Vol. 16, No. 7, 2021

scnat
swiss academy of sciences

swiss academies
reports

swiss-academies.ch

Neutron Science Roadmap

for Research Infrastructures 2025–2028
by the Swiss Neutron Science Community

SSSN
SGN

IMPRINT

PUBLISHER
Swiss Academy of Sciences (SCNAT) • Platform Mathematics, Astronomy and Physics (MAP)
House of Academies • Laupenstrasse 7 • P.O. Box • 3001 Bern • Switzerland
+41 31 306 93 65 • info@scnat.ch • map.scnat.ch • @scnatCH

CONTACT
Swiss Neutron Scattering Society • Paul Scherrer Institut
5232 Villigen-PSI • Switzerland
+41 56 310 46 66 • sgn@psi.ch • sgn.web.psi.ch

RECOMMENDED FORM OF CITATION
Rønnow HM, Gasser U, Krämer K, Strobl M, Kenzelmann M (2021)
Neutron Science Roadmap for Research Infrastructures 2025–2028 by the Swiss Neutron Science Community
Swiss Academies Reports 16 (7)

SCNAT ROADMAP COORDINATION
Hans-Rudolf Ott • Marc Türler

ELABORATION PROCESS
The present document is a community effort, with contributions from ‘core communities’ across Switzerland represented in the Swiss Neutron Science Society (SNSS), as well as from user communities across various disciplines working with neutron scientists to exploit neutron probes for specific applications.

EDITORIAL BOARD
Urs Gasser, PSI, SNSS Board member • Karl Krämer, University of Bern, SNSS Board member • Markus Strobl, PSI, SNSS Board member • Michel Kenzelmann, PSI and University of Basel, Head PSI Laboratory for Neutron Scattering and Imaging • Henrik M. Rønnow, EPFL, SNSS President

CONTRIBUTORS
Ueli Angst, ETH Zurich, Department of Civil, Environmental and Geomatic Engineering • Tom Fennell, PSI, Laboratory for Neutron Scattering and Imaging • Peter Fischer, ETH Zurich, Department of Health Sciences and Technolog y• Marc Janoschek, PSI & University of Zurich, Head PSI Laboratory for Neutron and Muon Instrumentation • Stefan Janssen, PSI, User Office • Fanni Juranyi, PSI, Laboratory for Neutron Scattering and Imaging • Bruce Normand, PSI and EPFL • David Mannes, PSI and ANAXAM • Marisa Medarde, PSI, Laboratory for Multiscale Materials Experiments • Florian Piegsa, University of Bern • Efthymios Polatidis, PSI and ANAXAM • Christian Rüegg, PSI, ETH Zurich, EPFL and University of Geneva, PSI Director • Sigita Trabesinger, PSI, Electro-chemistry Laboratory • Pavel Trtik, PSI, Laboratory for Neutron Scattering and Imaging • Evgenii Velichko, European Neutron Scattering Association • Jonathan White, PSI, Laboratory for Neutron Scattering and Imaging • Vanessa Wood, ETH Zurich, Department of Information Technology and Electrical Engineering

ACKNOWLEDGEMENTS
We thank all SNSS members and colleagues in the wider user community for the numerous inputs we have received.

LAYOUT
Olivia Zwygart (SCNAT)

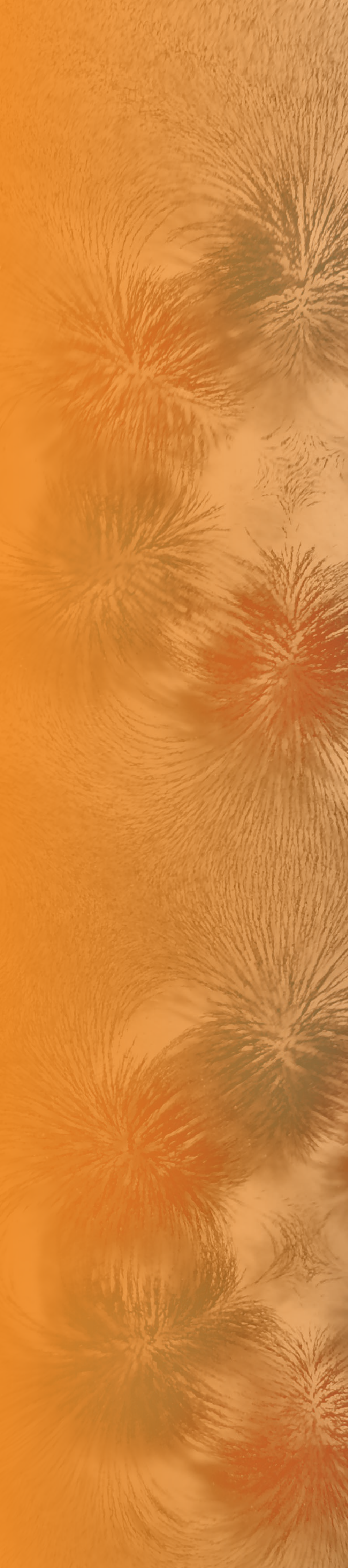
COVER PHOTO
Nicolas Gauthier
In 2020, an international team led by PSI researcher Romain Sibille established in neutron-scattering studies a fundamentally new state of matter, higher-rank multipole ice (Nat. Phys. 16, 546–552; 2020). The image shows a representation of a liquid of magnetic multipoles, obtained by immersing bar magnets and iron filings in water.

This report can be downloaded free of charges from scnat.ch/en/id/BGqdL

ISSN (print) 2297-1793
ISSN (online) 2297-1807

DOI: doi.org/10.5281/zenodo.4637661

Cradle to Cradle™-certified and climate-neutral
report printed by Vögeli AG in Langnau.



Neutron Science Roadmap

for Research Infrastructures 2025–2028
by the Swiss Neutron Science Community

Content

1 Executive Summary

This document presents a broad overview of the current status of neutron science in Switzerland and derives a set of recommendations for future developments.

The main objectives have been to survey and analyse

- the unique contributions that neutron probes provide across scientific and technological fields and disciplines;
- the growing and broadening Swiss neutron science community; and
- provisions needed to ensure continuing and sustainable success.

We identified an ever-increasing number of areas across a wide spectrum of disciplines in which neutron probes are used to address grand scientific, technological and societal challenges. These range from fundamental research in physics and material science to uses in energy research, health science and cultural heritage, among other fields, as well as in industrial R&D programmes. We stress that the list of topics is by no means exhaustive, and many area are only indirectly represented, for example structural biology and operando techniques.

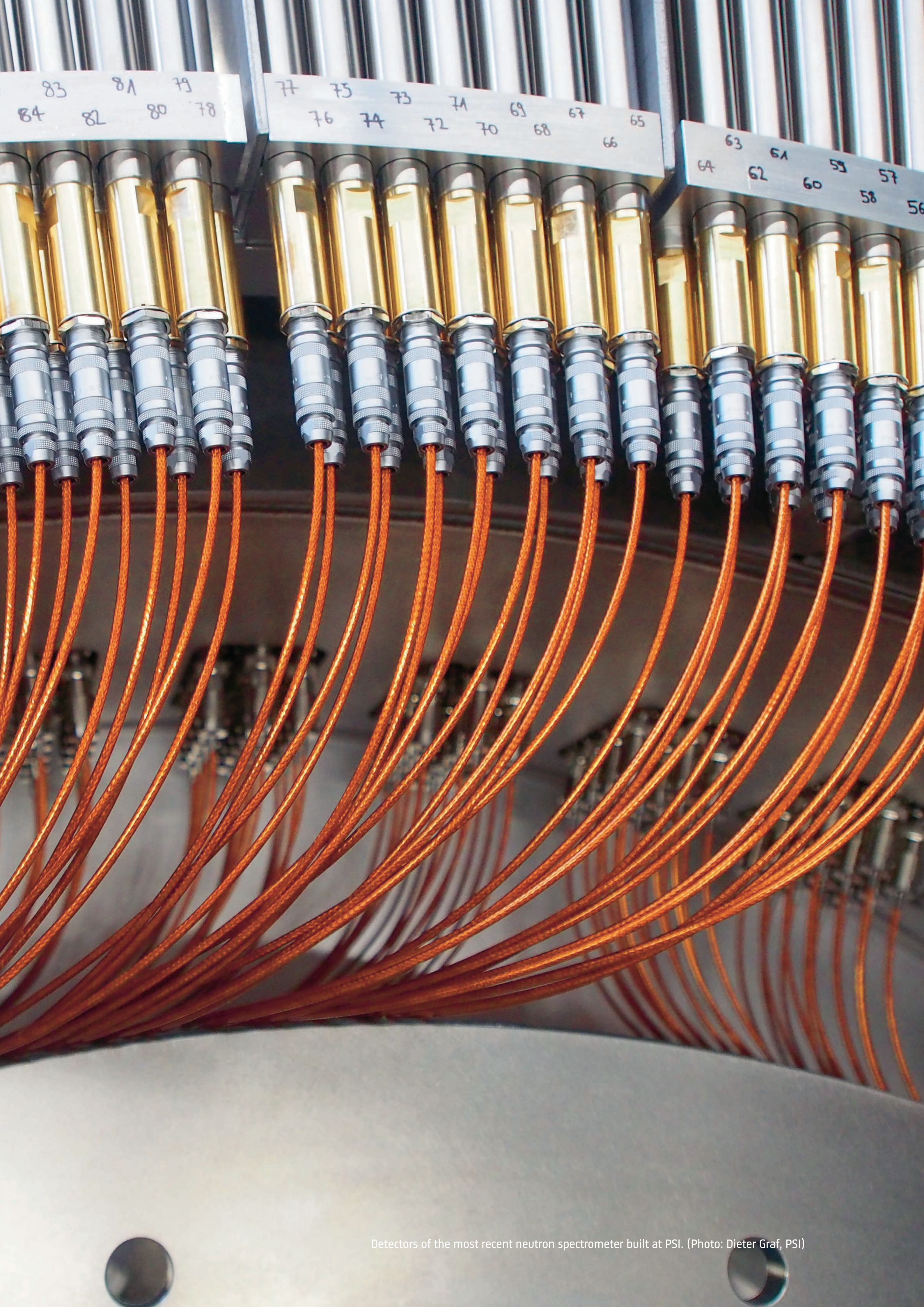
Our survey also portrays a vibrant and highly successful Swiss neutron science community, which is making remarkable impact both in fundamental sciences and on societal challenges, and at the same time provides education and training for the future generations of this growing and increasingly more diverse community. This is a central aspect especially for those communities that use neutron probes primarily as tools alongside other analytical techniques.

These developments are largely based on access to both a national neutron source (SINQ at the Paul Scherrer Institute) and leading facilities in Europe and worldwide. In order to sustain this progress, first and foremost provisions have to be made to ensure adequate access for Swiss-based researchers to the neutron experiments. This access should be commensurate with the growing need of a widening user community. Extrapolating from bibliometric analyses presented in this document, we project a 20% growth over the coming decade in the number of scientists using neutrons and a similar increase in demand for beamtime.

Our key recommendations are therefore to take adequate measures to ensure that

- Switzerland continues to have a state-of-the-art national neutron source; this can be accomplished by a continued upgrade programme of SINQ in the near- to mid-term, and forward-looking modernisation plans for the long term (beyond 2030);
- Switzerland remains a member of leading international facilities, in particular of the Institut Laue–Langevin (ILL) in Grenoble, France, and the new European Spallation Source (ESS) in Lund, Sweden; the level of membership has to reflect the strong and growing demand of the community, so as to guarantee a sufficient amount of beamtime.

The implementation of these measures will provide a solid basis for the Swiss community to remain at the forefront of neutron science and technology, and to react to emerging trends and new opportunities, which can be expected in particular in the context of ESS, which will be the most powerful neutron source worldwide when its user programme starts in 2023. Similarly, the upgrade programme for the national neutron source SINQ and planning for a potential new source should be informed by both the core group of those developing neutron methodology and technology, and the ever more diverse needs of the user community. Finally, the trend towards increased industrial use might further accelerate the demand for beamtime. In view of these anticipated developments, we recommend to review and update the present document in regular intervals.



Detectors of the most recent neutron spectrometer built at PSI. (Photo: Dieter Graf, PSI)

2 Findings and Recommendations

As detailed in the following chapters, the major findings of our survey and analysis are as follows.

Finding 1: Neutron probes provide essential contributions to a wide and increasing number of disciplines across the spectrum of grand scientific, technological and societal challenges, as well as to industrial R&D programmes (Chapter 3).

