

# **Strategy Paper on Neutron Research in Germany: 2020–2045**

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## 1 Summary

- From the outstanding scientific advances achieved with neutrons during the pioneering years to solutions of the grand scientific and technological challenges of the future: research with neutrons is and will remain at the forefront of science. In an ever-increasing number of disciplines, it provides unique information on condensed matter over many orders of magnitude in space and time.
- Research with neutrons **provides indispensable techniques** to solve scientific problems in materials research and is complementary to photon techniques (e.g. synchrotrons, FELs). Neutron techniques offer **unique characteristics** especially for investigations of magnetic properties or light elements, an indispensable tool in application-oriented fields like energy, mobility, IT or pharmaceutical research, that complements exciting improvements of photon techniques. There is a **high demand of using neutrons**, especially in materials science, research on soft matter and quantum materials.
- The availability of high-performance neutron sources with an optimized/coordinated range of instruments is an important research policy task for Germany and Europe. Within Germany, it is the mission of the Helmholtz-Association to operate large-scale facilities.
- A network of national and regional neutron sources is most important. This network must provide a co-operating eco-system with low flux experiments up to European top-class sources for neutron science, including both, continuous and pulsed sources.
- The status quo in Germany is based on a concentration of efforts on the Heinz Maier-Leibnitz Zentrum MLZ, while the research reactors of the Helmholtz Centers FZJ, HZG and HZB were permanently shut down in 2006, 2010 and 2019, respectively. In fact, 2019 saw the closure of three European research reactors central to the decades of success in the European neutron landscape: Orphée, used by the Laboratoire Léon Brillouin (LLB) near Paris, BER II at the Helmholtz-Zentrum Berlin, and JEEP II operated by the Institute for Energy Technology outside Oslo.
- The Heinz Maier-Leibnitz Zentrum MLZ is the German national neutron facility and one of the leading facilities worldwide. It brings together the main players in research with neutrons in Germany, offers outstanding instrumentation, education and professional user service. This statement was substantiated by an international MLZ review in late fall 2018 which attested MLZ an outstanding performance.
- It is of utmost importance that the cooperation contract between the MLZ partners, the Technical University of Munich (TUM), the Forschungszentrum Jülich (FZJ) and the Helmholtz-Zentrum, Geesthacht (HZG), is prolonged past the present term of 31st December 2020, keeping the established and successful cooperation scheme. As the number of facilities producing neutrons will decrease further, the capabilities of MLZ have to be expanded. Therefore, the new cooperation contract has to include an upgrade program for MLZ, the **“Vision MLZ2030”**. One element of this upgrade program is the transfer of suitable instruments from BER II to MLZ after 2020.
- The Institute Laue Langevin ILL in Grenoble has the role of the European top-class source and is the world-wide leading facility. It has the highest scientific output of all neutron facilities, underpinning the European leadership in this field of research. With the endurance program, ILL is currently extending its capabilities and capacities, securing its cutting-edge instrumentation. An agreement between the associates of ILL (France, Germany, United Kingdom) on the further operation of ILL after 2023 for another ten years is essential for a successful scientific exploitation of these investments in ILL’s instrumentation.

- The European Spallation Source ESS will be the most powerful spallation neutron source worldwide and is expected to play a leading role in the future. It will take a decade from the first proton hitting the target until all instruments at ESS are fully functional. It is therefore essential for the European neutron community that there remains an **overlap of the operation of ILL, ESS and the network of medium flux sources**.
- Together with international partners, Germany is building seven instruments for the **European Spallation Source ESS**. Moreover, it will deliver the moderator-reflector assembly and contribute to several work packages in instrumentation, sample environment and scientific computing. Thus, Germany is contributing to the future success of the ESS with the proven expertise in method development of its neutron community.
- The high-flux reactor **PIK** currently commissioned in Gatchina (Russia) could complement research opportunities in Europe in the medium to long term range. German involvement in the construction of instruments and components, their scientific use, and the establishment of an international user centre is an option within the Russian-German Roadmap.
- The future of neutron research will be complemented by **Compact Accelerator driven Neutron Sources (CANS)**. These conceptually new sources will be necessary to have a functional and resilient network, together with established science at reactors and spallation sources.
- **Compact accelerator driven neutron sources** have the potential to add value to the network of neutron facilities and provide a basis for the efficient use of top tier sources as ILL and ESS. CANS are scalable (also in price), don't need nuclear licensing and are inherently safe.
- The Jülich **High Brilliance Source project HBS** is a CANS which aims at a full-fledged medium size facility designed to maximize beam brilliance. It responds to the increased demand for experiments on small samples such as systems of biological macromolecules or nanomagnets. Together with other similar European sources, the HBS serves to fill the gap in instrument days anticipated with the ongoing closure of older neutron sources. A conceptual design report (CDR) for the HBS has been worked out by JCNS with many partners.
- **NOVA ERA ("Neutrons Obtained Via Accelerators for Education and Research Activities")** denotes a smaller version of a CANS, for which a CDR has been worked out by JCNS. Given its relatively low cost and its simplicity of operation, this type of source can revolutionize research with neutrons with the new paradigm to "bring neutrons to the users instead of users to neutrons". NOVA ERA type sources can become central facilities for universities, industry, museums or other research related institutions. Thereby, NOVA ERA devices could provide neutron diffraction and analysis methods accessible on-site, for the first time.
- With the changing European neutron landscape, coordination between the neutron facilities is becoming increasingly important. To this end, the **League of advanced European Neutron Sources (LENS)** has been founded. Working groups address pressing questions from European strategy all the way to research, education and application in a common manner.

## 2 Introduction

The development of new high-performance materials and more efficient active pharmaceutical agents is among the grand challenges facing our society. Tailor-made materials and material systems are required for all key technologies, from information technology, renewable energy concepts to more environmentally friendly transport systems and biocompatible medical applications. Many of these future materials, material systems and active pharmaceutical agents will be synthesized on the atomic or molecular level. This requires state-of-the-art, high-resolution (in situ) analytical methods to control the processes in a reliable manner.

Neutron probes are one of the pillars of the analytical techniques applied to solve these grand challenges, and are - due to the characteristics of neutrons – especially suited to investigate magnetic properties, light elements or big samples. They thus are especially suited to address scientific questions arising from grand societal challenges. Advanced neutron sources are large-scale instruments used in numerous disciplines across the entire range of science and technology development. The European GENNESYS Study (2009) summarized the future demand for analytical techniques involving X-rays and neutrons for all areas of research and technology development up to and including industrial applications /1/.

Germany is considered to be one of the pioneering countries in the development of modern neutron research. Its reputation is based on the design of powerful neutron sources and novel instruments as well as their scientific use.

Making available state-of-the-art high-performance neutron sources with an optimized range of instruments is an important research policy task for Germany and Europe. Within Germany, it is part of the mission of the Helmholtz Association to design, construct and operate large-scale facilities for users.

## 3 Note on the range of applications of neutrons in research as compared to other analytical methods

Materials research can provide many contributions to solve grand challenges that are currently on the political agenda. It is therefore one of the crucial technologies for Germany and Europe. Neutrons are one of many types of probes that have proven to be essential for understanding the structure, dynamics, and function of materials. Other important probes used for state-of-the-art materials analysis include X-rays, electrons, methods such as NMR, as well as different types of optical microscopes and scanning probes (STM, AFM, etc.) often combined with High Performance Computing.

In modern solid-state and materials research, these methods are often used to complement each other in gaining as complete a picture as possible of complex materials and processes by combining different types of information. This observation was driver for the foundation of a multi-method platform at FZJ, striving to integrate multimethod analysis based on the above techniques more deeply into research.

