal 4).

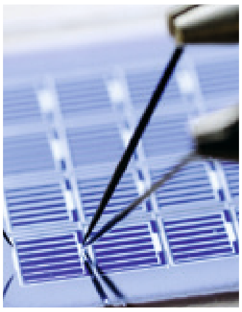
HZB Helmholtz Zentrum Berlin

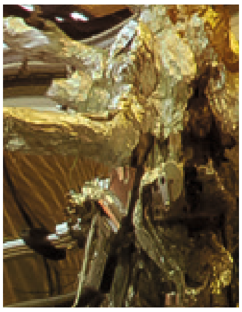
STRATEGY PAPER – EXECUTIVE SUMMARY

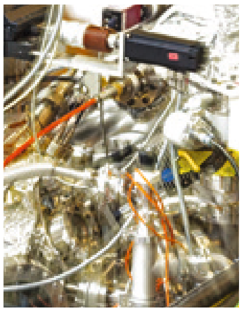
HZB INTERNATIONAL

– Preparing for the Future









CROSS-SECTIONAL ACTIVITY AT HZB

EXECUTIVE SUMMARY

PURPOSE AND AUDIENCE OF THE STRATEGY PAPER "HZB INTERNATIONAL – PREPARING FOR THE FUTURE"

This strategy paper, entitled "HZB International – Preparing for the Future" is intended to cluster present international matters at HZB and to outline the on-going process for further orienting the Helmholtz-Zentrum Berlin internationally during POF III (2015-2020) and beyond. Its primary audience is HZB's Perspective Commission.

It adheres to the "Pact for Research and Innovation", in which the Federal Government seeks to achieve two policy goals with particular relevance to international matters:

- Develop and implement new international cooperation strategies, and
- Obtain the best scientists for Germany

GENESIS OF THE STRATEGY PAPER

The discussions in preparation for this strategy paper took place with the Science and Technology Board, HZB participants in the evaluation of the POF III programmes, and with HZB staff participants in intercultural training seminars. A working group belonging to HZB organisational units (including scientific institutes, administration and PhD coordination) compiled the ideas and assumed the editorial tasks. A summary of the document was presented at the meeting of the HZB Science and Technology Board in October 2014 and April 2015 as well as at the autumn meeting of Scientific Advisory Council.

STATUS QUO OF INTERNATIONAL ACTIVITIES AT HZB

HZB is already an important international actor. This is reflected for instance in its widely international user communities of its two large-scale facilities BESSY II and BER II, as well as in the strong presence of HZB staff members in international scientific advisory committees for other large-scale facilities such as ESRF in France and the Bragg-Institute in Australia. HZB's leading scientists are also members of international committees for transnational initiatives that coordinate energy research like EERA – AMPEA (European Energy Research Aliance – Advanced Materials and Processes for Energy Applications) and international conference series like the IPAC (International Particle Acceleration Conference). Leading HZB scientists are guest professors at foreign universities and institutes, for example at the Chonbuk National University in South Korea and the National Institutes of Natural Sciences in Japan for outstanding contributions in the field of renewable energies.

HZB (about 1100 staff members in total) has more than 150 staff members of non-German nationality from 40 different countries. The large majority of these employees are scientists and students (more than 95 %) and administrative staff account for 5 %. HZB has set up programmes for improving incoming staff diversity, staff external career advancement options, and for attracting more young researchers and employees to Berlin, which will reinforce HZB's international reputation as a centre of excellence offering unique photon-related infrastructures for energy materials research.

Operating two large infrastructures for an international user community, HZB is a partner for many institutions outside Germany. Other strong players offering soft X-ray synchrotron radiation are: the Advanced Light Source ALS, USA, ELETTRA, Italy, and SOLEIL, France.

BESSY II has about 40 % of its users affiliated with organisations outside Germany, and BER II 65 % (average 2010 to 2013). Both BESSY II and BER II serve more than 550 user groups from over 40 countries annually. The scientific community including strategic partners is naturally involved in the development of instrumentation available at BESSY II. This is essential to take into account the requisites of new and specialised beamlines. Scientific cases for large future infrastructure projects, like e. g. BESSY-VSR with the pico second time resolution option, which together with EMIL@BESSY II will offer unique possibilities, are developed in close cooperation with the user community.

Furthermore, HZB will considerably strengthen its international competitive position in the design, operation, and use of photon-based large-scale facilities through BESSY II, BESSY-VSR (variable pulse-length storage ring), and eventually through BESSY III. BESSY II already plays an important role in the national and international light source communities as a world class, state-of-the art soft X-ray facility. BESSY-VSR will be the first photon source of its kind on the international scene.