Finding 2: The Swiss neutron science community is world-leading in the field and growing in number and diversity (Chapter 4).

Finding 3: The success of the Swiss neutron community is based largely on access both to the national neutron sources SINQ and UCN and to the currently world-leading facility ILL (Chapter 5).

From these findings we derive that it will be of vital importance that access to neutron instruments increases in the future, in line with the growing need of the widening neutron user community. In order to ensure such access, we recommend following measures:

Recommendation 1: The provision of a state-of-the-art national neutron source involves continued upgrading of SINQ and its proton accelerator at PSI until 2030 and beyond. This will ensure reliable national access to neutron scattering instrumentation for Swiss groups for the coming 10–15 years.
Recommendation 2: We recommend that SINQ is expanded with a northern neutron guide hall, allowing for a minimum of six new instruments. This is a cost-effective way to increase high-performance neutron capacity in Switzerland, and offers opportunities for Swiss universities and international partners to maintain or increase their involvement in SINQ.
Recommendation 3: We recommend the establishment of a national funding programme for innovative instrumentation, targeting consortia consisting of groups at universities and national laboratories. This will enable the development of unique instrumentation needed by university-based groups, and strengthen the synergies between universities and large-scale facilities.
Recommendation 4: For access of the Swiss neutron science community to world-leading facilities, Switzerland should remain member of the ILL facility at an adequate percentage for as long as ILL can continue operation, and must be a member of the new European Spallation Source ESS at a sufficient level to meet the strong Swiss demand. Alongside the financial commitment of direct Swiss membership to these facilities, we recommend to leverage international use of SINQ for increased Swiss access to leading European facilities.
Recommendation 5: For the time beyond 2030, plans must be made to either modernise the proton accelerator feeding SINQ and possibly the target–moderator systems, or to explore construction of a new high-brilliance source exploiting latest neutron technologies.


Aerial view of the European Spallation Source. (Photo: ESS)

3 Science Drivers

Neutron probes are advanced analytical techniques providing unique insight to an exceptionally broad range of systems of scientific, technological and societal importance, from the fundamental forces of our universe and quantum physics, to innovative smart materials, to energy technology, life science and industrial solutions. Alongside electrons and (optical and X-ray) photons, neutrons reveal structure and dynamics from atomic to microscopic length scales. Free neutrons interact with matter through the strong nuclear force and also electromagnetically due to their magnetic moment and, therefore, are truly complementary to electron and photon radiation, which predominantly interact electromagnetically. As neutrons are charge neutral, they can penetrate much deeper into matter than photons or charged radiation such as electrons. This is often a decisive advantage for studies under extreme environments, including low temperatures, high magnetic or electric fields, high pressure, or particular solvent conditions, which can severely limit the use of electron radiation and photon probes.

The production of neutron radiation for fundamental science and materials science happens through nuclear reactions that are realized in nuclear reactors or by bombarding a heavy-metal target with a high-energy beam of charged particles such as protons, as realized in the Swiss neutron spallation source SINQ. A neutron source therefore is a large-scale facility (Fig. 1), producing typically on the order of 1014 to 1015 neutrons per cm2 and second (see also Fig. 18).

The neutron radiation is guided to the experiment stations. Neutron beamlines are usually dedicated to the determination of structural (elastic measurements) or dynamic features (inelastic measurements) and a certain range of length and time scales. A neutron centre has typically 10 to 40 beamlines to cover the demands of the user community from all research areas.

The Swiss neutron science community includes experts pushing the technique forward as well as a wide range of scientific groups using neutron experiments as a central element in their research, and an increasing number of industries benefiting either from direct neutron measurements or from collaborating with scientific groups using neutron probes. The Swiss neutron community is remarkably productive, accounting for ~10% of neutron science publications in Europe (see Sec. 4.1), which is the leading neutron-science region worldwide (see Sec. 5.1). If normalized to population, Switzerland can therefore justifiably be considered the leading neutron science nation worldwide.

This leadership position is reached through the combination of an overall strong science and technology environment with access to neutron facilities, most notably the Swiss neutron source SINQ and the ultracold neutron source UCN at PSI. As the Swiss neutron science community grows both in number and into new scientific fields, it is imperative that Swiss scientists have sufficient access to state-of-the-art instruments of the type needed for their research.

When considering future directions of neutron science in Switzerland and worldwide, the importance of interdisciplinary research cannot be overstated. That research fields grow by reaching across disciplinary boundaries and connecting to other bodies of work seems to be an

Figure 1. Three of the main facilities used by the Swiss neutron science community: Institut Laue–Langevin (ILL) in Grenoble (France), the Swiss neutron spallation source SINQ at the Paul Scherrer Institute (PSI), and the European Spallation Source (ESS) in Lund, Sweden (under construction). (Credits: https://de.wikipedia.org/wiki/Datei:ILL_Grenoble_soleil.jpg, Scanderberg Sauer Photography/PSI, ESS)

intrinsic aspect of the scientific endeavour.[1] Neutron science is no exception. The European Neutron Scattering Association (ENSA) has recently conducted a natural language processing (NLP) analysis assisted by machine learning within the EU-funded BrightnESS2 project, and that study revealed clear signatures of growing complexity and interdisciplinarity in research involving neutron probes. The analysis considered some 46,000 journal papers published between 1956 and mid-2020 reporting results based on neutron probes; works related to, for example, neutron stars or particle physics were excluded. Over the period considered, the number of authors per 'neutron publication' increased clearly, a trend that was found to be somewhat more pronounced for publications with at least one European author (see Fig. 2).

The same analysis also classified the papers into coarse categories, revealing, among other things, that in the past 70 years neutron research as a whole has become less 'fundamental' and more 'applied'. For example, the number of publications related to biology and material science increased at a noticeably faster pace than those related to magnetism. However, in all categories the number of works increased.

This expansion in volume, scope, and interdisciplinarity is a development that we also witness in the Swiss neutron science community (see Sec. 4.1 for further results of the ENSA analysis, specific to Switzerland). For the purpose of this document, we selected a number of areas in which neutron probes have contributed substantially to the understanding of fundamental constituents of matter, material systems, and devices, with a focus on interdisciplinary research. The overview is not meant to be exhaustive; instead, we focus on areas where we expect that in the coming years neutron probes will help to address important scientific, technological and societal challenges.

1 See, for instance, a recent analysis of papers published in the journal Nature between 1900 and 2017 (*Nature* 575, 32; 2019).

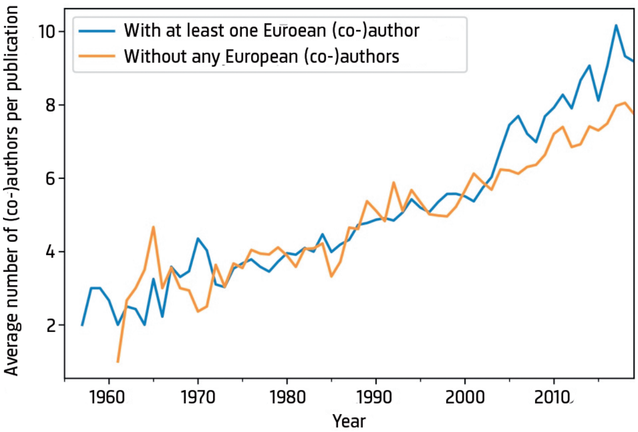


Figure 2. Number of authors per 'neutron publication' by year.

The sections of this chapter are organized in an order roughly proceeding from fundamental to applied research, including industrial R&D.

3.1 Fundamental Physics with Neutrons

Fundamental physics with neutrons addresses a broad spectrum of scientific questions and often has far-reaching implications in the realm of particle physics and cosmology. Low-energy experiments represent an important complementary approach to high-energy collider experiments, such as those performed at the Large Hadron Collider (LHC) at CERN. In low-energy physics, high-precision experiments are performed to search for smallest deviations from the Standard Model of particle physics (SM). The explored energies are up to 35 orders of magnitude lower than in present collider experiments, that is, in an entirely different regime of particle physics. Nonetheless, this research can provide indirect, but unambiguous, evidence for new physics at much higher energy ranges, for example probing supersymmetric theories at the TeV scale. The neutron represents the ideal tool for such investigations. Either the fundamental properties of the neutron itself are measured, or the neutrons are used as highly sensitive probes to search for new phenomena, exotic interactions, dark-matter candidate particles, neutron-to-antineutron oscillations, mirror-neutron oscillations, or to test gravitational interaction. Several international research groups, often organized in small and medium-sized collaborations, are presently conducting fundamental neutron physics at various large-scale facilities around the world.[2]

Particularly important properties of the neutron with respect to fundamental physics are its electric dipole moment (EDM), lifetime, decay coefficients, and electric charge. The discovery of a permanent EDM would violate parity (P) and time-reversal symmetry (T), and, invoking the CPT theorem, also the combined CP symmetry. In the 1960s, Sakharov pointed out that CP violation is one necessary ingredient for explaining the observed large dominance of matter over antimatter in our universe. However, so far the only known CP violation arises from the complex phase in the Cabibbo–Kobayashi–Maskawa (CKM) quark mixing matrix and is far too small to account for this matter–antimatter asymmetry. The search for an EDM therefore represents a highly promising pathway for testing new physics theories, i.e., extensions of the SM

2 For a recent overview, see for instance the proceedings of the 'International Workshop on Particle Physics at Neutron Sources (PPNS 2018)', EPJ Web of Conferences Vol. 219 (2019).

that naturally introduce new sources of CP violation. Although neutron-EDM searches have been performed since the 1950s, they are yet to produce a non-zero result. Currently, several research teams worldwide are aiming to perform next-generation EDM searches with ever-higher sensitivities.

Similarly, the lifetime of the free neutron is of major importance for the understanding of our universe and how it evolved. A few minutes after the Big Bang, free protons and neutrons started to combine and form nuclei in a process known as nucleosynthesis. This process and the abundance of helium as well as other light nuclei in our universe today is tightly bound by the number of available neutrons at that epoch, and thus to the neutron lifetime. Despite decades of performing increasingly accurate experiments using various different approaches, there is no agreement on how long neutrons live. The unsolved conundrum has been dubbed the 'neutron lifetime puzzle'. Decay coefficients provide an even more detailed way to characterize the neutron decay process. They describe the angular momentum (spin) and energy-dependent distribution as well as the correlation of the neutron with the other decay particles: proton, electron, and electron antineutrino. Studying these parameters leads to a determination of the (relative) strength of the axial-vector and vector couplings of the weak interaction, searches for discrete symmetry violations, and unitarity tests of the aforementioned CKM matrix, which provide important information regarding the completeness of the three-quark-family picture of the SM.

Last, the name of the neutron implies that it possesses no electric charge, which has been experimentally tested to an impressive upper limit of about 10^{-21} electron charges. However, the question of charge quantization and the neutrality of neutrons, neutrinos, and atoms remains under debate. Direct measurements of the neutron charge are additionally motivated by the possibility that the charge of a free particle might be slightly different in magnitude compared to its charge when bound in an atom. One immediate consequence of a finite neutron charge would be that a speculative neutron-to-antineutron oscillation is forbidden as long as charge conservation is valid.