The specific properties of neutrons provide information that cannot be obtained with other methods. These characteristics include:

- the nature of the interaction of neutrons with matter, which facilitates the observation of particularly light elements (e.g. hydrogen and lithium) and usually provides high contrast even between neighbouring elements in the periodic table,
- the energy of the neutrons used for scattering experiments, which is within the range of typical excitation levels for lattice vibrations, magnetic excitations, as well as diffusion and tunnelling

processes, makes neutrons a particularly suitable probe for studying the dynamics of materials,

- the high penetration depth for studying large objects or in complex sample environments,
- the magnetic dipole moment, which enables a simple analysis of magnetic structures and spin-based quantum phenomena,
- the very low radiation damage in comparison to X-rays and electrons (which is particularly important for biomaterials), and
- the sensitivity for different isotopes of an element.

It is often a combination of several of these properties that is crucial for analysing a material.

We give an example from applications-oriented research for future energy systems: using neutrons to study the processes that occur in a hydrogen tank during the filling process provides a wealth of information, because neutrons combine a high penetration depth (through the tank) with a high sensitivity for hydrogen. Such information, obtained at the German Engineering Materials Science centre (GEMS) of HZG, is of great significance for the development of modern hydrogen storage technologies.

In Germany, there are research groups, namely in solid-state and materials research, that use the entire analytical portfolio of synchrotron radiation, neutron methods, and electron methods (microscopy, spectroscopy) on a regular basis. Whether neutrons or other methods are more suitable always depends on the individual case, for example:

- In modern materials for spin-based information technologies (spintronics), functionalities are often based on complex magnetic structures. An example are multiferroics, which allow very energy efficient switching of the magnetic state under application of an electric field. Neutrons are typically used as a probe for magnetic structures and virtually all known magnetic structures have been obtained from powder- or single crystal neutron diffraction. The development of resonant magnetic X-ray scattering has enabled important new methods of analysis due to its element selectivity and capability of differentiating between the spin angular momentum and the orbital angular moment. However, the absolute determination of the total magnetic moment is often only possible with neutrons due to the much less complex magnetic interaction.
- State-of-the-art electron microscopy methods provide structural information with the highest resolution. However, this information is only available for thin samples prepared in a complex process and for surfaces, and the statistical information provided is limited due to the small volume of the samples that can be studied using this method. X-ray or neutron scattering considerably increases the information depth because samples with a larger volume can be studied; neutrons are the method of choice when their specific properties listed above are required (e.g. prevention of radiation damage and contrast variation by substituting isotopes, etc.).
- Neutrons can excel in providing a deeper understanding of condensed matter through combining experimental results from neutron spectroscopy with modern super-computer based up-initio theories or (Monte Carlo-, molecular dynamics-, micromagnetic-, ...) simulations. Neutron spectroscopy provides unique information on dynamic properties of condensed matter. Computer modelling of the inelastic neutron scattering cross sections allows one to obtain parameters of model Hamiltonians, such as inter-atomic forces or exchange constants, which enable the prediction of the macroscopic response of a material and thus lead to a microscopic understanding of the relation between structure and function. Neutron spectroscopy gives direct access in absolute units to self-, pair-, and spin-correlation functions,

which are the fundamental quantities derived by modern ab-initio theories or simulations. Thus, the simplicity of the neutron cross sections and the fact that they can be measured on an absolute scale allows benchmarking of ab-initio theories and computer modelling with huge impact in many different scientific fields. In this important aspect, neutrons are unrivalled, as no other method can provide such stringent test of microscopic theories.

## 4 Future scientific applications of neutron research

Already, neutrons have a wide range of applications in research and development. In the next years, we see several important areas of research, from

- **energy**, where light elements play the decisive role in the energy revolution striving towards the increased use of renewable energy sources. Examples include developing of economically attractive hydrogen storage systems, light weight batteries (Li, Na) or novel materials for electrolytes,
- **medicine and health**, where one aspect will be “drug design” and “drug delivery”,
- numerous applications in the fields of **engineering** and **industry**,
- to **quantum technologies of the 2<sup>nd</sup> quantum revolution**, which have a huge potential to revolutionize many aspects in technology and computing.

A more detailed description of the future flagship areas of research with neutrons can be found in the appendix. Additional information on future areas of application for neutrons in research and technology development are outlined in the German Committee for Research with Neutrons (KFN)'s 2013 framework paper on neutron research for the scientific challenges of the future (“Neutronenforschung für die wissenschaftlichen Herausforderungen der Zukunft”) /3/. More recently, the European Neutron Scattering Association ENSA published a brochure “Neutrons for Science and Technology” /4/ and further material can be found on-line at “Neutronsources.org” /5/. Aspects of a science case specific for CANS are detailed in /11/. These areas of application include fundamental studies on the structure and dynamics of matter as well as energy research, materials research, and research on active pharmaceutical agents.

## 5 Status and perspective of neutron sources worldwide

### 5.1 Situation as of 2019

The leading position of Europe in research with neutrons is based on national sources, which cater for the large number of users who perform experiments that do not necessarily require the highest neutron fluxes, and also on transregional top-class facilities for the cutting edge of neutron research.

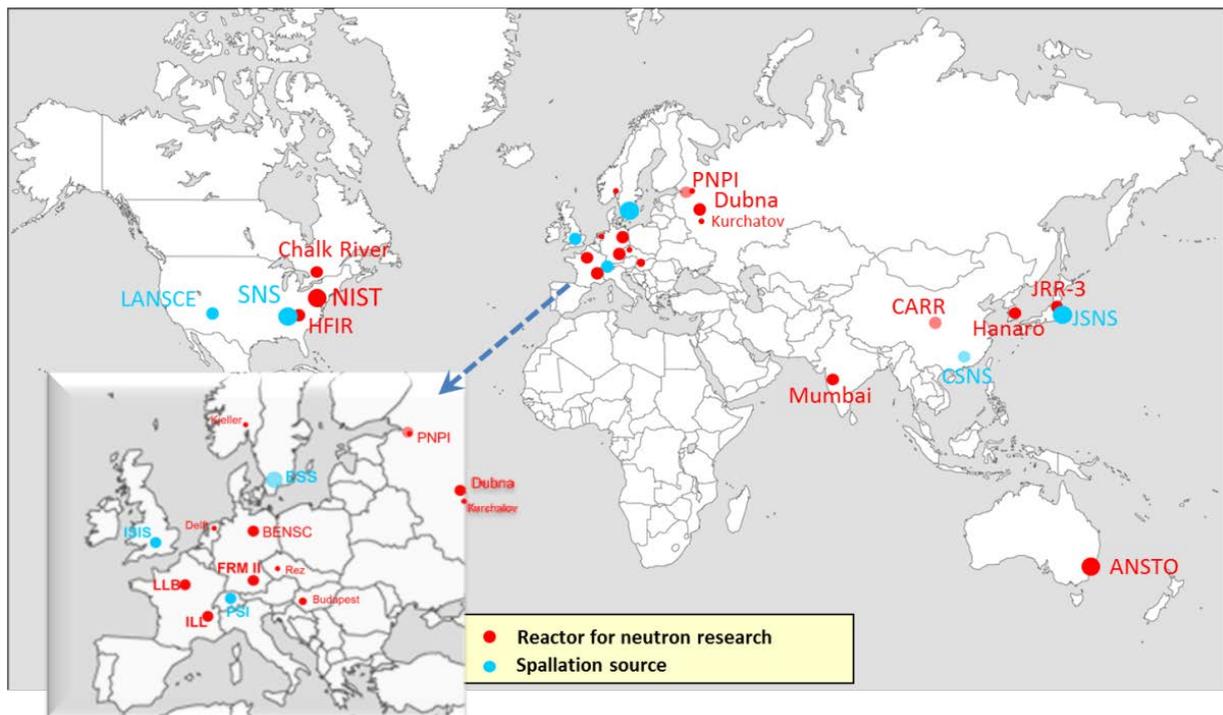


Fig. 1 Major worldwide neutron facilities for beam-tube experiments (BENS designates the user centre at the BER II reactor in Berlin). In 2019, the reactors JEEP II in Kjeller, Norway, Orphée in Saclay, France and BER II in Berlin, Germany, were permanently shut-down.