MAJOR ACTORS AND FUTURE TRENDS

The German public and the German Federal Government, as represented by the German Federal Ministry of Education and Research (BMBF), is the major actor and provides 90 % of HZB's funding. The German Federal Government has outlined its expectations for the development of German non-university research institutions in the "Pact for Research and Innovation".

In October of 2014, the German Ministry for Science and Education (BMBF) published their "International Collaboration" action plan. There, the goals of the Federal Government's Strategy for the Internationalisation of Science and Research are:

- Strengthening research cooperation with global leaders
- International exploitation of innovation potential
- Intensifying the cooperation with developing countries in education, research and development on a long-term basis
- Assuming international responsibility and mastering global challenges.

The Federal State of Berlin, represented on the Supervisory Board of HZB by SenWTF [1], contributes 10 % of HZB's institutional funding. The State of Berlin finances its universities, which are attractive collaboration partners for HZB and also important major actors. By operating BESSY II and BER II (the last until late 2019) for an international user community, HZB has a strong role in the visibility of science in the Berlin-Brandenburg region being in particular a strategic partner of Freie Universität Berlin (FU) and Humboldt-Universität zu Berlin (HU) within the German Excellence Initiative [2].

In 2012, **the Helmholtz Association of German Research Centres** of which HZB is a member adopted a strategy paper "Die Helmholtz Gemeinschaft in der Welt: Grundlage für ein Internationales Engagement" (The Helmholtz Association in the World: Basis for International Engagement) that defines three main objectives:

1. Strengthening Germany as a location for research
2. Collaborating with the best researchers and attracting them
3. Strengthening the visibility and presence of German research

The main measures to achieve these objectives are competitive funding programmes for recruiting internationally, and joint research programmes (e. g. Helmholtz Research Schools, Helmholtz Postdoc programme, Young Investigator Groups, virtual institutes, and joint research groups).

During the POF III evaluation, international reviewers recommended that HZB should continue to be internationally competitive, linked to international networks, actively follow international trends, apply international standards, and promote strong international collaboration with highly ranked international partners including internationally active companies that require a

1 Senatsverwaltung Wirtschaft, Technologie und Forschung
2 The Excellence Initiative of the German Federal Ministry of Education and Research and the German Research Foundation aims to promote cutting-edge research and to create outstanding conditions for young scholars at universities, to deepen cooperation between disciplines and institutions, to strengthen international cooperation of research, and to enhance the international appeal of excellent German universities.

qualified workforce with experience on an international level. The framework of **industrial collaborations** is outlined in the HZB strategy paper "Transfer to Industry and Society" (↘ in German, "Transfer in Wirtschaft und Gesellschaft").

For example for the Solar Fuels topic the reviewers stated that the future challenge is to become established as an outstanding platform on an international basis. The large investments proposed for HEMCP and EMIL@BESSY II will provide international visibility through their access to the international community.

Other future challenges for the international **scientific community** (including users, reviewers, and strategic partners), are implicit in the construction of more international infrastructures like XFEL, FAIR, and ESS that will increase the competition for financial and personnel resources.

The support programmes of the EU have an influence on international cooperation partners, such as support through the European Research Council (ERC grants) and through the HORIZON 2020 research and innovation programme which promotes collaboration and technology transfer between European partner institutes and access to research infrastructures, such as the Calipso project.

HZB has identified the following future strategic trends based on the analysis of its major actors:

- HZB is part of a worldwide competition and cooperation with other research centres operating large scale facilities and performing materials and energy research.
- HZB wants to continue to offer a competitive research environment to attract more top scientists from other countries.
- HZB wants to be internationally more competitive with its BESSY II and BER II sources, instrumentation, and science. To attract more leading scientists to use BESSY II and BER II, HZB will also to improve the quality of its user service.
- In energy science, HZB will further develop by building up and providing the best possible research environment and user service at EMIL@BESSY II, HEMF and Lab Cluster for an international user community.
- HZB will further invest in its branding and highlight its culture of diversity to recruit staff internationally, which for example will help to attract the best PhD students.