Fundamental physics experiments usually employ beams of cold or so-called ultracold neutrons (UCNs). As with an ideal gas, here the temperature is a measure for the mean velocity of the particles. For example, 'ultracold' neutrons are those with a speed of only a few metres per second – so slow that such neutrons can be stored for several hundred seconds in magnetic or material traps. These long observation times then allow high-precision measurements of the neutron's fundamental properties. In Europe, the main beamlines for fundamental physics experiments and UCN sources are currently located at the Paul Scherrer Institute (PSI UCN source and partially the BOA beamline at SINQ) and at the Institut Laue–Langevin in France (PF1b, PF2, the planned SuperSUN source, and other instruments). In Germany, another smaller-scale UCN source is operational at the TRIGA reactor in Mainz. At the FRM II in Munich, the PERC instrument is currently under construction, which will serve as an intense source for neutron decay particles to perform more precise measurements of neutron decay coefficients. At the European Spallation Source (ESS) in Sweden, which is under construction, exciting new possibilities are currently discussed. This includes a future fundamental physics programme and a cold-neutron fundamental physics beamline as part of the ESS instrument suite. The realization of these propos-

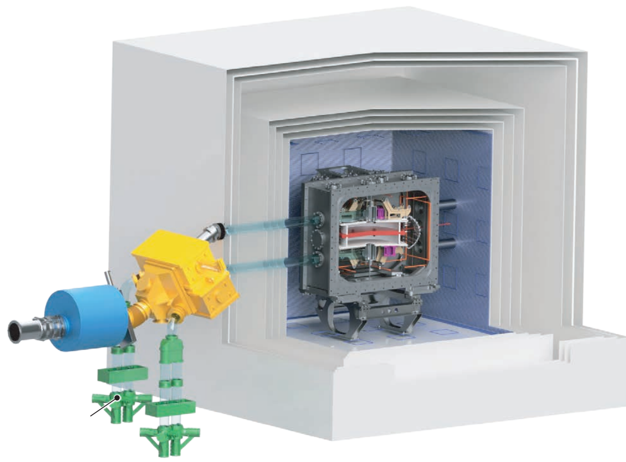


Figure 3. The new magnetically shielded room for the n2EDM experiment under construction at PSI (left) and design of the n2EDM apparatus (right).

als would largely strengthen the community and provide room for new ideas and projects in the field. Moreover, the pulse structure of the ESS with its high peak brightness provides tremendous advantages and novel possibilities for certain precision experiments with cold neutrons, for instance neutron velocity/energy-dependent measurements, beam-related background reduction, and the localization of the neutron pulse in space. These systematic advantages would be accompanied with an increase in neutron statistics.

In Switzerland, the main groups performing fundamental neutron physics research are located at the University of Bern, ETH Zurich, and PSI. These three groups are also members of a neutron EDM flagship experiment, which is performed within an international collaboration consisting of a total of 16 institutions from eight countries and more than 50 scientists. The so-called nEDM experiment is located at one of the world's strongest UCN sources at PSI (https://www.psi.ch/en/ucn). In 2020, after several years of installation and upgrades of the apparatus and careful data-taking, the collaboration finally published the most stringent limit on the EDM of the neutron.[3] The same nEDM apparatus has also been used in several side-analyses, such as searches for mirror-neutron oscillations, searches for Lorentz invariance violation, and searches for axion-like particles, which are candidates for dark matter in the universe. The Swiss members of the collaboration are also playing leading roles in the development and construction of the next-generation n2EDM project, with the goal of improving the sensitivity by one order of magnitude, to push the limit further or to discover a finite EDM (see Fig. 3). In addition, the group at the University of Bern currently pursues a second neutron EDM project, which aims to directly benefit from the planned ESS pulse structure. The project, entitled Beam EDM, is funded through an ERC grant and employs a novel concept to measure the neutron EDM using a time-of-flight Ramsey apparatus with a pulsed cold neutron beam. The advantage of this method is that a previously limiting systematic relativistic effect, which arises from the motion of the neutrons through an electric field, can be overcome. The project is currently in the proof-of-principle phase. The ultimate perspective would be to perform a competitive beam-type measurement with a full-size apparatus at the ESS in the coming decade.

Finally, an important point in fundamental physics with neutrons is the synergies and co-operations of scientists from this field with other researchers from neutron scattering and imaging. The transfer of knowledge and hardware is mutually beneficial and provides a route to improving instruments and experiments, and to developing novel ideas. A strong overlap of interests can be found in detector technology, spin-manipulation techniques, sample environment, neutron optics, and precision mechanics.

3 C. Abel et al., *Phys. Rev. Lett.* 124, 081803 (2020).

3.2 Quantum and Topological Materials

Quantum materials, whose properties include magnetism and superconductivity, already lie at the heart of our daily lives. Ferromagnets underpin technologies from data storage to electric transformers, and superconductors provide ultra-sensitive detectors and magnetic resonance imaging, as well as the promise of levitating-transport solutions. To achieve further technological gains, current research targets the ability to manipulate the all-important electronic wavefunctions. For example, despite the widespread applications of ferromagnetism, its drawbacks include a large associated stray magnetisation and a high energy cost for switching the magnetisation direction. These limitations can be overcome by using differently structured materials that instead promote antiferromagnetism, or possibly more exotic spatial arrangements such as magnetic spirals. These complex magnetisation distributions possess new magnetic properties that might themselves underpin functional behaviour of use to society. Current research in quantum materials aims to discover new forms of magnetic order and new phases driven by the quantum interactions of electrons, if possible at room temperature.

Because neutrons are an unparalleled probe of magnetism in all its forms, from the atomic scale to imaging macroscopic magnetic-field structures, they have an indispensable role both for investigating the fundamental physics of quantum materials and for developing the hardware on which the digital and quantum-technologies revolutions will be built. Here we highlight representative areas of quantum and topological materials research, illustrated in Fig. 4, that can only be pursued experimentally using neutron-science instrumentation.

3.2.1. Quantum Magnetism

At the fundamental level, quantum magnetic materials provide the cleanest realisation of interacting many-body systems with complex, correlated and non-commuting degrees of freedom. The challenge one may address is therefore nothing less than understanding the entanglement structure of the quantum wavefunction. Elastic and inelastic neutron scattering experiments continue to reveal new forms of exotic quantum order and topology in the ground state and fractional or collective excited states. This makes neutron experiments integral both to revealing elementary physical models and, by extension,

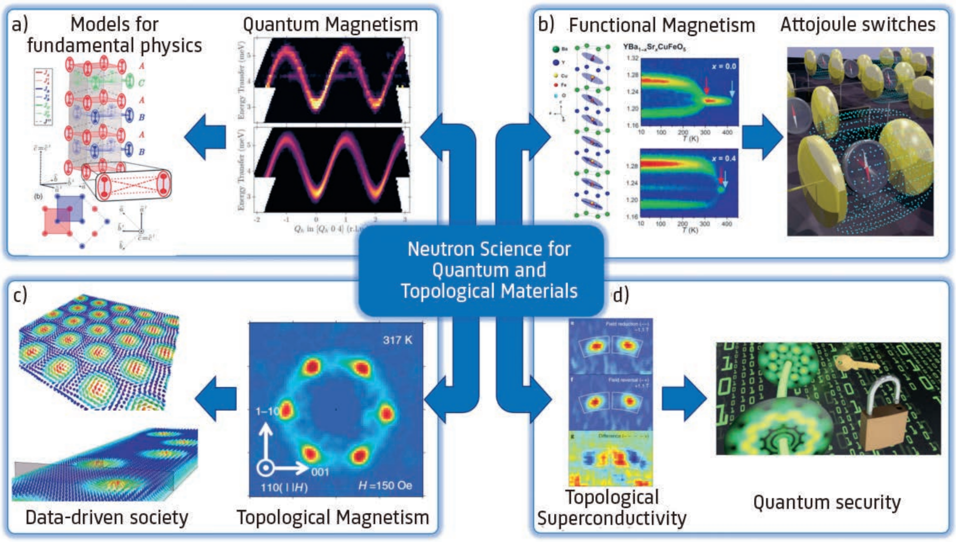


Figure 4. Applications of neutron science in quantum and topological materials research. The data shown in panels a–d were obtained from four different experiments at SINQ. Also indicated are the domains in which the research is expected to have a broad impact, which range from deeper physical understanding to the needs of a green and digital society.

to their adaptation for future applications. In Fig. 4a, we show state-of-the-art neutron spectroscopy measurements obtained at SINQ from a quantum magnetic dimer material, which led to a quantitative model description of the microscopic interactions and hence to an understanding of quantum critical scaling in any modulated layered system.

3.2.2 Functional Magnetism

The periodic table provides a wealth of combinations for building quantum magnetic materials. These are often oxides of 3*d* transition-metal ions or of 4*d*, 4*f* and 5*d* magnetic ions, which by their spin–orbit coupling introduce a variety of interactions between electronic orbitals of varying extent. In this context we highlight magnetoelectric multiferroics, a class of system being investigated with the goal of near-lossless control of the magnetisation by applied electric fields, rather than by magnetic fields, whose components are energy-intensive and hard to miniaturise. The challenge is that nearly all such multiferroics display their spiral magnetic texture only far below room temperature. Figure 4b highlights a recent breakthrough achieved at SINQ, in which neutrons revealed unambiguously that the temperature range of the spiral order in an oxide system can be raised to room temperature by careful control of the chemical composition.[4] This development paves the way for using quantum materials in high-speed, low-power switches. Neutrons are also integral to research into materials for antiferromagnetic spintronics, a technology that will extend high-speed, low-power operation to information storage and manipulation with classical digital bits.

3.2.3 Topological Magnetism

Tailored spin anisotropies and non-centrosymmetric geometries can be used to build Ising or XXZ magnets, simple models with discrete quantum bits, and the Dyzaloshinskii–Moriya interactions that are crucial to create the most complex magnetisation textures. These include magnetic helices, vortices and skyrmions, whose topological properties in real space mean that the organising principles of their magnetism are in a class fundamentally different from common, more trivial forms such as ferromagnetism. Consequently, these topologically nontrivial magnetic structures are robust against decay, which makes them extremely attractive for information-flow and data-storage applications. The prospects for such applied topology received a huge boost from recent observations made at SINQ of the first topological skyrmion phase to be discovered at room temperature,[5] which is shown in Fig. 4c. Complementary to nontrivial magnetic topology in real space are systems with topological electronic structures, most notably Dirac and Weyl materials, which offer the most promising route to topological magnetic properties in reciprocal space. The use of topological magnetic excitations for the transmission and manipulation of protected quantum information has already gained the moniker 'topological magnonics', and its development to-

4 T. Shang *et al.*, *Sci. Adv.* 4, eaau6386 (2018).

5 Y. Tokunaga *et al.*, *Nat. Commun.* 6, 7638 (2015).

wards the end goal of quantum computation will be possible only through the capabilities of neutron experiments to characterise the full spectrum of topological excitations in suitable magnetic materials.

3.2.4 Topological Superconductivity

Superconductivity is perhaps the ultimate form of macroscopic quantum coherence, and fundamental open questions in this field range from quantitative details of the pairing mechanism, required to enhance critical temperatures, fields and currents, to qualitative issues of symmetry and topology, which are required to protect and manipulate quantum information. In the latter context, Fig. 4d highlights recent neutron studies of the vortex phases in a chiral spin-triplet superconductor, again performed at SINQ.[6] These results revealed that the superconducting state is protected topologically, meaning that the electron pairs cannot decay trivially and that the vortices should contain fractional Majorana fermion excitations. The topological nature of Majorana fermions makes them further candidates for use in quantum computing and quantum information security. Future studies mandate the exploration of unconventional superconducting symmetries and topologies as a route to qubit protection, while the range and sensitivity of technologies based on superconducting switches and devices needs to be improved. Also in this context, neutron scattering will provide an essential underpinning for both microscopic investigations, meaning of electrical and magnetic properties at the atomic level, and for imaging of functional devices.

In summary, neutron scattering is a technique vital for the development of new quantum materials, because the use of electron spins and collective spin states as bits and qubits forms the backbone of quantum information storage and manipulation, now known as the quantum technologies revolution. Figure 4 represents a sample of present research into quantum and topological materials where neutron science plays an unrivalled role. Further areas of intense activity include quantum spin liquids, spin ices, proximate Kitaev physics, quantum phase transitions, and magnetically mediated superconducting phases. In all cases, the initial aim is to discover new physical paradigms but the critical end goals include the generation of new applications to enable the transition to a digital and green (i.e., low-power) society. Decades of development in both neutron sources and instrumentation have made neutron scattering the tool of choice for investigating all facets of bulk quantum and topological quantum materials, but the drive towards smaller or thinner samples and faster processes provides a continual mandate for technical development.

3.3 Innovative Smart Materials

Materials are considered as ‘smart’ – or, functional – when they possess one or several properties that can be readily tuned. Some such materials show also intrinsic coupling among their tuneable properties, which can be exploited for cross-control of multiple properties. These characteristics make them particularly appealing for magnetic, optical and electronic applications, an increasingly growing sector in the continuous search for cheap, fast and low-power technologies. Similarly, properties of soft materials can be tuned, for example, by changes in temperature or pH value.

Understanding the origin of the properties of smart materials is of fundamental importance for material design, and requires the use of neutrons for accessing information about the atomic and magnetic structures, as well as about the fundamental interactions at the origin of their unusual properties. This is due to the superior capabilities of neutrons for detecting light atoms such as hydrogen or oxygen, which are directly linked to the ability to tune properties in many such materials. As neutrons interact with magnetic moments, they provide unique modalities for accessing complex magnetic properties of materials, a necessary information to unravel their intriguing multifunctionalities. Moreover, the wavelength of cold neutrons is, combined with small-angle scattering techniques, well suited for probing mesoscopic length scales, which makes cold neutrons indispensable probes for many complex materials.