The most important national sources in Europe are SINQ at PSI (Switzerland), ISIS in Rutherford Lab (UK), and FRM II of MLZ (Garching) in Germany. The French national research reactor, Orphée of the Laboratoire Léon-Brillouin LLB, the BER II reactor of HZB in Germany, and the JEEP II reactor in Kjeller, Norway, were permanently shut down during the year 2019, leaving a large gap in the European neutron landscape. The transregional top-class facility in Europe is currently the Institute Laue-Langevin (ILL) in Grenoble (France), which has the highest-flux reactor (HFR) and the highest number of instruments (approx. 40). ILL also takes a leading position in an international comparison. There are few large centres world-wide that combine a high neutron flux with a broad range of instruments (see Tab. 1 and Fig. 1). At all of these centres, beam time is allocated in a peer-review process by independent experts. The overbooking factor is typically 2 to 3.

Outside Europe, apart from the MW spallation sources SNS at ORNL in Oak Ridge, USA, and JPARC in Tokai, Japan, above all NIST in Gaithersburg near Washington D.C., USA ( $2 \cdot 10^{14} \text{ n/cm}^2 \text{ s}$ ) and the HIFR reactor at ORNL ( $10 \cdot 10^{14} \text{ n/cm}^2 \text{ s}$ ) are of particular importance. In the Asia-Pacific region, the OPAL research reactor was put into operation in 2007 at ANSTO in Sydney, Australia, ( $2 \cdot 10^{14} \text{ n/cm}^2 \text{ s}$ ), and South Korea operates the Hanaro reactor, which has a comparable flux. China, with its expanding economy, has realized the importance of research with neutrons for the development of innovative materials. User facilities are the CARR reactor near Beijing ( $8 \cdot 10^{14} \text{ n/cm}^2 \text{ s}$ ) and the CSNS spallation source in Dongguan, which went into operation in 2017, hosts 3 instruments and is designed for a beam power comparable to ISIS target station one (100 kW) at present. Upgrade plans to 500 kW and a full instrument suite exist.

Facility (Source)	Start of operation	Thermal power [MW]	Nominal integral flux [ $\text{cm}^{-2} \text{s}^{-1}$ ]	Nominal peak flux [ $\text{cm}^{-2} \text{s}^{-1}$ ]	Nominal op. time [days/a]	User instruments	Potential no. of instruments	User stays /a	Ann. op. budget
<b>MLZ (FRM II)</b> (special role of univ.) <b>national</b>	2005	20	$8 * 10^{14}$		240	26 operational 8 under construction + positrons	35	1000	€ 55 m + fuel cycle
<b>ILL (HFR)</b> <b>25 %</b>	1971 (1995)	58	$1.5 * 10^{15}$		200	29 + 10 CRG + 4 jointly funded	> 40	1600	€ 103 m + CRGs
<b>ESS</b> (under negotiation)	under construction  (first user oper. planned for 2023)	5 MW LP		$4 * 10^{16}$	200	15 initial	> 22		€ 140 m
<b>PIK</b>	under construction  (user operat. planned for approx. 2025)	100 MW	$1.5 * 10^{15}$			approx. 25	up to 40		---
<b>SINQ</b> ----	1996	1 MW cont.	$1.5 * 10^{14}$		180	17	20	800	€ 30 m
<b>ISIS/ISIS-II</b> ----	1985/ 2009	nom. 160 + 32 kW (TS1 & 2)		$4.5 * 10^{15}$	120	20 + 11	35	1500	€ 55 m
<b>IBR-2</b> BMBF Dubna contract	1984/ 2010	2 MW	$10^{13}$	$10^{16}$	108	13 public	20		

Table 1: Relevant neutron sources in Europe (sources highlighted in colour play an important role in the national roadmap)

## 5.2 Changing European neutron landscape

Over the last decades, the success of research with neutrons has been based on the network of medium flux sources supporting ILL as the flagship facility. This network largely consisted of research reactors. Most of them have reached or are reaching the end of their lifetime. Examples for important research reactors, which have been closed are: Siloé (Grenoble, France) in 1997, DR3, (Risoe, Denmark) in 2000, FRJ-2 (Jülich, Germany) in 2006 and FRG-1 (Geesthacht, Germany) in 2010. The JEEP II reactor in Kjeller, Norway, will not start up again and two important neutron research reactors have been taken out of operation by the end of 2019: BER II (HZB, Berlin, Germany) and Orphée (LLB, Saclay, France). The present status and future perspectives of neutron scattering facilities in Europe has been analysed by the neutron landscape working group of the European Strategy Forum for Research Infrastructures ESFRI in 2016 /6/. A main result is depicted in Fig. 2, which shows the possible future development of the number of instrument days, i.e. the number of days of facility operation times the number of instruments. A drastic decrease occurs when major facilities such as Orphée, BER II and eventually ILL are shut down. The reduced availability of neutron instrument days and the concentration on very few facilities represents a threat for this field of research – and for the respective application fields. A possible way out is discussed in section 5.3.

In terms of instrument days, MLZ will then be the most important reactor-based facility in Europe, complemented by the UK national spallation source ISIS in Rutherford Laboratory. MLZ will provide a basis for education and method development for the German user community and facilitate a huge number of experiments, which do not require the highest neutron flux. However, MLZ will not be able to fully compensate for the loss of beam days within Europe. On the other hand, instruments at ESS will outperform the best existing neutron instruments by several orders of magnitude of its peak flux. They will enable entirely new science to be done and not “just more of the same”. The ESS is being realized in a truly European effort (with 17 countries participating) from the very start. It will become the world leading neutron facility within a decade after the first ramp up of its accelerator (first beam on target expected end 2022) and allow German neutron users to perform experiments, which are not possible elsewhere. Especially during its ramp-up phase to full operation, expected to cover the first ten years, ESS will be strongly dependent of other neutron sources like ILL, MLZ SINQ and ISIS that allow testing, development of instrumentation and preparation of experiments. Thus, focusing all efforts on ESS will hinder the functioning of the whole eco-system of neutron sources.

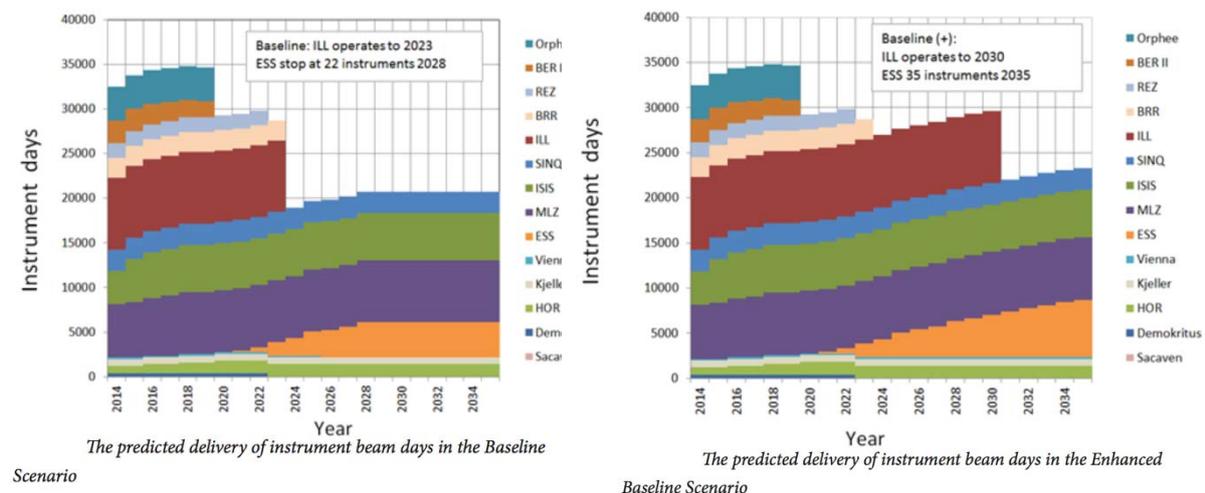


Fig. 2 Two scenarios for the development of the delivery of instrument days discussed in the ESFRI Neutron Landscape Report /6/.