STRATEGIC FIELDS OF ACTION FOR HZB

Based on the requirements of its major actors, internationalisation policies in science, objectives formulated in the strategies of the BMBF and the Helmholtz Association for international matters, and its own status quo and future plans (as outlined in the HZB strategy papers (↘ "A Strategy for the Photon Source BESSY II", "The Road to BESSY III", and "Energy Materials Research at HZB"). HZB has identified its strategic fields of action (Fig. 1). They meet the needs of HZB as a centre that provides world-class photon-related research infrastructures to the international user community and that focuses on materials and energy research.

GOALS AND MEASURES FOR INTERNATIONAL DEVELOPMENT OF HZB

Goals and measures have been formulated for the above-mentioned four fields of action and many of them will be accomplished within the POF III period. They will be first steps into the direction of internationalisation at HZB and have to be further extended in the subsequent years.

Field of action 1

Energy research, infrastructures and user community

GOAL 1

To increase HZB's international visibility for materials science and energy research with its large-scale facilities BESSY II, BER II, and also with EMIL@BESSY II, HEMF and the Lab Cluster, to attract more international users and to meet international standards for the user service.

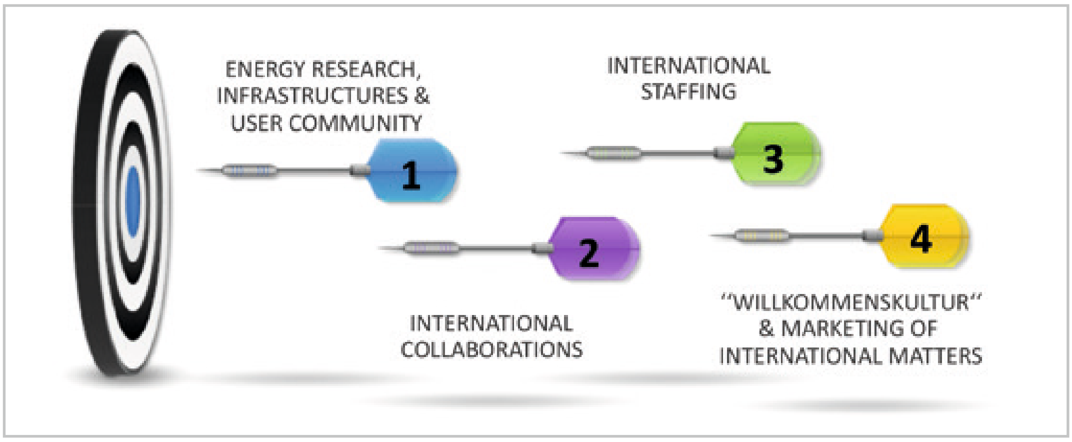


Fig. 1: Strategic fields of action for HZB's further internationalisation

SUBGOALS

Reputation and large-scale infrastructures

- The worldwide reputation of the BESSY II synchrotron radiation source and BER II neutron source for materials science and energy research will be reflected in mid-term review (2017) and POF III evaluation (2019).
- EMIL@BESSY II will become a user facility for external users from academia and industry worldwide. EMIL@BESSY II will be open for the international user community (beginning of 2017).

International user community

- The number of external users at BESSY II coming from foreign countries will be increased from 41 % in 2014 to 50 % in 2020.
- EMIL will have 25 % international users (2019).
- The number of international external users at HEMF will be 25 % in 2020.

User service

- A Quality Management system for user service will be installed (2016).
- More than half of the members of HZB's Scientific Selection Panel will come from abroad (2017).

HZB will reach the goal and the subgoals defined above by the following

MEASURES

Reputation and large-scale infrastructures

- HZB will invest in user infrastructures for energy materials research to enhance the international visibility and competitivness
- HZB will invest in the BESSY II source (BESSY-VSR), beamlines, and end stations to guarantee the high international standards of user experiments.

International user community

- The organisational units operating EMIL@ BESSY II and HEMF will actively recruit users through their scientific and industrial collaboration partners and at international conferences and fairs.

User service

- User service at BESSY II, BER II and at the energy lab clusters will be performed by scientists with substantial international experience.
- HZB will apply quality standards and control systems to user service, and will seek and incorporate feedback from users about user service, with regular reporting to boards.
- HZB will perform user service at BESSY II in accordance with international standards at European infrastructures.

Field of action 2

International collaborations

GOAL 2

To continue to be part of an international network of long-term and sustainable collaborations with strategically important partners worldwide.

SUBGOALS

- HZB will increase the number of collaboration agreements with strategic partners worldwide in energy and synchrotron research from 22 in 2015 to 30 in 2020. For this, the existing and successful German-Russian and German-Swedish collaborations and their respective end-stations at BESSY II will serve as role models.