3.3.1 Crystalline Smart Materials

Among smart materials, correlated transition-metal oxides (TMOs) occupy a prominent place, due to their remarkably large palette of electronic, magnetic and optical properties. Moreover, the recent progress in thin-film and heterostructure fabrication enables the growth of many of them in forms that are more suitable for technological applications. A distinctive aspect of these materials is the competition of phases with very different electric/magnetic and/or optical properties close to a phase boundary. Tiny structural changes, or small external stimuli such as temperature, pressure, electric or magnetic fields, can therefore result in very large changes in properties of such materials. This can be exploited in devices requiring robust switching between two different states. For example, resistive switching devices know as memristors incorporating TMOs with spontaneous metal-to-insulator transi-

6 K. Avers *et al.*, *Nat. Phys.* 16, 531 (2020).

tions such as VO_2 or $SmNiO_3$ have generated considerable interest, with a view to uses in memory, logic and neuromorphic applications.[7] Due to their deep penetration into matter, neutrons are ideally suited for investigating in-situ property switching in bulky sample environments.

An example of multifunctional smart materials are the so-called magnetoelectric multiferroics, characterized by an intrinsic coupling between (ferro)magnetism and ferroelectricity, two properties that were for a long time believed to be mutually exclusive. The experimental demonstration that both types of order cannot only coexist but also be strongly coupled in the same material has challenged the scientific community, resulting in a rapidly growing interest at both fundamental (see Sec. 3.2.2) and applied level during the past two decades. These discoveries have raised enormous expectations about the possible cross-control of the magnetic and electric properties, and its use in low-power data-storage technologies. In most of today's hard disks, the information is stored in magnetic bits that are written using magnetic fields generated by electric currents. If instead a voltage pulse could be employed, energy dissipation and heat accumulation could be significantly reduced, reducing the enormous, continuously growing energy consumption associated with data storage. A spintronic logic device prototype incorporating the multiferroic oxide $BiFeO_3$ has been recently proposed by Intel,[8] and it is important to underline that the details of the magnetoelectric coupling used in this prototype could be established with neutron probes.

3.3.2 Soft Matter

Many materials with building blocks on the mesoscopic scale, from nanometres up to a few microns, are 'soft', as the density of their building blocks is much smaller than in atomic or molecular crystals and, therefore, the energy density due to the interaction of the building blocks is much lower. This general class of soft condensed matter comprises diverse systems, including polymers, amphipiles, liquid crystals, and complex fluids such as colloidal suspensions. As a consequence, current soft-matter research focusses on fundamental properties and applications of a range of materials classes, including proteins and cell membranes, polymers used in the production of plastics, and liquid crystals, for example for display applications.

The contributions of research using neutrons to this broad field are similarly diverse. Neutron scattering and imaging are often the tools of choice for the study of soft matter, as the mesoscopic length scales can be covered with thermal neutrons and, in particular, with small-angle neutron scattering. Furthermore, many soft-matter materials are aqueous systems, for which contrast matching with light and heavy water is an advantage that only neutron scattering and neutron imaging can offer. In addition to their structures, also the dynamics of mesoscopic systems such as macromolecules or membranes can be studied with quasi-elastic neutron scattering or neutron spin-echo spectroscopy.

As an example, smart polymer nanoparticles are an active research field, as polymer particles can react to changes in their environment such as temperature, pH, or (osmotic) pressure, therefore offering great promise with regard to applications. Such polymer nanoparticles (microgels) can, for instance, be used to carry drugs and release them, when triggered by a change in pH, at the desired location in the body (see also Sec. 3.6). Similarly, the response of microgels to a change in temperature can be used to control the viscosity of biomedical, pharmaceutical, or cosmetic products, or they can serve as the basis for smart microlenses or photonic crystals in optical sensing applications.

Whereas many potential applications are pursued, the fundamental properties of the collective (colloidal) behaviour of concentrated microgels is not sufficiently understood, particularly for soft and deformable microgels. In contrast to the hard and rigid colloidal particles, these materials change their volume and shape when they interact. As a result, the particle–particle interaction and phase behaviour of microgels is more complex, because not only the colloidal but also the intrinsic degrees of freedom of the particles are relevant.[9]

Small-angle neutron scattering (SANS) is an ideal tool to study both the internal structure of microgels and their collective (colloidal) behaviour. Contrast matching and the controlled deuteration of microgels makes it possible to follow the structural change of these smart nanoparticles even in the most concentrated environments, and their interactions and phase behaviour are directly linked to the structure factor, which is also obtained in SANS experiments.[10, 11]

A further example of using neutron probes in soft matter research is given in Sec. 3.4.1, in the context of work towards optimized polymer membranes for fuel cells.

7 W. Yi *et al.*, *Nat. Commun.* 9, 4661 (2018).
8 S. Manipatruni *et al.*, *Nature* 565, 35 (2019).
9 A. Scotti *et al.*, *Proc. Natl. Acad. Sci. USA* 113, 5576–5581 (2016).
10 U. Gasser *et al.*, *J. Chem. Phys.* 141, 034901 (2014).
11 A. Scotti *et al.*, *Phys. Rev. E* 96, 032609 (2017).

3.3.3 Designer Nanomaterials

Nanocrystalline materials consist of inorganic particles (up to 100 nm in size) that are stabilized by attaching a layer of surfactants to their surface. These materials have properties that are distinct from their bulk counterparts, making them interesting for a variety of applications. The small grain size gives the surface of the crystallites extraordinary relevance, where the missing continuation of periodic order leads to altered structure and dynamics. It is increasingly recognised that ligands and surface chemistry have an active role and that, when used wisely, can contribute to the success of devices. Neutron scattering can uniquely contribute to the understanding of static and dynamical properties of this type of materials and pave a path toward future developments.

Neutron diffraction can be applied to study the atomic-scale structure, with emphasis on magnetic properties and light-element positions or, together with X-ray powder diffraction (XRD), to solve complex, for example, phase-change problems. The SANS technique, together with isotope contrast variation, delivers structural information on the mesoscale (shape and core-shell structure and superlattices), while allowing to characterize macroscopic sample volumes, contrary to high-resolution imaging techniques. A recent example with Swiss contribution demonstrates the possibility of three-dimensional reconstruction of nanostructured materials, following the way of data analysis applied in the field of biological macromolecules.[12]

The dynamics of nanocrystalline assemblies – superlattices extend over several decades – can be well addressed with neutron spectroscopy. For example, the long-term collaboration between ETH Zurich and PSI explored the dynamics in semiconductor PbS colloidal nanocrystals (also known as quantum dots), which is a well-established material for various opto-electronic applications. The phonon spectrum of the PbS nanocrystals, and its alteration at the surface, is strongly related to their optical properties due to unexpectedly high electron–phonon coupling. The combination of inelastic neutron scattering, computer simulations and thermal admittance spectroscopy has enabled the identification of a new electronic-transition pathway, mediated by the large number of low-energy phonon modes, which arise from the softened nanocrystal surface.[13] Depending on the application, this effect can be useful or undesired. The targeted control of its magnitude by surface chemistry is therefore expected to lead to reliable and enhanced device performance.

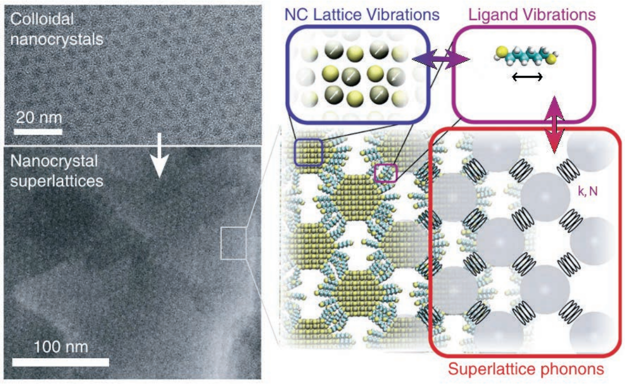


Figure 5. Phonons in nanocrystal superlattices. Schematic of classes of vibrations and phonons in nanocrystal superlattices. (From ref. [14])

Colloidal nanocrystals can form highly periodic, crystalline superstructures. In analogy to the atomic lattices, one expects therefore the existence of superlattice phonons (see Fig. 5), which was confirmed by inelastic neutron scattering.[14] The superlattice phonon spectrum can be tuned by the size and composition of the nanocrystals, and their interaction by the choice of ligand shell. Ongoing work addresses the dynamics of ligands, which act as an elastic medium, and can be characterised by an effective spring constant. Quasielastic neutron scattering is used here to understand the localised rotations of the ligands, and high-resolution neutron spectroscopy to extract the temperature-dependent mean square displacement, from which the effective spring constant can be calculated. This work also aims to provide a deeper understanding of molecular elasticity, which is highly relevant to biological functionality of, for instance, proteins.

Another example of nanocrystal application are battery materials. $LiFePO_4$ is an extensively used cathode material, which conducts lithium ions predominantly along one direction. Defects can therefore easily block the conduction channels, leading to passive regions in the interior of the crystals. This is the main reason why only the nanocrystalline form can be used. Building on the work on PbS nanocrystals, inelastic neutron scattering provided evidence that typical surface passivation (e.g., with carbon) has a measurable effect on the surface vibrational modes.[15]

In summary, neutron spectroscopy (in the examples presented here performed at SINQ and at ILL), backed up with computer simulations and complementary methods leads to deeper understanding of the dynamics of the whole, hierarchical system of colloidal nanoparticles, and of the interplay between different components.

12 Z.Luo *et al.*, *Nat. Commun.* 9, 1343 (2018).
13 D. Bozyigit *et al.*, *Nature* 531, 618–622 (2016).
14 N. Yazdani *et al.*, *Nat. Commun.* 10, 4236 (2019).
15 P. Benedek *et al.*, *Sustain. Energy Fuels* 3, 508 (2019).

3.4 Energy Materials and Processes

Finding energy solutions for the future is of key societal relevance, requiring novel technologies and corresponding advanced energy materials to fulfil the needs of the energy transition (Energiewende). Neutrons are particularly well suited to provide comprehensive insight into the structure and dynamics of such materials on multiple length and time scales, not only in model systems but in particular also in operating devices. Operando studies with neutrons enable observations from the atomic length scale, where intercalation and crystalline phase changes govern processes in batteries, to macroscopic length scales of swelling inner components and the redistribution of constituents. Similarly, probing various time scales enables covering diffusion on atomic length scales as well as full process timescales of minutes to hours. Neutron probes are unparalleled and indispensable for understanding processes involving, for example, hydrogen, which is key in the hydrogen economy of fuel-cell solutions, or lithium, the central element in Li-ion battery technology. Swiss scientists and neutron instruments have enabled some of the first seminal detailed process observations for fuel cells, hydrogen storage, and batteries. However, the impact is not limited to these key conversion technologies supporting the energy revolution, but is critical in numerous related technologies such as biofuels, catalytic processes or generating fundamental understanding of the supercritical state of water, to name but a few examples where Swiss neutron science has made core contributions already.

3.4.1 Fuel Cells

In the transition to renewable energy sources, polymer electrolyte fuel cells are of great interest for mobile applications, in particular automotive propulsion, where hydrogen and oxygen are used as reactants. The key processes in these fuel cells take place inside and close to the polymer membrane that separates hydrogen and oxygen and simultaneously allows ions (H^+) to pass and react with oxygen. This process is supported by catalyst nanoparticles located at the surface of the membrane.

Taking advantage of the unique contrast for light water (H_2O), heavy water (D_2O), and H^+ ions obtained with neutron scattering, it was shown that the structure of aqueous pathways with typical length scale from several nanometres up to a micron has a direct impact on the performance of the fuel cell.[16] Small-angle neutron scattering (SANS) and quasi-elastic neutron scattering give direct insight into the involved structure and dynamics.[17] For instance, the introduction of a preferred direction into the fractal and predominantly disordered polymer membrane has been found to optimize the aqueous pathways by reducing the tortuosity[18] of the maze-like aqueous channels through the membrane, and to improve the performance of the fuel cell. Such a structural improvement can be obtained by mechanical means during the functionalization of the base polymer with sulfonic acid. Neutron scattering is the method of choice to analyse the membrane structure and to link the structure with membrane performance.