### 5.3 Future Sources: Compact Accelerator Driven Neutron Sources CANS and the project of High Brilliance Neutron Sources HBS

Recent technological and scientific developments open the path to new types of neutron facilities. These provide a response to the changing neutron landscape in Europe by offering the possibility to add to the network of research reactors, which will be shut down due to being over their prime, with neutron sources based on low energy ion accelerators. Due to societal opinion and political aspects, a replacement by new reactors is extremely unlikely, although a combination of neutron origins would be preferable. Such sources are simple to operate as in most countries they do not require nuclear licensing. They are scalable and allow one to realize neutron facilities adapted at one's need and budget. Small sources with a limited set of instruments (e.g. diffraction, small angle scattering, reflectometry, imaging or prompt gamma activation analysis) can serve as central facilities at universities, industry, museums etc. Full-fledged high-performance sources offer instrumentation which can compete favourably with existing state-of-the-art instruments, but for a significantly lower price-tag. Thus, such Compact Accelerator Driven Neutron Sources **CANS** can fill the gap opened by the decommissioning of research reactors in Germany by providing for specialized experiments, regional user needs and recruitment, user education, method development, or mere capacity and capability. These tasks cannot be realized at facilities like ILL or ESS alone, due to the sheer number of users there.

Smaller sized CANS with their relatively low cost and simplicity of operation, can revolutionize research with neutrons with the new paradigm to "bring neutrons to the users instead of users to neutrons". Having a neutron source at hand, just like a laboratory instrument, allows one to develop new neutron techniques and to train students (e.g. at universities), to shorten the development and optimization cycle in materials design by providing immediate feedback from neutron analytics into the production process (e.g. for industry) or to avoid risky transport of valuable artefacts to distant facilities for inspection (e.g. at museums). At JCNS in Jülich, a Conceptional Design Report CDR for a small CANS named **NOVA ERA** ("Neutrons Obtained Via Accelerators for Education and Research Activities") has been published in 2017 /7/. NOVA ERA type sources can be of high interest for industry applications. Examples include quality control in production, environmental science e.g. recycling of materials, or inspection of infrastructures.

Small CANS can spread neutron technologies and reach new user groups which require immediate feedback, e.g. in academics and industry. However, they have clear limits when it comes to more challenging experiments, including the entire field of neutron spectroscopy. For such applications, more powerful facilities are needed, which can be based on the same CANS principle. Trends in research with neutrons go to smaller samples, e.g. systems of biological macromolecules or nanomagnets. Therefore, JCNS is developing a "High Brilliance Neutron Source" **HBS** /8/ together with partners, which maximizes the beam brilliance and not the source strength as has been done in the past. Brilliance<sup>3</sup>, i.e. neutron flux per source area, solid angle of emission and energy interval, is conserved by conservative neutron optics and is thus the quantity, which determines the performance of an instrument if it comes to small samples. HBS type sources produce less neutrons than spallation sources, but use them much more efficiently. In this way, instruments at HBS perform favorably compared with instruments at today's medium flux reactor- or spallation based sources /12/, while the facility comes at significantly lower cost. Fig. 3 shows the layout of a typical HBS facility, which can host some 20 to 30 different neutron instruments. However, for the top-tier of experiments, spallation as realized at ESS, will remain the neutron production method of choice. The combination of ILL, MLZ and SINQ as continuous sources on one hand, and ISIS and ESS as pulsed spallation sources on the

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<sup>3</sup> Here we use the terminology of the German language area, while in the anglo-saxon language the term "Brightness" is used for the same quantity.

other hand, together with the described CANS facilities has the potential to lead neutron science from being at stake to a new prime.

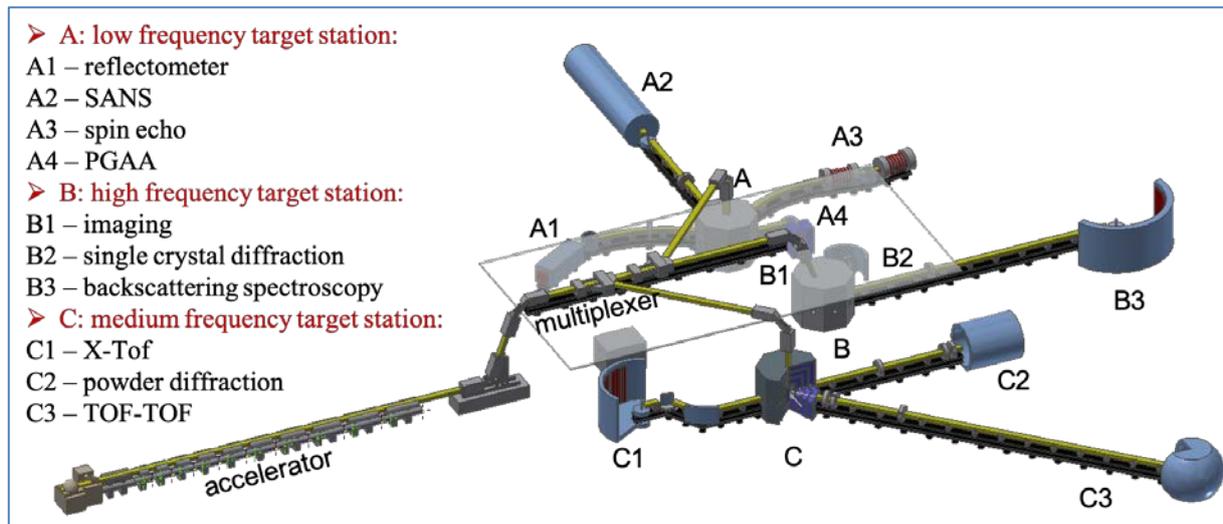


Fig. 3: Possible layout of a High Brilliance Neutron Source HBS. Instrument with the same requirement for pulse time structure are grouped around the same target station. Different target stations with different pulse structure are being deserved by multiplexing the ion beam from the accelerator. Each instrument has its own dedicated moderator /8/.

## 5.4 Cooperation of Neutron User Facilities in Europe: the LENS consortium

The **League of advanced European Neutron Sources (LENS)** was founded in view of the changing neutron landscape in Europe. LENS is a non-profit consortium formed to promote cooperation between European-level neutron infrastructure providers offering transnational user programmes to external researchers. The nine LENS founding members are: (1) Budapest Neutron Centre (BNC), Hungary; (2) European Spallation Source (ESS), Sweden; (3) Forschungszentrum Jülich (FZJ), Germany; (4) Heinz Maier-Leibnitz Zentrum (MLZ), Germany; (5) Institute for Energy Technology (IFE), Norway; (6) Institut Laue-Langevin (ILL), France; (7) ISIS Neutron and Muon Source, UK; (8) Laboratoire Léon Brillouin (LLB), France and (9) Paul Scherrer Institut (PSI), Switzerland.