Funding
- Increase the number of funded EU projects to 5 new EU projects annually (2015 / 2016), with HZB coordinating at least one EU project (2020).

Networking and advertisement
- HZB will increase the number of guest professorships at HZB to two professorships for stays of approximately three months annually (2016 – 2020).
- HZB will develop an alumni network and related activities (2017 ALUMNI).
- HZB will use the Helmholtz offices in Brussels, Moscow and Beijing as well as representative offices of other science organisations worldwide for networking

MEASURES

- HZB will use its scientific network to invite partners of interest for BER II instruments and to present opportunities for scientific collaborations at HZB

Funding
- The third-party funding department will implement a newsletter containing important information about EU calls and advertised funding programmes.
- HZB will support joint applications with partners of strategic fields to country-specific calls, e. g. with China and Russia.
- HZB will apply for at least one Helmholtz International Fellow Award and at least three other fellowships (DAAD, Alexander-von-Humboldt Foundation, etc.) per year.

Networking and advertisement
- An ALUMNI-Officer will be appointed responsible for developing an ALUMNI Concept (2016).
- Directors and leading scientists will regularly visit strategic partners for maintaining contacts and networking
- Collaboration agreements will be yearly updated and strategically assessed.
- Scientists from the Energy division will participate in the development of curricula for energy- and materials science studies at the Turkish German University in Istanbul.

Field of action 3

International staffing

GOAL 3

To welcome more colleagues from abroad and respect numerous cultures.

SUBGOALS

Current staff
- Increase intercultural experience and staff mobility for administration and technical staff at HZB. Implementation of diversity-orientated recruiting policies: Percentage of non-German administration and technical staff is 2 % (as of March 2015); target is to increase this to 8 % by 2020.
- International standards for administration processes will be adopted in 2016.
- All PhD students at HZB will participate in a graduate school with one of HZB's partner universities (2020).

Recruitment

- Establish substantial international experience as an important recruitment criterion for all scientists at and above Post-Doc level and for key administrative staff (2016).

MEASURES

Current staff

- Administrative processes will be performed in German and English.
- Intercultural and multilingual knowledge will be added to competence profiles of administrative and technical staff.

Recruitment

- All jobs in science, administration, and technical departments will be advertised in international platforms like EURAXESS, EURESS – The European Job Mobility Programme.
- Apprenticeship training positions will be advertised in EU internet platforms like EURESS.
- Emphasize international recruitment in the W2- / W3-Programme for Excellent Women in Science and via recruitment initiatives
- An International Officer will enhance networking with foreign offices and branches of scientific organisations like international offices of DAAD, DFG and universities in order to improve International recruitment of the best scientists worldwide.

Field of action 4

“Willkommenskultur” and marketing of International Matters

GOAL 4

To have a corporate culture that embraces diversity, an international mindset, and equal opportunities for employment.

SUBGOALS

- HZB will increase the visibility of its international activities
- HZB will continue to organise international workshops, schools, and conferences in the fields of photon, neutrons (until late 2019), and / or energy research by HZB (2016-2020).
- HZB will enhance international marketing as an employer that offers an international environment, an excellent scientific infrastructure, and attractive prospects for professional development (beginning in 2015).
- HZB will encourage a “Willkommenskultur” in all working relationships (beginning 2016).

MEASURES

- Appointing an International Officer responsible for internationalisation (2016).
- Define key metrics for international activities and establish a reporting system to the management board (2016).
- Summarise international actions and themes of HZB on the HZB homepage by 2016.
- Engage in active international marketing through regularly participation at international career fairs like Nature Jobs Career Fair, Gain, or European Career Fair (beginning 2015).
- Yearly organisation of international student summer or winter schools in the fields of photon, neutron (until late 2019), and / or energy research
- Establish a welcoming procedure for international employees like a visit plan, welcome events, or a welcome week.

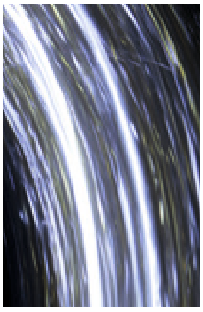
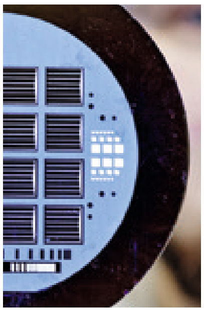
In **conclusion**, a future international development of HZB requires that organisational and structural conditions as well as processes are installed. Additionaly, necessary finances should be planned.