In addition, a large body of works in the academic and industrial context is performed to advance fuel cell technology and materials through direct operando observations of water formation and transport depending on design, materials and operation conditions. Neutron imaging enables such direct observations in operating and fully functional cells. Neutrons easily penetrate such fuel cells and are also extremely sensitive to the time-dependent water distribution in the cell, which is a key property for their performance. These investigations have in the past enabled market readiness of sustainable products of specific companies and are still invaluable for advancing and improving this technology.[19] Recent breakthroughs enable to study performance under extreme environmental conditions, tackling issues of fuel cell operation in vehicles in harsh winter weather.[20]

3.4.2 Catalysts

The production and the demand for catalysts is increasing with the trend towards energy-efficient processes for the production of an abundance of chemicals and materials, and also for the transition from fossil to renewable energy sources. For the best catalytic activity, the active surface of catalysts has to be maximized, and the behaviour of the reactants close to the catalyst need to be understood on the atomic and nanoscale to optimize catalytic processes. Further, many catalysts consist of heavy elements, while the processes that they expedite often involve light elements. Neutron scattering is the method of choice to study a large number of catalysts, as it is sensitive for light elements in the presence of nanoparticles containing heavy elements, so that the structures as well as the dynamics on the atomic and the nanometre scale can be probed.

For the transition to renewable energy sources, for example, the production of fuels from biomass and increasingly from organic waste is of great interest and is expected

16 S. Balog *et al.*, *Macromol. Chem. Phys.* 211, 635–643 (2010).

17 V. Sproll *et al.*, *Macromolecules* 49, 4253–4264 (2016).

18 S. Balog *et al.*, *J. Membr. Sci.* 383, 50–59 (2011).

19 A. Forner-Cuenca *et al.*, *Adv. Mater.* 27, 6317 (2015).

20 J. Biesdorf *et al.*, *Phys. Rev. Lett.* 112, 24, 248301(2014).

to increase by orders of magnitude in the coming decade. The most effective production of methane from organic waste is the catalytic gasification using ruthenium nanoparticles on an active carbon matrix as catalyst. This process takes place under supercritical-water conditions (~400 °C, 24 MPa).

One obstacle in the production of methane from organic waste is the deactivation of the catalyst used, as sintering of the ruthenium nanoparticles reduces the active area and because of organic deposits on the catalyst. The rejuvenation of the catalyst is therefore of high interest and has been shown in a recent study to be feasible for used but still partly active catalysts. Neutron scattering (SANS) with contrast matching is sensitive to the organic material on the ruthenium nanoparticles of the catalyst and has provided detailed structural insight into catalyst deactivation by organic deposits, a deactivation mechanism that is being studied for the further optimization of catalysts.[21]

3.4.3 Batteries

Lithium-ion batteries is the most advanced and the most efficient energy-storage technology available today, not least as processes within this type of electrochemical cell are very well characterized and understood. Neutrons have a unique role in lithium-ion battery research, as they are sensitive and selective probes for hydrogen and lithium atoms, as well as for protons and lithium ions. They are employed on various length scales, from atomic resolution in structure determination, to centimetres, where whole battery cells can be imaged (see also Sec. 3.3.3).

The active materials of batteries intercalate (or alloy) and de-intercalate lithium ions, and neutron probes are used to track structural and chemical changes as batteries are going through charge–discharge cycles. Electrolytes, on the other hand, contain hydrocarbons and lithium ions, and neutron technique provide information about concentration gradients and their interphase decomposition near the surface of the active materials. Structural determinations, for example the atomic positions of different species in the typically complex active materials of batteries, are often not possible without neutron scattering, as X-rays are blind to such element-dependent structural changes. Such studies, especially those working in operando mode, guide the design of improved battery materials.

Neutron probes can help not only in structural determination and in understanding the working mechanism of nanoscopic materials, but also in optimizing battery manufacturing processes and in avoiding battery failure caused by poorly understood production steps. One example is the neutron imaging of electrolyte filling, where it was established which level of vacuum and how much time is required for the filling process.[22] The understanding thus obtained enabled an optimization of the process, resulting in a logarithmic slow-down of the filling procedure and isotropic soaking.

The ongoing race for high-energy batteries also brought renewed interest in metallic-lithium electrodes (or anode-less configurations) in combination with both current liquid electrolytes and solid-state cells, which bear great promise for future applications. In both cases, dendritic lithium growth is a main issue. Neutrons, with their high sensitivity to lithium isotopes can provide unique insight into these systems, especially if neutron-imaging technology will develop further towards higher spatial resolution.

3.5 Engineering Materials

Neutrons have a long history as a probe to investigate and progress the advancement of engineering materials. As such, they have a key role also in the current industrial revolution, where the development of metal additive manufacturing requires in-depth observations of detrimental stresses and microstructures induced by the complex thermomechanical printing process. Also in many other cases, only neutrons penetrate deep enough to observe porosities, deformations, strains, and structural flaws deep in the volume of complex samples and components.

3.5.1 Additive Manufacturing

For 3D-printed samples, neutrons provide quantitative and representative information in the context of printing parameters and material quality. The non-destructive nature of neutron investigations enables in-situ studies assessing specimen throughout sophisticated processes, including service conditions and post-processing.

A team from PSI and Empa, for example, investigated the effect of service load and microstructure on transmission-induced plasticity, in order to unlock the potential of additive manufacturing to tailor local material behaviour to the service needs of components. In the framework of the Scientific Focus Area Advanced Manufacturing (SFA-AM) of the ETH Domain, neutrons contribute to a number of projects, from additive manufacturing of precious metals involving the Swiss jewellery and watch industry

21 S. Bjelić *et al.*, *ChemCatChem* 11, 1747–1755 (2019).

22 W.J. Weydanz *et al.*, *J. Power Sources* 380, 126–134 (2018).

to the development of sensors in additive manufacturing machines. For instance, neutrons are used to characterize strain fields induced by printing and to identify improvement strategies through sophisticated operando measurements and post-processing.[23]

3.5.2 Electric Steels

The magnetic moment of the neutron enables as well studies in the field of magnetism of engineering materials, such as electric steels, where domain structures and magnetisation behaviour have a decisive role for the efficiency and losses of electric machines, which is highly relevant with a view to energy consumption. Advanced neutron imaging methods developed in Switzerland enable unparalleled observations of magnetic domains in the bulk of magnetic materials,[24] which has made it possible, for example, to better understand the effect of production methods on the material quality, and thus to optimize materials such that related losses in energy efficiency are avoided. In particular cutting technologies led to deterioration of the material quality in the vicinity of the edges and laser methods were developed to improve the material characteristics, based on neutron observations.

23 M. Morgano *et al.*, *Addit. Manuf.* 34, 101201 (2020).

24 I. Manke *et al.*, *Nat. Commun.* 1, 125 (2010).

3.5.3 Corrosion

Neutron imaging is also an important scientific tool is the study of corrosion of metals. In many engineered composite materials, metals are surrounded by porous media and the study of the internal corrosion processes requires non-destructive investigation methods. Corrosion is generally closely linked to the presence of moisture within the porous medium surrounding the metal. Neutron imaging has therefore a key role in studying the relevant processes. The high sensitivity for hydrogen also entails that some corrosion products lead to an increased contrast in the neutron data, despite the lower density in the affected areas. An example is the study of the corrosion mechanism affecting reinforcing steel in concrete. A team from ETH Zurich and PSI uses combined X-ray and neutron imaging to study the role of entrapped air voids at the steel–concrete interface and to study the influence of capillary water movement through the cementitious matrix and the related corrosion processes at the reinforcing steel.

3.5.4 Nuclear Safety

Owing to their high sensitivity for hydrogen and low sensitivity — and therefore high transmittance — for many high-Z materials, neutrons have long been utilized as a probe for investigation of materials relevant for nuclear safety. Neutron imaging in particular has been instrumental in providing information relevant for the safety

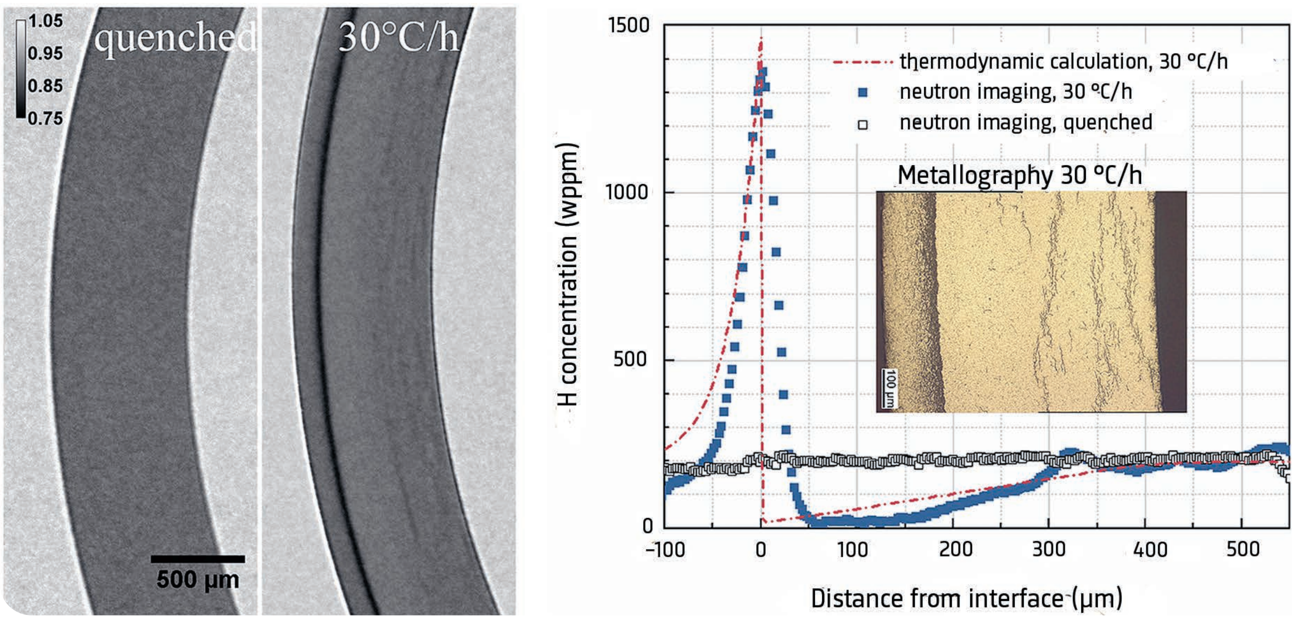


Figure 6. Left: High-resolution neutron radiography of nuclear-fuel cladding tubes hydrogenated to 200 wppm and treated to different cooling rate. Right: The derived hydrogen concentrations in the samples shown on the left. (From ref. [27], with permission.)

aspects, for example on the hydrogen distribution and concentration in zirconium-based materials,[25, 26] which are the material of choice for nuclear-fuel cladding tubes. The diffusion of hydrogen into the cladding is inevitable and poses a safety risk throughout the lifetime of the nuclear fuel assembly. In order to assure safe handling, transportation and (intermediate dry) storage of nuclear fuel, the spatially resolved quantification of hydrogen within the cladding is highly important. Especially for cladding that is fitted with liners that improve the corrosion resistance of the cladding or the interaction between the nuclear-fuel pellet and the cladding. Recent advances in the high-resolution neutron imaging lead to a much improved understanding of the hydrogen/hydrides distribution in zirconium nuclear-fuel cladding tubes[27] and in particular enabled spatially resolved hydrogen quantification (see Fig. 6).

Due to the intrinsic activation of the studied specimens, the neutron-based techniques are also primed for the investigations of radioactive samples. Recent advances in the instrumentations enables high-resolution neutron imaging of cladding tubes that underwent the entire life-cycle in a nuclear power plant. Using this novel technology,[28] the hydrogen distribution in realistic samples (with dose rates up to 10 mSv/h) were recently obtained in pilot investigations at SINQ. Further work in this direction will be of interest for all parties involved, from academia to industrial partners and regulators. For samples emanating even higher dose rates, PSI is equipped with worldwide unique test equipment. With the NEURAP add-on at the NEUTRA beamline, neutron radiography of samples with up to several Sv/h is possible, enabling imaging investigations of nuclear fuel. The future upgrade of the NEURAP facility will provide the basis for imaging at even higher spatial resolution and for tomographic investigations, opening the path to investigations answering important questions on safety aspects related to spent nuclear fuel.