The individual members remain independent but together through LENS join forces to support and strengthen European neutron science by creating an effective, collaborating eco-system of neutron facilities. The LENS activities are executed by standing and ad-hoc Working Groups on (i) Strategy, Promotion & Policy; (ii) Neutron Usage and Innovation; (iii) Synergies in Technological Development and Operation; (iv) Computing, Data and (v) Compact Neutron Sources. For more information on LENS, see /13/.

## 6 German user community

Germany has a long tradition of science-driven method development and instrument construction in neutron research and there is no doubt that it is one of the leading countries in this field worldwide. Germany has the expertise for building high-intensity neutron sources, as exemplified by the compact core design of FRM II and the development of spallation neutron sources.

The German Committee for Research with Neutrons KFN records about 1900 **registered neutron users** in Germany. They come from all sectors of the German science system (universities, Max Planck Society, Helmholtz Association, Leibniz Association and industry). This analysis shows an upwards trend compared to an analysis of the utilization of the high-flux reactor by the ILL Associates /9/, which shows that the HFR was used by **1300 users with a large number of publications from Germany** between 2000 and 2009 (France: 1700 [location of ILL], UK: 1100). A bibliometric study performed in 2016 provides a survey of peer-reviewed publications in the field of research with neutrons for the years 2005 – 2015 /10/. The survey resulted in 49769 individual publications in this period, giving an average publication record per year of 4524. More than half of all publications were published by European groups, see Fig. 4, left, which gives an update for the period 2005 - 2018. Within Europe the strongest countries are France (10109), Germany (10262) and UK (7164) (Fig. 4, right, update 2005 - 2018). Since the number for France contains all papers published with scientists working at the European facility ILL, it becomes clear that in terms of the number of publications, Germany has the most productive neutron user community in Europe /10/.

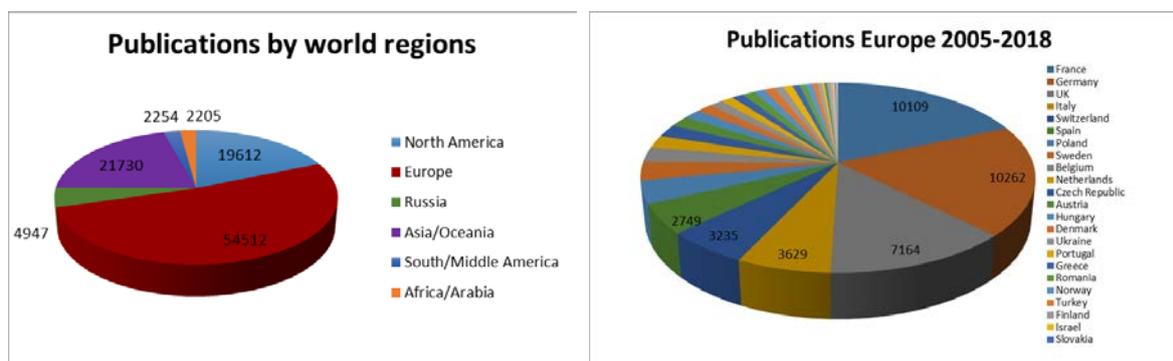


Fig. 4: Number of peer-reviewed publications in the field of research with neutrons in the period 2005 – 2018 classified by world regions (left) and countries within Europe (right) /10/.

One of the strengths of the German neutron user community is the strong networking between the operators of the neutron sources, the user facilities, and the universities. This network is supported by collaborative research funding (“Verbundforschung”, within the framework program **ErUM** – “Erforschung von Universum und Materie”) of the Federal Ministry of Education and Research BMBF, which enables groups from universities to set up instruments and ancillary equipment at neutron sources. This kind of support widens the range of opportunities developed for using the sources and for training excellent young researchers.

The scientific focus of the neutron users has changed substantially. Today, it is characterized by a multitude of scientific disciplines that are increasingly governed by current societal and scientific challenges instead of the conventional categories of science (see Fig. 5).

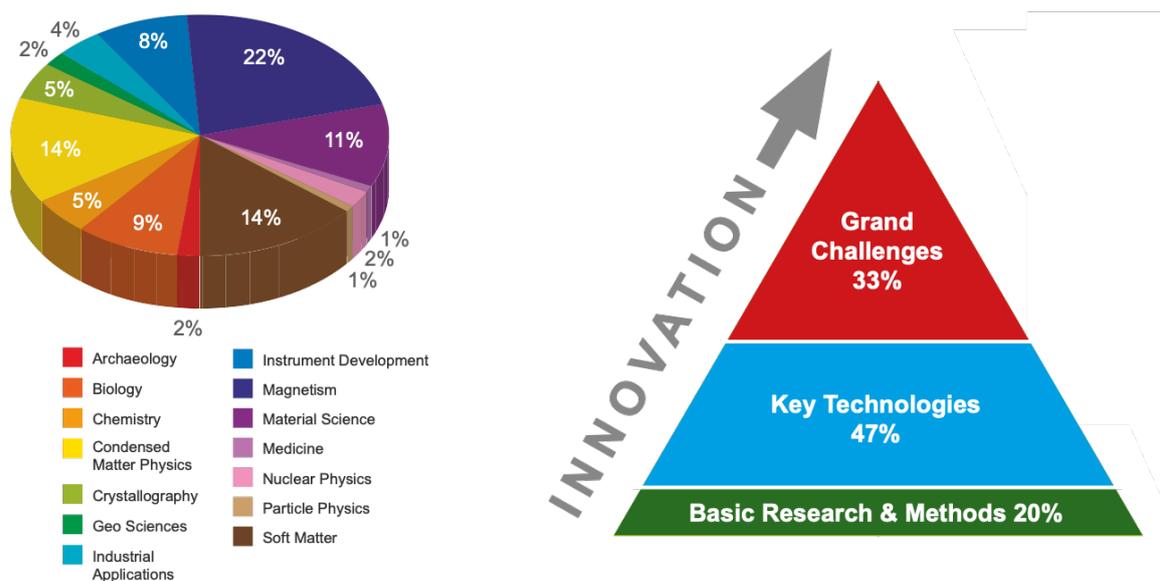


Fig. 5: Left: Distribution of performed scientific experiments at MLZ according to scientific fields 2014 – 2017 (taken from /14/). Right: The journal articles at the MLZ can be pictured as a pyramid: Basic Research & Methods (20%) required to tackle the Key Technologies (47%) and articles that address directly the Grand Challenges of our society today (33%) (taken from /15/).

## 7 National roadmap for neutron research 2020–2045

The long lead times for the realization of new neutron sources require long-term planning to ensure that science and industry can continue to work with powerful neutron sources in the future without any prolonged interruptions.

It is to be assumed, that Forschungszentrum Jülich and Helmholtz Zentrum Geesthacht HZG, will remain the most important research institutions in the Helmholtz Association for research with neutrons providing user support in the foreseeable future.

The experiments by German neutron users currently focus on the following sources:

- FRM II of MLZ in Garching / Munich,
- HFR of ILL in Grenoble.

German scientists also perform a considerable number of experiments at ISIS, SINQ, and the American reactor and spallation sources NIST and SNS. In 2019, two sources with major importance for German users, the BER II reactor in Berlin and the Orphée reactor in Saclay have been permanently shut-down.

The neutron landscape in Germany and Europe is set to change significantly during the next few decades:

- The European Spallation Source (ESS) is scheduled to be put into operation in the years from 2022 (first beam on target) onwards (2023 first science with three instruments).
- The high-flux reactor HFR (ILL) in Grenoble is expected to be operated until around 2030.
- The Russian high-flux reactor PIK in Gatchina will ramp up to full power till 2021 with commissioning of instruments expected to start in 2024.