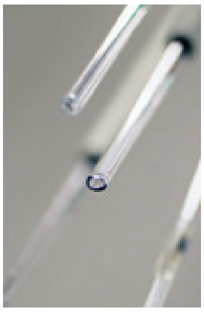
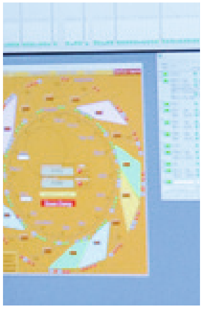
By implementing this strategy, HZB is committing itself to its further internationalisation and continuation of its efforts to promote international networking and exchange. Solid existing international collaborations with Russian and Swedish groups constitute successful examples of mutual benefit that will serve as role models. HZB will pursue to strengthen international collaborations with other strategic partners such as China, USA, India and Brazil. The strong presence of HZB staff in international scientific advisory committees for other large-scale facilities, energy research, specialised conferences, workshops and schools, as well as active recruiting of international users and staff members will nurture the implementation of measures in all four fields of action.

HZB Helmholtz Zentrum Berlin

STRATEGY PAPER – EXECUTIVE SUMMARY

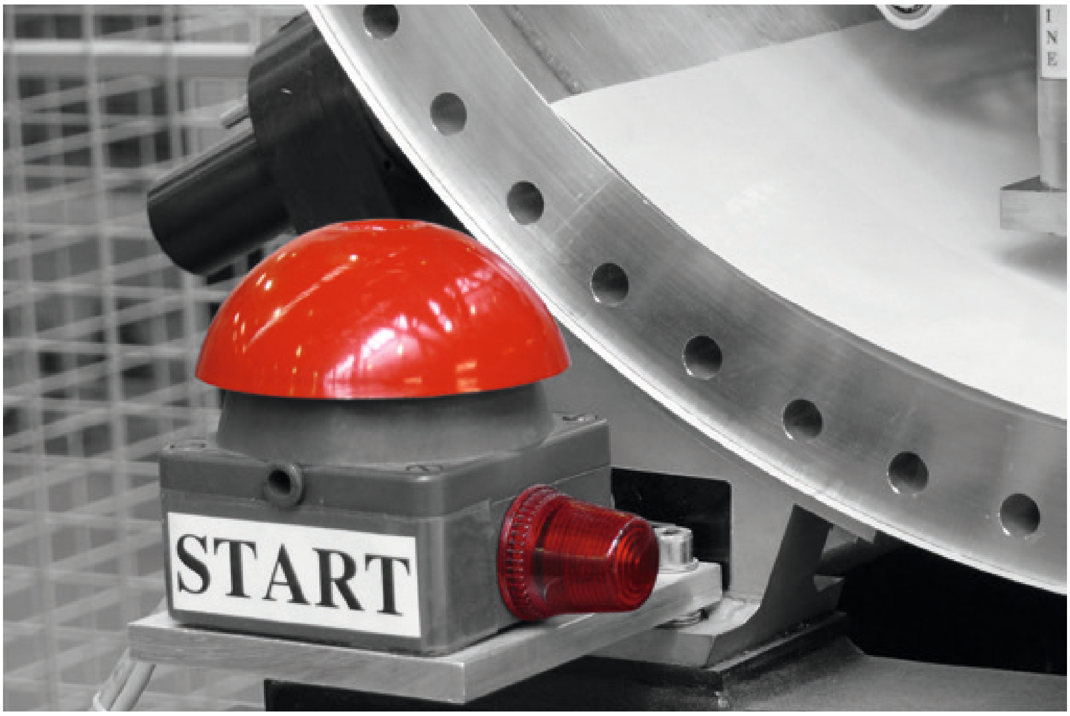
TRANSFER INTO INDUSTRY AND SOCIETY


CROSS-SECTIONAL ACTIVITY AT HZB

EXECUTIVE SUMMARY



AIM AND GENESIS OF THE STRATEGY PAPER “TRANSFER INTO INDUSTRY AND SOCIETY”

The new *Hightech-strategy* (HTS) of the German government aims to bring forward Germany as a Leader in Innovation. Based on the discussion regarding the new HTS and inspired by the key policy paper “Strategische Weiterentwicklung des Technologietransfers in der Helmholtz-Gemeinschaft” of the Helmholtz Association, a working group at HZB developed a new strategy for HZB’s Transfer into Industry and Society. In this strategy paper, the goals and measures for an improvement of Transfer into Industry and Society in the near future are put forward. Primary addressee of this strategy paper is HZB’s Board of Governors and HZB’s perspective commission. Based on insights from structuring the HZB research work (↘ strategy papers “Energy Material Research”, “A strategy for the photon source BESSY II” and “A road to BESSY III”) options will be generated to deliberately offer and transfer results and know-how of Energy-Materials-Research to Industry and Society.