25 M. Grosse *et al.*, *Nucl. Instrum. Methods Phys. Res.* A 651, 253 (2011).
26 N.L. Buitrago *et al.*, *J. Nucl. Mater.* 503, 98 (2018).
27 W. Gong *et al.*, *J. Nucl. Mater.* 526, 151757 (2019).
28 Trtik *et al.*, *Rev. Sci. Instrum.* 91, 056103 (2020).

3.6 Health

Neutron probes provide unique opportunities for the health sciences, typically in combination with other modalities. Water is the foundation of all life, and neutrons offer a unique contrast for water-based materials by means of contrast variation with light and heavy water. We highlight here three examples to illustrate both the promise and breath of the contributions of neutron science and technology to the health sciences.

In recent work, a combination of neutron reflectivity measurements and interfacial rheology was used in designing emulsion systems stabilized with natural biopolymer particles to realize specific lipid digestion kinetics. Such systems are important in the context of addressing malnutrition, which includes overeating as well as nutrient deficiencies and is one of the most pressing problems with a view to a healthy population and personal well-being. Among a variety of approaches, the stimulated release of satiety hormones offers a soft control on food intake. The use of stimuli-responsive particles such as nanocelluloses received increasing recent attention. The

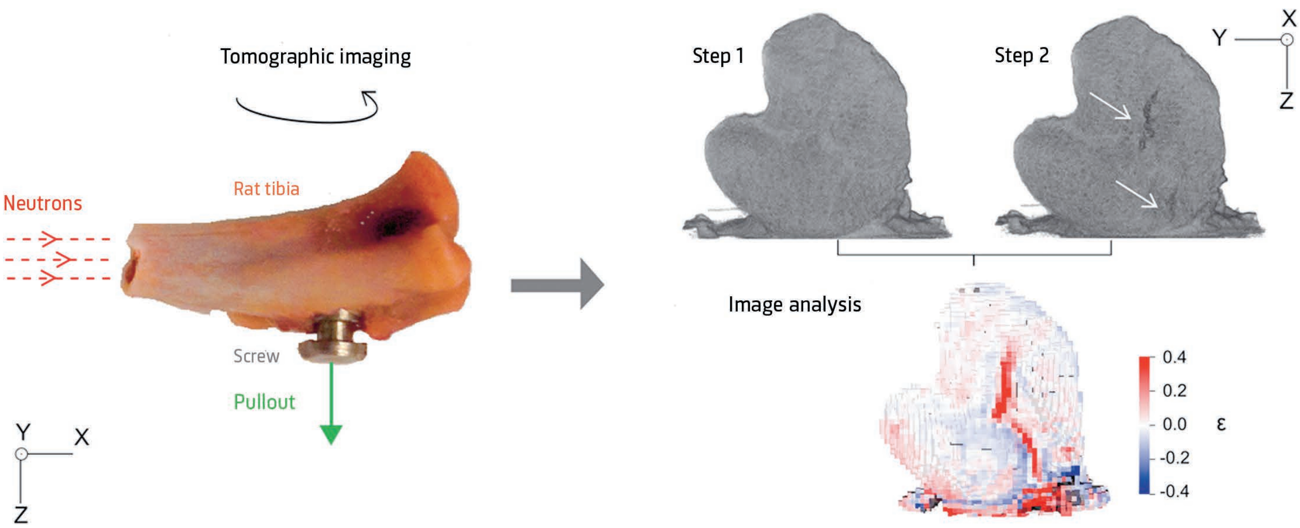


Figure 7. Neutron tomographic imaging provides insight into bone-implant interfaces and can be used to characterize their mechanical response under in-situ loading, including crack formation during the loading of the implant. (From ref. [30], with permission.)

adsorption of nanocellulose and nanocellulose–protein composites at oil–water or air–water interfaces facilitates the formation of stable and biocompatible emulsions and foams. Neutron reflectivity measurements at SINQ have been used to monitor the structure of differently designed adsorption layers as a function of physico-chemical boundary conditions (pH and salts), surface properties of the cellulose crystals and protein addition (i.e., concentration). Scattering-length density profiles obtained from neutron reflectivity measurements provided information about the thickness and roughness of the adsorption layer, and in case of nanocellulose–protein composites, their spatial composition. Supported by atomic force microscopy (AFM) images and interfacial rheological of the adsorption layer, the design principles of nanocellulose-stabilized emulsions and foams for food and drug delivery vehicles were rationalized. In a feedback loop between neutron reflectivity, interfacial rheology, in-vivo gastric magnetic resonance imaging (MRI), and physiology in humans and rats, not only the in-vitro/in-vivo correlation of fat digestion was established, but also pathways to limit or stimulate food uptake.[29]

In other work,[30] neutron tomography was used to characterize the interface between bone and metal implants (Fig. 7). The integration of implants used for numerous orthopaedic conditions is of outmost importance for the long-term success of corresponding surgical treatments. The imaging of commonly used metallic implants is challenging for conventional X-ray imaging and MRI, but their integration and behaviour under realistic load conditions can be studied efficiently with 3D neutron imaging. Corresponding model studies at PSI to, for instance, reveal and quantify bone ingrowth around implants and the mechanical response of a system of metal screws implanted in rat tibiae have provided quantitative insights up to load states leading to cracking and finally failure of the bone–implant interface.

A third example is the use of SINQ in the development of innovative radionuclides and radiopharmaceuticals. At PSI, the Center for Radiopharmaceutical Sciences (CRS), a joint endeavour between PSI, ETH Zurich and the University Hospital Zurich, works on clinical application of radiopharmaceuticals, with a focus on the development of novel radioactive drugs for non-invasive diagnosis and therapy of metastatic cancerous lesions. For further information and future perspectives on radiopharmaceutical innovation using neutrons, see Sec. 5.6.

3.7 Cultural Heritage

Non-destructive testing methods are typically the only possibility to investigate invaluable objects of cultural and natural heritage, in order to understand their origin, meaning or underlying technologies. In particular when X-rays fail, neutrons are generally the only means that can provide information on the interior and interior structure, contents, and conservation state of objects of significant value and interest. In addition, neutrons in general provide complementary information, for which Swiss researchers have pioneered combined X-ray and neutron imaging, which is of interest not only for cultural heritage. Today the method is applied around the world to numerous cultural heritage and materials science questions.

Neutron instruments at PSI have a long tradition, when it comes to investigations of cultural heritage objects. Neutron imaging in particular has enabled over the years close collaborations with many Swiss and international muse-

29 N. Scheuble *et al.*, *ACS Appl. Mater. Interfaces* 10, 17571 (2018).

30 S. Le Cann *et al.*, *J. Mech. Behav. Biomed.* 75, 271–278 (2017).

31 D. Mannes et al., *Physics Procedia* 69, 653–660 (2015).

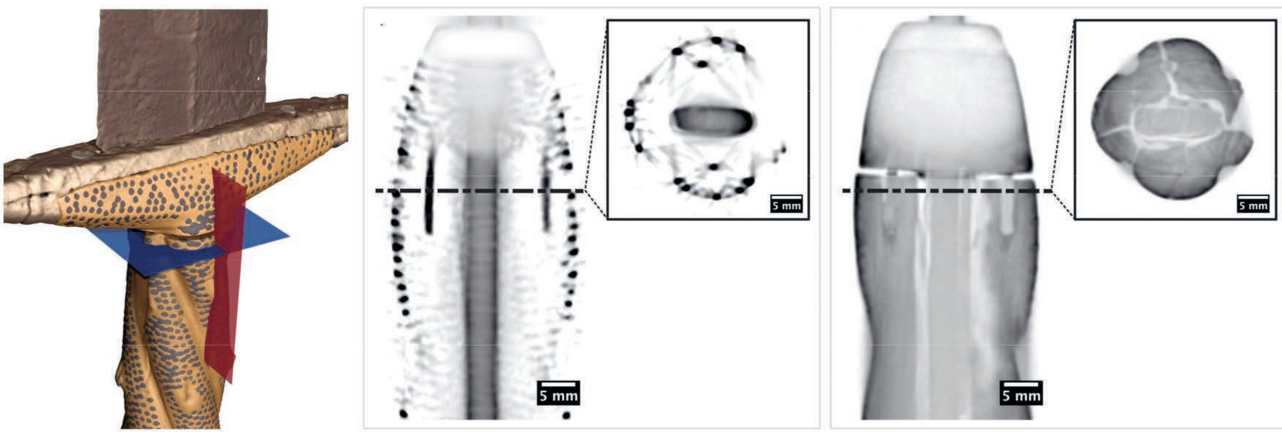


Figure 8. Neutron images of the 'Swiss Degen'. (From ref. [31])

ums (including the Swiss National Museum, the Museum Rietberg in Zurich and the Museu Nacional d'Art de Catalunya in Barcelona), research institutions, universities and cantonal authorities. An example of particular Swiss relevance is the investigation, in collaboration with *Kantonsarchäologie* Zug, of a short sword found in lake Zug in 2010. The weapon was later identified as the 'Swiss Degen'. Though the blade was heavily corroded, the highly ornamented wooden hilt was still in very good condition. The hilt is also what makes the object so special, as it is the only one of the three remaining swords of that type that is still in its original constellation. The hilt shows spiral carvings and is abundantly decorated with tiny metal inlays. These ornamental inlays contain mercury and are hence highly attenuating for X-rays. It was therefore in this case impossible to retrieve information on the actual wooden parts of the hilt by X-ray imaging alone. Therefore, the sword was inspected using neutrons and X-rays. Computed tomography revealed all complementary information and the neutron data provided images of the wood structure (such as annual rings and knots) as well as position, size and shape of all the wooden parts of the hilt. X-rays on the other hand visualize only the structure of small inlays (see Fig. 8). The reconstructed data sets were merged to obtain the complete virtual 3D volume of the object.

3.8 Industrial R&D

While the major share of societal and industrial impact of neutron science derives from academic and collaborative academic/industrial R&D innovations, there is also a more direct relation of neutron science and industry, in particular in the field of non-destructive testing. This means that industry increasingly leverages neutron-science methods for solving specific problems — be it a failing product, large deficient production rates, or lack of understanding of a product issue or failing development. Neutron imaging, which enables direct non-destructive insight into complex and bulky products, is often the means of choice, but also neutron strain scanning or small angle scattering and diffraction can often solve such problems and provide immediate feedback and solutions through commercial beamtimes.

Typical customers at neutron facilities are the automotive and aerospace industries, but also the energy and health sectors are well represented. Many such services are by their nature proprietary and therefore protected by non-disclosure agreements. However, a few examples have been published and can be revealed. They are presented in the following.

3.8.1 Automotive

Many components in automotive applications are bulk-metal devices that contain hydrogenous materials, in particular oil. These can be penetrated only by neutrons to observe the oil content and even changes in its distribution during operation. But also the results of a number of joining technologies, including welding, soldering and gluing, can be readily inspected with neutrons. A specific

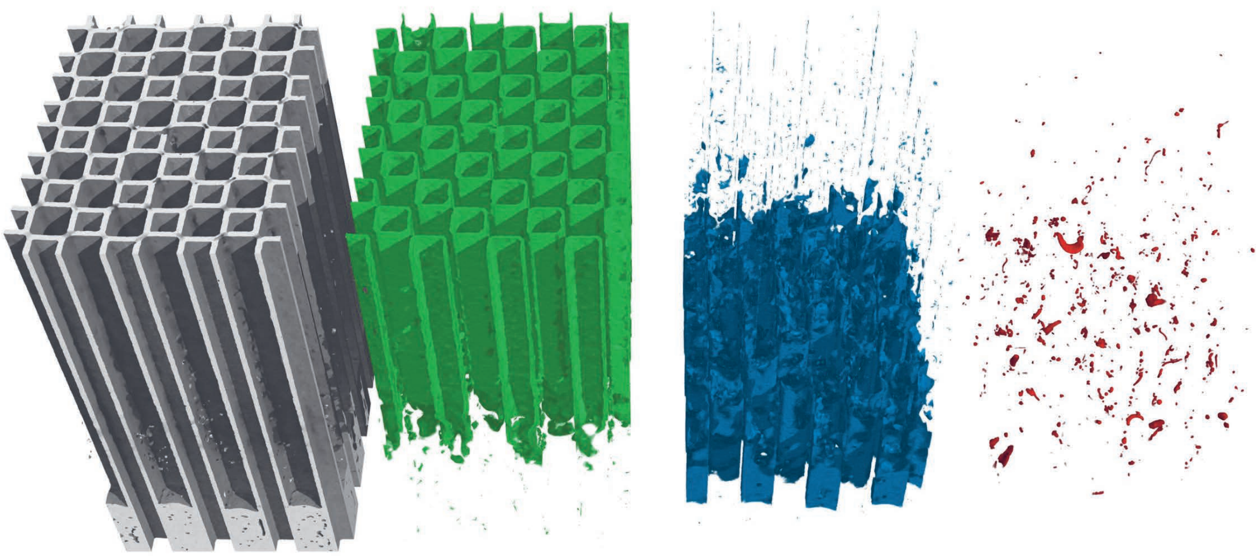


Figure 9. Investigation of a diesel particle filter showing (from left to right) the support and deposited soot (green), ash (blue) and metal particles (red). (Photo: https://www.psi.ch)

example of an automotive application is regular support in the R&D of diesel particle filters (see Fig. 9), which were urgently required when they became mandatory for vehicles in order to reduce the environmental impact of transportation. It was demonstrated at SINQ that neutron imaging can probe full-scale filters and provides all relevant information on their inner status of load and contained sediments, to comprehend their functionality and shortcomings. Subsequently neutron imaging, in particular at PSI, supported extensively the entire automotive sector in the development of particle filters.