**Based on this scenario of developments in the European neutron infrastructure, this paper proposes a national roadmap for neutron research for 2020 – 2045 that**

- takes into account the long-term strategic development of the portfolio of neutron sources to cover the demand of science and industry in Germany,
- taps the special potential of neutrons for research and innovation further,
- exploits future possibilities for German users from science and industry in an optimal manner,
- builds on the successful synergy between European top-class sources and a network of medium- and lower-flux sources,
- guarantees the operation of at least one national neutron source for research and training,
- and, at the same time, ensures that
- the financial margins for research with neutrons funded by Germany do not exceed the current order of magnitude,
- and that known international framework conditions/obligations are taken into account.

The following considerations are based on the assumption that neutron sources typically have an operating life of 40 to 50 years. A national roadmap 2020 – 2045 is outlined, starting with the relevant international and European sources, and then focussing on the national German facilities:

## 7.1 HFR, ILL, Grenoble

ILL is currently by far the leading neutron facility in the world, both in terms of the quality of its neutron beams and the instrument suite available. It provides German researchers with unique research opportunities. Germany bears about 25 % of the costs of the operation of the ILL in Grenoble. FZJ as the German Associate is directly involved in the user operation of three instruments in cooperation with other partners and contributes to two further instruments.

Future role and further plans:

- Negotiations started in 2018 for an extension of the ILL's Intergovernmental Convention for the period 2024 to 2033. Negotiations with ILL's Scientific Members towards renewing the membership agreements for the next five years will be concluded in 2020.
- Until the ESS is fully functional, operation and use of the ILL are of vital importance for the German research groups in order to contribute to the solution of the grand societal challenges of our age, in order to fully exploit the scientific, technological and financial asset of the ILL, namely the neutron source, the cutting-edge instrumentation and the skills and know-how of ILL's staff and users. The overlap between ILL and ESS operation should therefore be as large as possible, at least a decade, which is the typical time for ramp-up of a new large facility like ESS to full performance. This overlap is also necessary for the support of ESS in order to allow full functionality.
- Until then it has to be ensured that with appropriate investment into instrumentation, ILL stays top tier to maintain expertise and secure the leading position of Europe in research with neutrons (compare ILL Endurance program, see /16/).
- Since ESS alone cannot cover the future demand of neutrons, novel concepts have to be developed in time. The aim is to maintain a cooperating network of neutron sources serving different user demands. Existing facilities like ILL or MLZ can act as a nucleus for these developments. The establishment of LENS, currently chaired by the ILL director, Prof. Helmut

Schober, is an important step towards a closer collaboration and strategic development of neutron centres. The internationally recognized role of ILL with the system competence of its personnel and the existing infrastructure in terms of effective operation, instrumentation, sample environment, computing and user services offers an excellent opportunity to continue with a versatile follow-up project.

## 7.2 Contribution to the European Spallation Source ESS, Lund

The European Spallation Source ESS will be a pulsed source in the MW range. Since it will be of similar importance as ILL in Grenoble in the long term, the ESS is of great strategic significance. According to the current status of planning, it will be the most powerful spallation neutron source in the world. It is envisaged that the European Spallation Source ESS, a collaborative project of 17 European countries, will be put into operation in the years from 2022 (first beam on target) onwards. Designed for maximum power of 5 MW, ESS will start in the initial configuration with a thermal power of 2 MW, where all funded instruments will already be world-leading. First science with three instruments is foreseen for 2023, followed by the user operation of initially 3, then 8 first instruments. At present, 15 instruments are being realized, but expansion of the suite up to 22 instruments is anticipated. Seven of the initial 15 instruments are being built by German centres, in collaboration with international partners: four by FZJ, two by TUM and one by HZG. Moreover, FZJ will deliver the moderator-reflector assembly and the partners contribute to various work packages in instrumentation, sample environment and scientific computing. This underpins the strong German expertise in method development and instrument construction and shows the importance of already operating facilities like MLZ and ILL as a hub to develop this expertise.

- In the medium and long term, ESS in Sweden will become the leading European neutron source. Future role and further plans:
- The contribution agreement between FZJ and the ESS ERIC has been signed beginning of 2019.
- Seven instruments for ESS are being built together with European partners by German groups. It is envisioned to contribute to their commissioning. The Helmholtz Centres involved would be FZJ and HZG.
- After successful installation and commissioning of the instruments build with German involvement, instrument operation will be transferred to the ESS. A cooperation model has to be established which ensures that the groups involved in instrument construction can on the one hand further support the future instrument development and on the other hand take part in their scientific usage. Such cooperation agreement will benefit all partners involved in the ESS project.

## 7.3 Contribution to the American spallation source SNS, Oak Ridge

SNS at Oak Ridge National Laboratory is currently the most powerful pulsed neutron source. FZJ's contribution to SNS is laid down in a cooperation agreement, and JCNS provides German users with access to the neutron spin echo spectrometer and two other instruments (beam time allocation through the MLZ user office).

- Future role and further plans:
- The use of instruments at SNS by German users is of significance for preparing the German user community for ESS operation.
- The term of the current agreement between FZJ and SNS is ten years, ending in 2021.

- With the start-up of ESS, FZJ will decrease its commitment at SNS, shifting resources to the instrument operation at ESS. Discussions about the further scientific collaboration with SNS are ongoing in a positive manner.

#### 7.4 German contribution to the Russian high-flux reactor PIK, Gatchina

The new high-flux reactor PIK (neutron flux for beam-tube experiments comparable to ILL) in Gatchina near Saint Petersburg, Russia, can play a significant role in the European neutron landscape in the long term. The Ministry of Higher Education and Science of the Russian Federation (MON) and the Bundesministerium für Bildung und Forschung (BMBF) have agreed on December 10th 2018 upon a joint research roadmap resting on 4 pillars: I. Cooperation in the area of large research infrastructure development; II. Joint research projects in the fields of scientific and technological cooperation; III. Mutually beneficial development of the scientific talent pool; and IV. Science and research to build bridges between science, society and business in both countries. Pillar I includes the option for the joint implementation and operation of an international user platform at the PIK research reactor, which comprises development and construction of excellent research instrumentation with a perspective for closer association of the PIK scientific program into the international neutron community. In parallel, plans for the other pillars are being discussed.

- Funding for the instrumentation upgrade has been earmarked within the Russian-German Roadmap signed in 2018. Current negotiations aiming at specific cooperation agreements as basis for the International Centre of Neutron Research (ICNR) are ongoing. Model should be the successful cooperation of FZJ, HZG and TUM within MLZ. Construction and operation of about 3 new instruments is a part of the German in-kind contribution to ICNR within a ten years period.
- In order to enable research operation and access to measuring time in accordance with international standards, an International Neutron Scientific Advisory Board has been established.
- HZG transferred seven instruments from the FRG-1 research reactor, which was taken out of operation in 2010, to the PIK reactor to Gatchina. At least two of these instruments will be upgraded and adapted to the high flux neutron beams of PIK. The relevant contract stipulates that, in return, HZG is allocated 15 % of the beam time on these instruments for an unlimited period of time.
- The EU (HORIZON2020) funded CREMLIN project has supported coordination between the German and Russian partners. A follow-up proposal (CREMLINpluss) has been granted.

#### 7.5 Cooperation with China

Powerful modernized instruments were sold to the new CARR research reactor in China when the DIDO research reactor in Jülich was decommissioned. Jülich researchers provided support for installing and commissioning the instruments before handing over operation to the scientists at CARR. Apart from affording the right to a German share in beam time, this cooperation serves as a focal point for future German-Chinese cooperation in neutron research and beyond.