The strategy paper was presented to the Science and Technology Board (Wissenschaftlich-Technischer Rat / WTR) for discussion. The executive summary was discussed by the Scientific Advisory Council (SAC) in November 2014.

STATUS QUO OF TRANSFER INTO INDUSTRY AND SOCIETY AT HZB

An important element of the mission of the Helmholtz Association and HZB is transferring knowledge and technology to the industry and society. HZB meets its obligation to provide the results of its research to the public through Transfer into Industry and Society.

HZB benefits from Transfer into Industry and Society through:

- third party funding, revenues from cooperation and licensing resulting in an increased budget for its scientific activities, to reinvest these in research and to maintain know-how,
- higher status of the HZB from industry’s perspective and subsequently stronger

evaluation results in the POF evaluation for example, and
- joint development and equipment qualification with suppliers of scientific components.

Compared to other Centers within the Helmholtz Association, HZB maintains a mid-position in its acquisition of third-party funds (the third-party funding rate today is 17 % of the total budget, third party funding here includes both competitive funding from public sources and direct funding from industry). This reflects HZB’s mission of operating two large-scale research facilities and providing service for the user community. This absorbs human resources that would otherwise contribute to third-party funded projects.

Instruments currently used for Transfer into Industry and Society at HZB

- contract research (R & D agreements, services),
- protection of property rights and licensing,
- spin-offs, and marketing activities facilitating the transfer of scientific results into industry,
- through use of high-tech devices and equipment (collaborations and user agreements),
- communications to media and the public, teaching, and advanced training.

MAJOR ACTORS AND FUTURE TRENDS

Besides the shareholders (government and Land) other Major stakeholders of the HZB in terms of the Transfer into Industry and Society are the Society, the federal government, the centers of the Helmholtz Association, the Industry and also the scientific community and the HZB employees.

Society expects benefits from research that receives support from and is facilitated by public funding. In Germany the public recognizes the importance of basic research, even when it does not produce immediately tangible or marketable results, and of applied research. Technologically oriented basic research and applied research are supposed to address socially relevant challenges (such as healthcare or energy supplies) and to contribute to securing the standard of living.

Research policies over the last decades have increasingly emphasized the importance of the interaction between science and industry. Proof of innovations made possible through basic research will be increasingly demanded of HZB and increasingly viewed as an assessment quantity for the success of HZB by its stakeholders.
The **Centers of the Helmholtz Association** recognized the improvement in Technology Transfer to be made and agreed in a key policy paper in spring 2014 entitled “*Strategische Weiterentwicklung des Technologietransfers in*

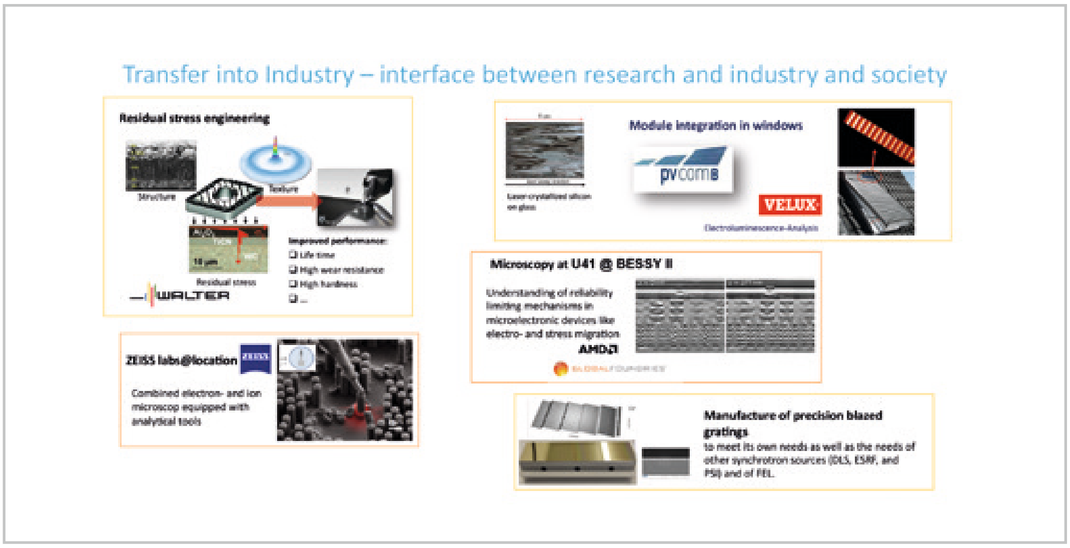


Fig. 1: Transfer into Industry – interface between research and industry and society