3.8.2 Medical

In the medical sector, a published study drawing on neutrons is one performed with La Roche at SINQ. The issue investigated is related to clogging in staked-in needle pre-filled syringes (SIN-PFS) during storage and before use (Fig. 10). Depending on storage conditions, including temperature and humidity, needles of syringes containing high concentrations of drug-product solutions tend to clog. After the initial demonstration that neutrons enable remote observation of the filling states and clogging of the needles, a number of studies were performed, to investigate, for example, the influence of water-vapour transmission through the needle shield. The published results have created significant international interest in this industry for additional studies.

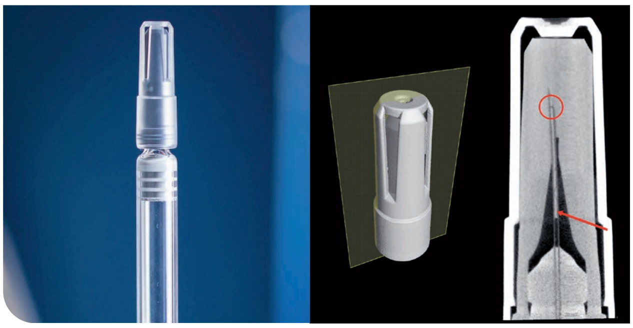


Figure 10. Investigation of syringe needle clogging. (Photos: https://www.psi.ch)

3.8.3 Energy

The energy sector constituted the biggest share of industrial use of neutrons before fuel cells for mobile applications reached market readiness, a development that was significantly supported by insights provided by neutron imaging. Customers from around the globe requested neutron imaging at SINQ in order to facilitate key advances. A more recent example of completely different nature is a seminal investigation for ABB in Aargau, where neutron experiments enabled clear practical recommendations to increase the production efficiency and thus output in the manufacturing of ceramic varistors. Varistors are voltage-dependent resistors used, for example, in electrical transmission lines for overvoltage protection. Neutron images provide a clear picture of the binder burn up and in particular the residual binder content — which is not accessible otherwise — depending on heating conditions in the ovens utilized during production.

Figure 11. Launch of an ESA Ariane 5 rocket. (Photo: ESA/CNES/ARIANESPACE-Service Optique CSG; JM Guillon)

3.8.4 Aerospace

For the European Space Agency ESA and its component suppliers, neutrons are an indispensable tool for guaranteeing the quality of key parts that decide about success or failure of a mission, in particular in the launching phase of their rockets Ariane 5 and Vega (Fig. 11). Moreover, neutrons are also regularly used for investigations and inspections of conventional airplane components.

In addition to the direct utilization of neutrons for commercial products, neutron science centres create synergies for the technology companies in their vicinity, which depend on close ties to these large-scale facilities. Two specific examples in Switzerland are SwissNeutronics, who produce high-quality neutron optics utilized at neutron sources around the world and are developing and testing their products at SINQ. RC Tritec, on the other hand, has developed in close collaboration with PSI a product line of neutron scintillator screens, which are standard screens used around the globe today.

The direct commercial innovation use of neutrons underlies fluctuations and depends strongly on the proactive action of neutron scientists in creating awareness and specific market needs, which in turn can lead to booming requests for certain periods of time, such as in the phase shortly before market readiness of fuel cells. Another limiting factor, in addition to awareness, has been identified in the resources of scientist and institutions to react to industrial needs, such as complex sample environments tailormade for specific product studies.

The number of average yearly requests show an increasing trend (Fig. 12), which led to the situation that currently the available beamtime for these projects is typically fully booked, calling for the addition of further imaging instruments in order to be able to satisfy the growing demand.

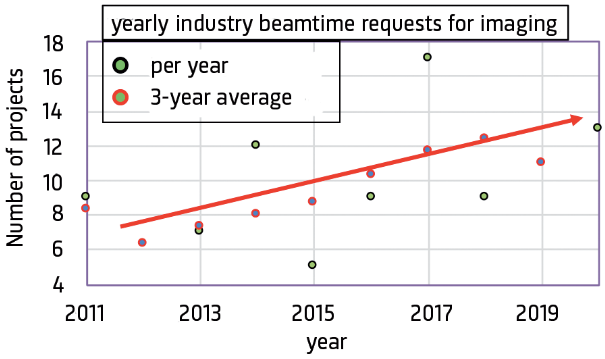


Figure 12. Number of yearly neutron-imaging industry projects at SINQ.

In an important development, in 2019 the Technology Transfer Centre ANAXAM (Analytics with Neutrons And X-rays for Advanced Manufacturing) has been founded by the Kanton of Aargau, PSI, the Swiss Nanoscience Institute (SNI), and the University of Applied Sciences and Arts of Northwestern Switzerland (FHNW), under the umbrella of the Strategic Focus on Advanced Manufacturing of the ETH Domain.

ANAXAM establishes a link between industry and the academic analytics infrastructure, in particular the large-scale facilities and hence the neutron source SINQ. It serves as a portal for industrial requests, acquires customers through marketing of the potential of the available methods, and supports studies and in particular their technical needs. Thereby ANAXAM offers in particular the opportunity to open a path for the industrial use of neutron methods other than imaging, such as scattering techniques, where the entry barrier for non-academic players has been typically prohibitively high so far.

Thermal neutron triple-axis spectrometer EIGER of the SINQ at PSI. (Photo: PSI)

4 The Neutron Science Community

4.1 Analysis of Swiss Neutron Science Community

4.1.1 Impact

Working closely with the team that has recently conducted a machine-learning-assisted natural language processing analysis of around 46,000 journal papers published between 1956 and mid-2020 in the broad field of neutron science, we present here parts of the results that relate specifically to the Swiss neutron science community.

Figure 13 shows the output of the Swiss community between 1998 and 2018. The number of 'neutron articles' with at least one author with Swiss affiliation grew from ~150/year in the period 1998–1999 to ~300/year in the period 2015–2018. Of the European 'neutron articles', around 10% include authors with Swiss affiliation (whereas Switzerland has only 2% of Europe's population).

When comparing the numbers of the European and worldwide (without Europe) communities, we can see that articles from outside Europe have since 2010 started to outnumber European output. This trend has to be seen against the background of the expressed concern by the European neutron users that the coming decade will see a clear reduction of available neutron beamtime,[32] with direct consequences for the European community. This is a genuine threat for European leadership in the field: In 2019, for example, three national neutron-scattering facilities have been closed, in France, Germany, and Norway.

The unbiased machine learning algorithm classifies papers into topics that were subsequently identified by human inspection of the key words associated with each. Inspecting the individual topics produced by the algorithm, the following observations can be made (see Fig. 14):

- Decline in pure diffraction. This is likely because specialized forms of diffraction such as protein crystallography or engineering samples shift into dedicated fields, such as fundamental physics and lattice dynamics, both of which have seen significant growth in the past two decades.

- Continual strong activity in spectroscopy of magnetic materials

- Significant growth in the following topics:
  - Life, food and polymer science
  - Neutron sources and neutron instrumentation, driven by SINQ upgrades and ESS instrumentation, where Switzerland is a remarkably strong contributor
  - Neutron imaging

32 https://www.esfri.eu/neutron-landscape-group

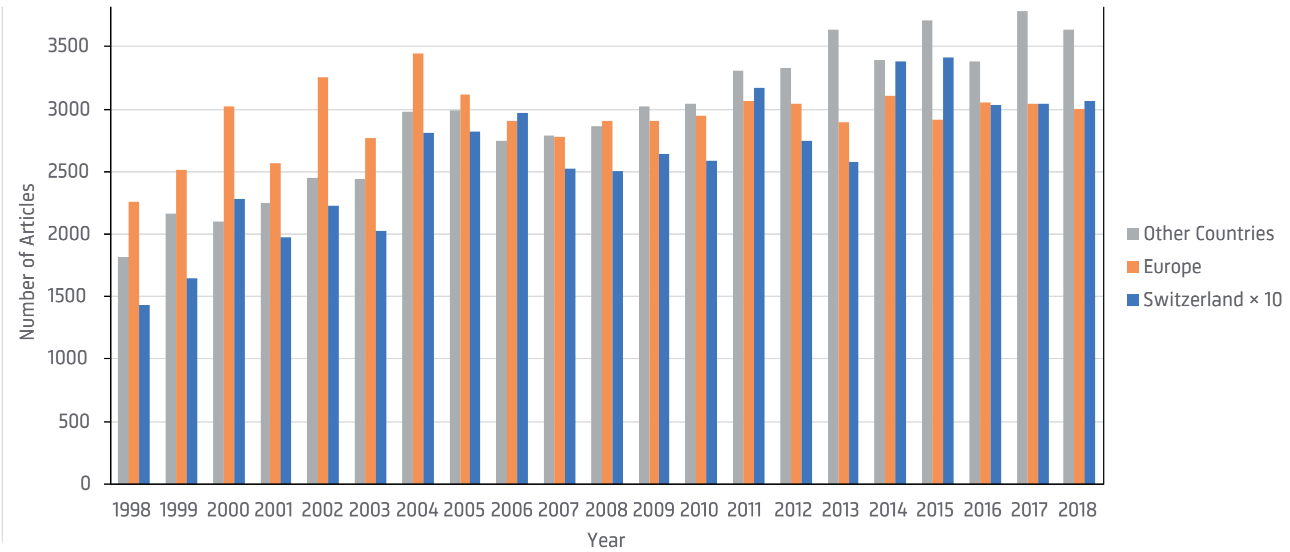


Figure 13. Numbers of articles published per year with author lists affiliated entirely outside Europe (grey), within Europe but with no Swiss authors (orange), and those including at least one author with a Swiss affiliation (blue).

- Neutron electric dipole moment
- Fundamental physics, i.e., the n-TOF experiment at CERN

The analysis also highlights the breadth of applicability of neutron probes, with several more topics with continual and important contributions such as reactor physics, medicine, lattice dynamics, nuclear physics, soft-matter dynamics, and superconductors.

4.1.2 Needs

Access to neutron experiments proceeds mainly through peer-reviewed beamtime proposals. Exceptions to this are in-house research at facilities and longer-running projects and collaborations, such as electric dipole measurements. The needs of the Swiss neutron science community with regard to neutron experiments can be quantified by the historical numbers of beamtime proposals.

Analysing data for Swiss proposals to neutron facilities demonstrates a trend of increasing requests for neutron beamtime from Swiss researchers for SINQ (Fig. 15) and ILL (Fig. 16) — in both cases more than doubling from 1999 to 2015, which is also seen at several other sources, including FRM II, ISIS, and SNS. This trend is capped by the available beamtime allocations at the corresponding sources, which leads to a self-regulating reduction in proposals from each user group. This effect is particularly pronounced for beamtime requests to ILL (Fig. 16), where for the period from 1999 to 2016, the excess Swiss need ('oversubscription') was a factor of two. Since 2016, a combination of factors led to drastic decrease in beamtime allocation to Swiss scientists, which has resulted in a self-regulating slight reduction in requests, but more importantly has had a detrimental effect on the many scientists who have not been able to carry out their research programmes, especially PhD students who need to get results within the time of their doctoral studies.