Future role and further plans:

- German–Chinese cooperation in research with neutrons should be explored further.
- There will be no financial obligations.

Within the above international setting, we now discuss the neutron landscape within Germany.

## 7.6 BER II, HZB, Berlin

BER II has been operated by HZB in Berlin till December 10, 2019, when it has been permanently taken out of operation. By focusing on complex sample environments in connection with state-of-the-art instruments, the source has been a top-class facility for international neutron research despite its relatively low flux. For example, the combination of very strong magnetic fields and very low temperatures had enabled unique experiments with neutrons.

Future role and further plans:

- BER II has been taken out of operation December 10<sup>th</sup>, 2019. It is important to offer the users of BER II an alternative for their research after 2020, naturally at MLZ, ILL and upcoming, at ESS.
- The transfer of 3 instruments from BER II to MLZ is part of the first phase of the MLZ2030 vision. These instruments cannot be installed at MLZ as they are, but they all need to be adapted to the situation at MLZ.
- Transfer of the High Magnetic Field Facility for Neutron Scattering HMF from BER II to MLZ has been evaluated in detail by specialists from both sides and has been found to be technically not feasible.

## 7.7 Heinz-Maier-Leibnitz-Zentrum (MLZ)

With the FRM II, the Technical University of Munich TUM operates the reactor with the highest power density in the core world-wide. Scientific user operation at this unique neutron source is done jointly between TU Munich and Helmholtz (FZJ and HZG) with about equal shares. MLZ is the result of implementing BMBF's strategic goal of optimizing the possible uses of the most powerful German neutron source as part of a cooperation agreement between TUM and the Helmholtz Centres. The integration of universities in the construction and operation of instruments is a particularly important element in this process. At FRM II, 26 neutron instruments are currently being operated (FZJ 11, HZG 2). Eight additional instruments are in the construction phase (FZJ 2).

In future, the Helmholtz Association will play a key role in the operation and further development of the research instruments through its relevant competence centres, JCNS at FZJ and GEMS at HZG.

Future role and further plans:

- MLZ will be the only national facility in the medium term. It is one of the leading facilities worldwide and brings together the main players in research with neutrons in Germany, offers outstanding instrumentation, education and professional user service. Therefore, MLZ plays a key role for German users. This statement was substantiated by the extensive MLZ review in November 2018, which concluded among other things that *"The suite of instruments and user operation at MLZ is outstanding"*.
- To enhance its productivity, it is crucial that the cooperation contract between the MLZ partners, TUM, FZJ and HZG, is prolonged past the present term of 31. December 2020. Due to the concentration of research with neutrons on less facilities, the capabilities of MLZ have to be expanded. Therefore, the new cooperation contract should include an upgrade program for MLZ, the **"Vision MLZ2030"** (see /14/) with an improved and extended instrument suite, new neutron delivery and user access schemes, increased support in scientific computing etc. One element of this upgrade program is the transfer of instruments from BER II to MLZ after 2020.

## 7.8 Network of Compact Accelerator driven Neutron Sources CANS

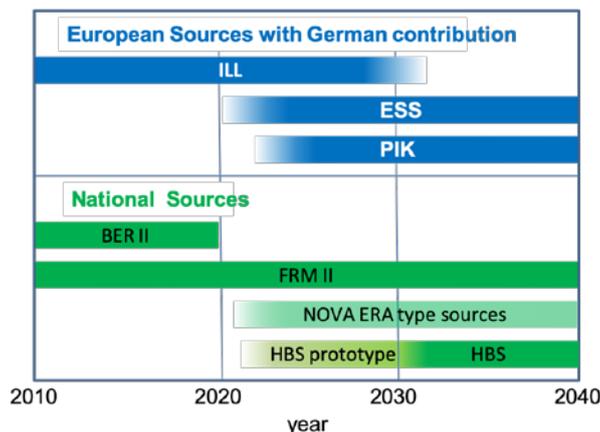
Europe’s leading position in research with neutrons is based on a network of smaller and medium flux sources, mostly reactor based, providing the basis for ILL and later on ESS as the world’s flagship facilities. These smaller to medium size sources are indispensable for user recruitment, user education, method development, fast and easy access, and allow specialized experiments that cannot be realized at larger facilities due to the user pressure and instrument overload. With the fading of research reactors, it is necessary to establish a new network of neutron sources within Europe. As has been shown by the recent development work of JCNS /7, 8, 11, 12/, compact accelerator driven neutron sources CANS have the potential to replace the ageing network of research reactors. CANS are scalable, come with a much smaller price tag than spallation or reactor-based facilities, don’t need nuclear licensing in Germany, and are inherently safe.

Future role and further plans:

- Smaller “NOVA ERA”-type CANS sources can open entirely new applications of neutron methods in science and industry by providing local and immediate access to neutron instruments. A strategy has to be developed how to realize such CANS, make potential user groups aware of their potential and propose appropriate funding schemes.
- Given the long lead time for the realization of large scale facilities, concrete timely planning for the realization of a future accelerator based national neutron source is urgent. Such a source has to be in place latest when the ILL ceases operation.
- This future source could be a High Brilliance Neutron Source as proposed by JCNS and its partners, which offers new possibilities for science and industry particularly in promising fields like life sciences or quantum phenomena.
- A Conceptual Design Report (CDR) for a full-fledged High Brilliance neutron Source (HBS) will be published in the beginning of 2020, a Technical Design Report (TDR) will be available by end of 2021.
- Before realization of a full-fledged HBS, a smaller scale prototype has to be realized, which will allow for optimization beyond what is possible with modern simulation tools. Ideally, such a HBS prototype should become available shortly after BER II is decommissioned in order to offer possibilities for method development and experimental opportunities for part of the former BER II users.

## 7.9 Proposed neutron scenario

A rough timetable based on 7.1–7.8 is shown in the figure below.



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## 9 Acknowledgements

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## 10 Appendix: “Flagship Areas” of Research with Neutrons

The multidisciplinary nature of current neutron sources, as well as the future ESS, has an effect on the entire range of science and technology development. It is therefore impossible to predict whether individual future flagship experiments will be successful. However, we can project with considerable certainty those areas of science and technology where research with neutrons, particularly at the ESS, will have a major impact. The following is a brief outline of these “flagship areas”:

### 10.1 Energy

The continuous availability and affordability of energy is one of the foundations of our industrial civilization. A sustainable energy economy is therefore one of the key challenges facing society in the 21<sup>st</sup> century. Neutrons provide ideal access to the structure, kinetics, and dynamics of numerous materials and processes that are of great importance for energy generation, conversion, and storage. For example, neutrons can be used to optimize the structural materials that play a key role in mobility concepts and energy generation, from steam turbines and rotor blades for wind turbines to materials for fusion reactors. Hydrogen is an ideal fuel for mobility solutions. The technological challenge consists in developing hydrogen storage systems that combine low costs and weight with a high capacity. Neutrons with their high sensitivity for hydrogen atoms are an ideal probe for this purpose. All solid-state Li-ion batteries are promising power sources for electromobility. With neutron depth profiling, the Li distribution can be observed in-operando with three-dimensional resolution during charging and discharging allowing one to optimize the batteries with respect to capacity, power density, aging effects etc. Self-assembly is an important principle in the development of solar cells from organic polymers. The contrast variation made possible by neutrons will play a decisive role in unveiling the prerequisites for this process. This is also true for the elucidation of the processes involved in the production of biofuels and for research into novel materials for electrolytes, which are one of the key components of batteries and fuel cells.