der Helmholtz-Gemeinschaft"[1] (Strategic Development of Technology Transfer in the Helmholtz Association). This key policy paper expresses the view that the transfer of knowledge and technologies into society and industry is part of the mission of the Helmholtz Association. This applies to basic research with its long-term orientation as well as to application-oriented research. The Helmholtz Centers have stated the following common goals for their technology transfer activities:

- establishing a transfer culture,
- expansion of inducements for transfer and commercialisation,
- a stronger connection between commercialization strategies and research planning, and
- professionalization of transfer support (expertise, organisation, and tools).

Industry and commerce have an interest in well-organized transfer of knowledge and technology, basic as well as applied research. Technology companies expect consulting services, involvement in externally funded projects, and education and training of specialized personnel.

For the **organisational units of HZB** Transfer into Industry and Society can provide options for career development for their young scientists and technical staff and thus make them attractive for PhD students and technical staff in an early career stage. Transfer into Industry and Society can be an opportunity to establish technology-oriented companies and creating patents and licenses.

Based on the analysis of the interests of the Major Actors, HZB has identified the following future trends:

- In order to be able to solve the grand challenges facing **society**, science has to perceive itself as a provider of solutions.
- HZB core competences (energy-material research and research infrastructure) create opportunities for Transfer into Industry and Society and can meet the Industry's needs for technical solutions in the sustainable energy conversion and storage.
- As a result of the energy policy, the Industry claims an increasing interest for renewable energy technologies. Taking this chance and for support, HZB needs to be open for technologies and application oriented solutions.
- In order to be perceived by the **funding bodies** – BMBF and SenWTF – as contributing to wealth creation in Germany and Europe the relevance of HZB and its research results must be apparent to regional and national companies.
- In order to enhance its performance in the Transfer into Industry and Society HZB has to increase its visibility in **industry** and has to analyze the requirements of industry.
- The **funding bodies and the society** expect HZB to contribute to Transfer into Industry and Society by innovation. In order to turn ideas and inventions of its research activities into marketable innovations, the HZB needs to establish a process to identify the potential of inventions.
- Success in Transfer into Industry and Society has become a relevant criterion for the **POF** evaluation process and thus for HZB's future funding. In order to excel at the POF-assessment HZB has to improve its Transfer into Industry and Society.
- In order to gain **societal relevance**, the HZB should furthermore participate in cooperation and interdisciplinary projects between science and industry, funded by federal and Land sources.
- The **scientific community** and HZB's researcher expect access to complex and partly unique infrastructures for their research. These infrastructures also need to be available for industry.
- The **institutional funding** of HZB must be utilized for the operation and maintenance of the scientific facilities. At the same time, effective Transfer into Industry and Society requires resources both in budget and manpower. In order to use the available resources efficiently, HZB has to find the right balance between Transfer activities and its core activities to ensure basic research remaining competitive; in this regard, know-how and expertise in technology and processes relevant for Transfer into Industry and Society have to be developed and maintained.
- In order to evaluate the performance of Transfer into Industry and Society and the efficient use of its resources, HZB should

1 "Strategic Development of Technology Transfer in the Helmholtz-Association", Key policy paper „Strategische Weiterentwicklung des Technologietransfers in der Helmholtz-Gemeinschaft", passed the general meeting of the Helmholtz-Association, 10.04.2014

develop and define criteria to measure the success of Transfer into Industry and Society.
- To transform ideas and inventions from research activities into marketable innovations, HZB (even with external consulting) needs to create processes and initiate a cultural change.