### 10.2 Medicine and health

Neutron research will have an impact on three areas in this field: (i) It will help to optimize materials in biomedicine, e.g. for implants. (ii) It will play an important role in studying the molecular causes of diseases. (iii) It will play a part in elucidating underlying biomolecular processes. Examples for (i) include the optimization of biocompatible surface layers for artificial hip joints and the use of hydrogels to improve surgical procedures. The molecular causes of diseases (ii) include topics such as amyloid aggregation, in particular in the early stages of Alzheimer's disease, and the interaction of drugs with the target molecules, specifically taking into account the dynamics. Special examples are cholesterol transport and its effects on neurodegenerative diseases and heart disease, and the distribution and dynamics of neurotransmitters in polymeric eye implants. (iii) For the elucidation of underlying processes, a combination of neutrons and X-rays is of great significance. While X-ray radiation provides information on the molecular structure, neutrons can be used, for example, to clarify the detailed protonation states in close proximity to the catalyst atoms in enzymes. In particular, neutrons also lend themselves to understanding the role of the dynamics in biophysical processes, e.g. allostery and functional dynamics in enzymes, and in the movement and function of proteins in dense environments such as cells. The functionality and dynamics of membrane proteins in their environment can become another new field of research. The ESS will make a huge difference to answering most of these questions. Many of the current neutron sources are unsuitable for research into these topics due to their limited intensity.

### 10.3 Electronics and information technology

The discovery of the giant magnetoresistance effect (GMR), i.e. magnetic fields that influence the electric resistance, was honoured with a Nobel Prize in 2007 and became the starting point for a field of research referred to as "spintronics", an information technology that is based on the electron's spin. This has numerous advantages, for example, ohmic heat loss can be avoided, which enables further miniaturization. Today, the GMR effect is the basis for the read heads in magnetic storage media. Deciphering the underlying magnetic structures was made possible by the use of neutrons and their high sensitivity for magnetic properties. More recently, topologically stabilized spin vortices, so called Skyrmions, have been discovered with neutron small angle scattering. They are promising candidates to realize high density, low power racetrack memories. For the future development of this technology, the use of neutron beams to optimize spin structures and kinetics will be of the essence. In future spintronics, novel materials and thin-film material systems will be used, many of them based on complex transition metal oxides. At their interfaces, these materials display unexpected emergent properties that lead to new functionalities. Neutrons enable a depth-resolved determination of the order of the degrees of freedom of spin, orbit, and charge, which is the most important prerequisite for understanding the interface phenomena and therefore for developing novel components. Examples include multiferroic materials that combine magnetic, electrical and mechanical properties. They could become the foundation for non-volatile, fast data storage systems with an ultras-small switching power suitable for a multitude of sensors. Neutrons play an essential role in deciphering their structural and magnetic properties. Further miniaturization will lead to the development of molecular magnets, which are already being discussed as possible qubits for quantum information processing. Neutron radiation is important for investigating their structural and dynamic properties. Another field of research is the coupling of electronic circuits with biomolecules and cells. The circuit surface is of decisive importance for their function. Neutron reflection experiments will provide important insights.

### 10.4 Industrial applications and engineering

Materials science and engineering are the key to new technologies, growing prosperity, and sustainable growth. Numerous diagnostic tools are used to optimize materials, processes, and components. Neutrons provide insights into the structures as well as the kinetics and dynamics. In construction materials, for example in aircraft engineering, controlling internal stresses is of the greatest significance. Airbus, for example, is currently in the process of replacing rivets with weld seams in aircraft. Since internal stresses add up to outer loads, controlling them is extremely important for the safety of an aircraft. Neutrons are used to validate the welding processes. In vehicle construction, increasingly lighter components prevent unnecessary fuel consumption. One example is the optimization of multiphase materials made up of aluminium and silicon. Their strength depends on the exact control of the casting processes as well as the solidification process. In situ neutron experiments with the high-intensity neutron beams at the ESS will extend the knowledge base considerably. The same is true for the in-situ characterization of welding processes, which requires fast measuring techniques with a high intensity. Neutrons penetrate deep into materials and, at the same time, they are particularly sensitive for light atoms. In this way, the behaviour of lubricants in engines during operation can be observed and optimized. In batteries or fuel cells, it is possible to investigate the lithium distribution and the evolution of water in the catalytic conversion during operation. The exchange between light and heavy hydrogen also makes it possible to study the kinetics of exchange processes.

### 10.5 Materials in the chemical industry

Materials in the chemical industry often consist of numerous components that assemble themselves on the scale of nanometres and micrometres, thus determining the behaviour of the entire system. Examples include functional materials that react to external stimuli, such as stress, temperature, and

electrical fields, in a very controlled manner, and soft matter, which displays both solid-like as well as liquid-like behaviour. Soft matter comprises colloids, e.g. varnish, paint, or micro-emulsions of detergents, pharmaceutical products with active pharmaceutical agents, solvents for tertiary oil recovery, or gels in the form of ointments, creams, and other personal hygiene products, and many more materials. The contrast variation offered by neutrons is an indispensable tool for deciphering the structures of individual components and their movements. This applies to the molecular causes of rheological behaviour, a key factor in polymer processing, as well as the stability of foodstuffs, which are usually a highly complex combination of a wide variety of substances. An example from industry is the use of CO<sub>2</sub>-based solvents for the extraction of oil from reservoirs, which boosts oil output by up to 30 %. Neutron experiments can provide information on the underlying formulations. The same applies to replacing organic solvents with ionic liquids in the pharmaceutical industry. Here, structure investigations with neutrons are of great significance. Another field is the optimization of catalysts, such as the Lindlar catalyst from Evonik and catalysts for PVC synthesis from Ineos Chlorvinyls. Since the materials under consideration are complex and the processes must be studied with a high temporal resolution, the intensity of the neutron radiation is a decisive element. The ESS will make it possible to considerably broaden the currently small range of applications in industry.

## 10.6 Quantum technologies

Even today, technologies based on findings from quantum physics contribute more than a quarter of the gross national product in modern industrialized societies. Examples of quantum technologies include magnetic resonance imaging and X-ray imaging in medicine, photovoltaic cells in energy technology, and semiconductor components in information and communications technology. Macroscopic quantum phenomena in solids, such as magnetism and superconductivity, are particularly fascinating, because they reflect quantum mechanics in properties that can be observed on a macroscopic level. Ever since the discovery of superconductivity in compounds of copper and oxygen and the finding that the high transition temperatures can be attributed to electronic correlations, it is generally assumed that, in principle, room-temperature superconductivity can be realized. This would be a spectacular breakthrough for energy technology, because superconducting power cables would be associated with much lower losses during energy transmission and storage. Although the principle behind high-temperature superconductivity is still not fully understood, neutrons have already made a significant contribution to a better understanding of the fundamental principles, because they are able to throw light on the interaction between superconductivity and magnetism as well as superconductivity and lattice vibrations. In particular, magnetic fluctuations were found in the superconducting state that some theories consider to be decisive for the high transition temperatures. In the past few years, iron-based high-temperature superconductors were also discovered in which neutron scattering unveiled a similar phenomenon: another milestone on the road to a targeted search for room-temperature superconductors. More recently, scientists were able to demonstrate by means of neutron scattering that a collective ground state exists in magnetism that is produced by the Higgs mechanism in analogy to superconductivity. This collective state of magnetic monopoles will allow innovative approaches to be developed for a new kind of spin-based energy-efficient information technology (spintronics). The Nobel Prize in Physics in 2016 gave tribute to the concept of topology in condensed matter research. Skyrmions, topologically stabilized spin vortices, have been discovered by neutron scattering and are now being discussed as possible elements of future spintronics. This requires a better understanding of the magnetic spectrum – and this is where neutron scattering comes into play once again.