GOALS AND MEASURES

Based on the analysis of stakeholder development and the future trends HZB has identified the following action fields for Transfer Activities:

1 **Visualize the achievements and benefits of transferring knowledge and technology,**

2 **Stimulate inventions and improve innovation performance at HZB**

3 **Creation of a corporate culture**

4 **Transfer into Industry and Society as an interface between research and industry and society**

Action field 1

Transfer into Industry and Society

GOALS

1. Transfer into Industry and Society incorporated into the Missions-Statement of HZB (2015)
2. A regular structured report of achievements in Transfer into Industry and Society including revenues is provided for each HZB organizational unit to the internal and external panels of HZB (2016)
3. Increase of revenues from Transfer into Industry and Society by 10 % (2019)
4. Bi-annual awarding of the Technology Transfer Prize (2016, 2018, 2020)

EXAMPLES OF MEASURES

- Results from Transfer into Industry and Society are provided in internal and external evaluations of HZB organizational units (OU) results. Achievements in Transfer have an impact on internal funding and performance bonuses.
- Results in Transfer into Industry and Society are assessment criteria for
  – heads of HZB organizational units and key staff positions.
- Deficiency guarantees provided by HZB to enable hiring and employing well-trained

Fig. 2: HZB Technologies for Industry

personnel, experienced in dealing with industrial projects if adequate revenues have been provided by the organizational units in the past. Stronger support from OUs that are involved in industry-related research:
- Establishing regulations for using measurement stations, devices, and equipment operated by the respective OUs for industrial applications
- Creating financial incentives for the OU for activities concerning Transfer into Industry and Society e. g. bonuses for patent applications or contract measurements for industry

Action field 2

Allocation of Third Party Funding in order to strengthen (the strategy of) HZB

GOALS

1. Increase of Third Party Funding by 20 % (2019)
2. Increase the numbers of ERC-Grants, on the basis of the 2015 numbers 3 new ERC Grants (2019)
3. Establishment of a project monitoring, which entails structured processes and reports (2016)
4. Increased success rate of Third Party proposals from 66 % in 2014 to 75 % in 2017

EXAMPLES OF MEASURES

- Regular updates about the possibilities of Third Party Funds for heads and key staff of HZB's OUs
- Establishing proactive activities in order to identify Third Party Funding sources
- Presentation of funding, costs and achievement for all projects to the internal panels
- Establishing of a structured project management and controlling for Major projects (> 5 Mio. Euro)
- Establishing an internal HZB forum for discussing Third Party proposals

Action field 3

Creation of a corporate culture

GOALS

1. Annual Information events for various occupation groups referring the options concerning Transfer into Industry and Society (2015, 2016, 2017, 2018, 2019, 2020)
2. At least one spin-off company by HZB staff every two years (2016, 2018, 2020)
3. One proposal per year at the Helmholtz validations fund or Helmholtz enterprise fund (2016, 2017, 2018, 2019, 2020)
4. Maintain the number of patent applications and increase the revenues of licenses by 10 % (2019)
5. Bi-annual report about benchmarking of Transfer into Industry and Society in comparison with 6 institutions of science or research (2015, 2017, 2019)
6. Annual report about the realization of the action recommendations stipulated in the Key policy paper of the Helmholtz Association (2015, 2016, 2017, 2018 , 2019, 2020)

EXAMPLES OF MEASURES

- Creating awareness for commercialization and protection of intellectual property for staff members
- Publication of scientific and technical results in national and international journals, and news reports aimed at the industry
- Bonus systems, back flow of funds from contract research (or licensing or services) to OUs allowing the development of working conditions and of the research infrastructure.
- Provision of financial support of collaborations and interdisciplinary projects with industry

Action field 4

Transfer into Industry and Society as an interface between research and industry and society

GOALS

1. Establishment of an industry advisory board (2016)
2. Establishment of a position as „Contact-Point“ (originated in industry) (2016)
3. Annual assessment of all Transfer activities enabling adjustments and reorientation; annual meetings searching options for commercialization (2015, 2016, 2017, 2018, 2019, 2020)

EXAMPLES OF MEASURES

- Establishing an unit for Transfer to professionalize the transfer management:
  - Act as a contact for companies interested in innovation
  - transmitting research advances to technologies
  - Act as a communicator to companies and society
  - visualization of the patent portfolio of the HZB and advertising the potential of the scientific facilities; set-up and recovery of contacts to industry
  - competitive advantage through protected property rights
  - marketing of the technologies by structured acquisition
  - detailed market research to discover the intersections of HZB know-how and the requirements of industry
- publication of remarkable results within Transfer into Industry and Society in internal and external media, supporting publication which increase visualization, accessibility via social media
- attendance and representation at exhibitions
- Facilitating internship at industrial facilities through close cooperation
- Setup of an Alumni-Network

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