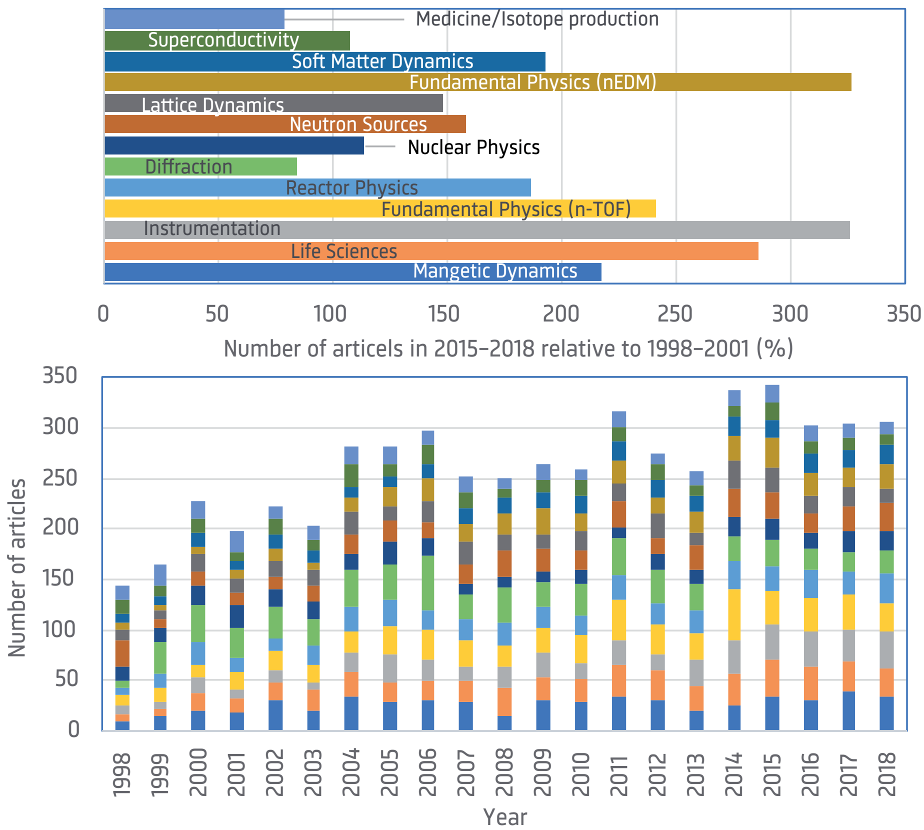


Figure 14. Lower panel: The time evolution of the topics of 'neutron articles', as identified by the NLP analysis. The topics were named by inspecting the key words for each of the 13 topics identified by the algorithm. Upper panel: Growth by topic, determined by comparing the number of articles published in the period 2015–2018 relative to those published in the period 1998–2001.

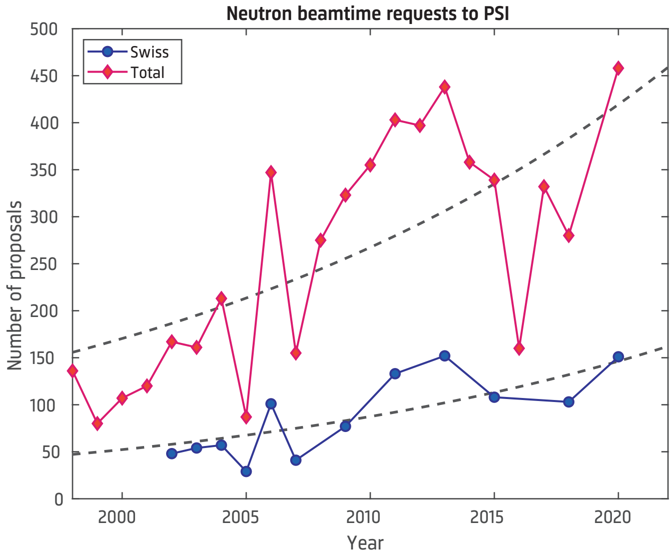


Figure 15. Number of neutron beamtime requests to SINQ 1999–2020. The exponential fit corresponds to a 5.1% annual increase in Swiss proposals.

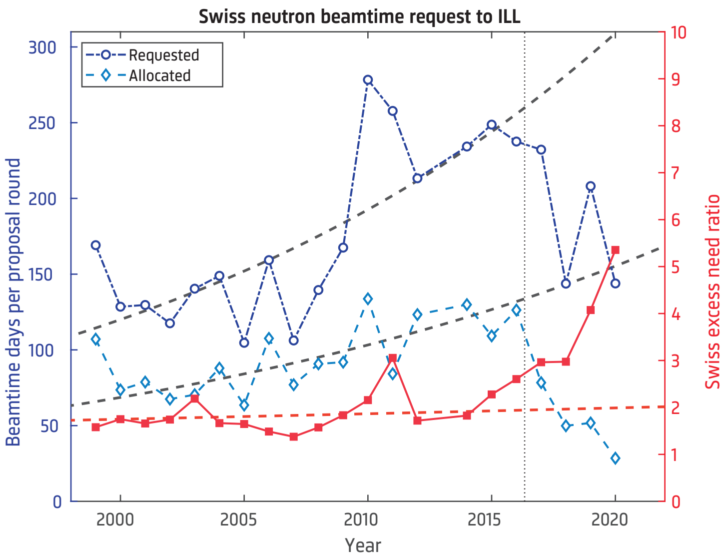


Figure 16. Swiss usage of the neutron source ILL, Grenoble. The requested (dark blue line) and allocated (light blue line) number of beam days was increasing 4.7% per year (dashed black curves) from 1999 to 2016

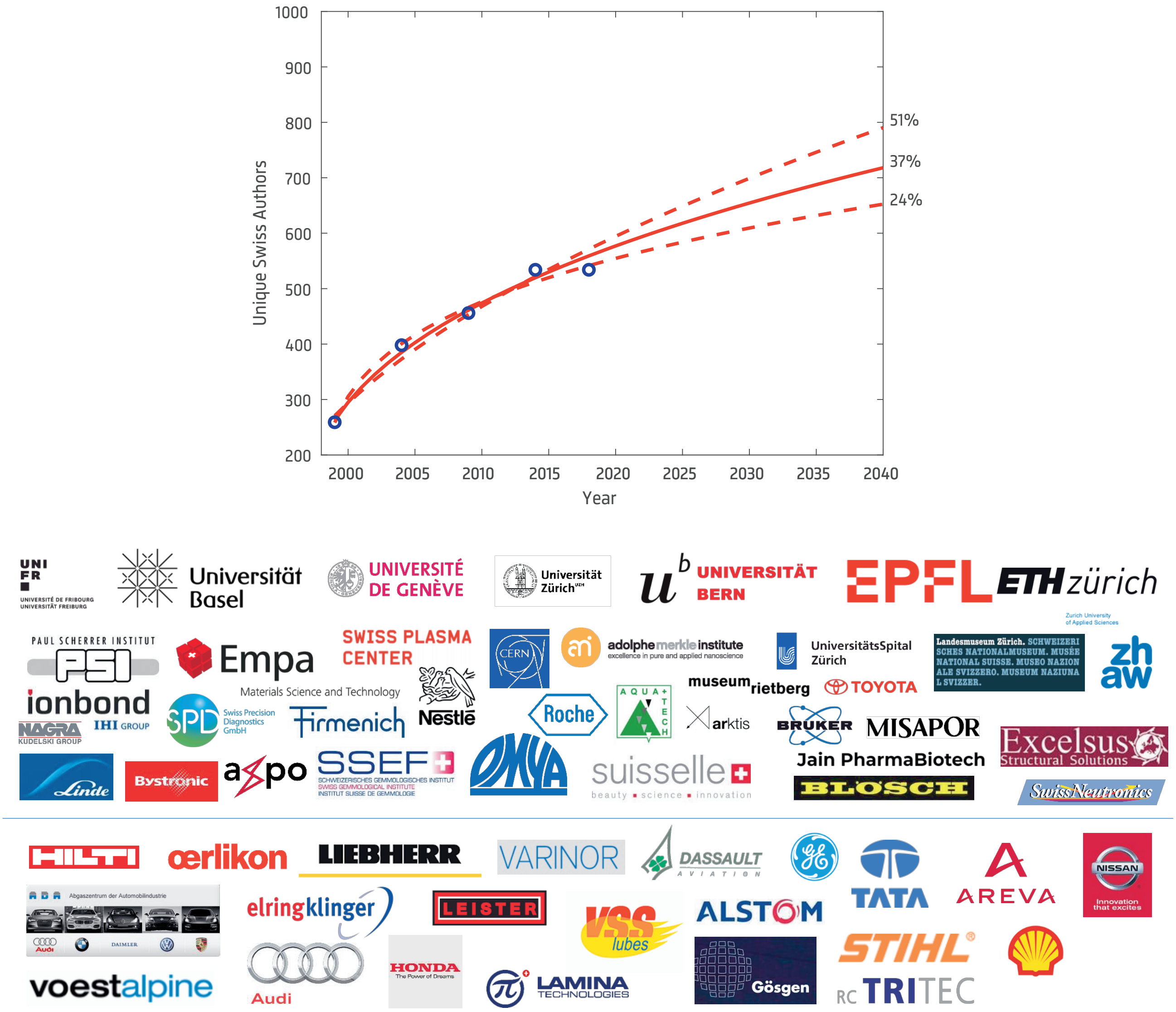


Figure 17. Growth in the number of unique authors of neutron science articles with Swiss affiliations since 1999. The extrapolations show the size of the community in the near future, for different rates of growth that may all be compatible with the current and historic community sizes, but which do not take into account the catalytic effects that can be expected from the inauguration of ESS and from the strong increase in industrial use. The logos represent affiliations on articles and non-publishing industrial neutron users, illustrating the remarkable span of the Swiss neutron science community (above the thin blue line are the affiliations on articles, and below companies involved in industrial collaborations).

4.1.3 Size

To further quantify the neutron science community, we counted the number of unique authors with Swiss affiliation for selected years. We found that the number of unique authors grew from 257 in 1999 to 534 in 2018. The full result is shown in Fig. 17 (note that the number of years for which this analysis was carried out is restricted as it had to be done manually).

The counting shows that the number of unique authors active within the Swiss neutron science community has grown steadily since 1998, in fact approximately doubling. The figure also includes conservative estimates of the size that the community might reach in the coming decades, assuming steady (as against sudden or discontinuous) growth, underlining our recommendation that funding and facilities for such a growing community must expand to match (see Chapter 2). This recommendation is all the more urgent as we expect for the coming decade accelerated growth, with the user programme at the ESS starting in 2023, and likely increased use of neutron probes in industrial R&D, which is a global trend we also see in Switzerland (see Sec. 3.8).

4.2 Education and Training

The education of PhD students and scientific training of postdocs are essential for an active research community and our society in general. The participation in neutron experiments introduces the students to demanding experimental processes, a broad variety of analytical tools for data analysis, and complex theoretical modelling. After their PhD studies, these highly qualified young people are open to continue their careers in science, industry, business or politics, thus making important contributions to our society.

In Switzerland, 20–30 PhD students graduate per year on research topics relying on neutron and muon beams, as revealed by analysing the 2018–2019 PhD theses in the Swiss National library data base (e-helvetica.nl.admin.ch). Another 80 to 100 postdocs work in all areas of neutron sciences in Switzerland. Their diverse activities cover fields from basic research to applied sciences and services, such as those provided by beamline scientists. These young researchers are located across essentially all the Swiss research institutions, including the ETH Domain at ETH Zurich, EPFL, PSI, and Empa as well as at the cantonal universities at Basel, Bern, Fribourg, Geneva, and Zurich.

Neutron sciences require access to neutron beams for experiments. The Swiss Neutron Spallation Source SINQ is the national host for neutron research and education in Switzerland. At SINQ the PhD students acquire first hands-on experience on neutron experiments, data collection, and evaluation. Far beyond the basic education, SINQ offers a strong neutron source, high-performance instruments, and dedicated sample environments, such as low temperature, high magnetic field, and high pressure. These ingredients, together with Swiss high-precision engineering and reliable operation, make SINQ an internationally competitive source for cutting-edge neutron research. Aside from SINQ, the access to international neutron sources is granted via collaborative contracts. The most important centres are currently the ILL (France), ISIS (UK), and starting from 2023 the ESS in Sweden. Access to neutron sources is competitive, and is granted through a proposal system evaluating the scientific merit of the planned experiment. Therefore, the research-based access has to be complemented by an educational approach for students. The availability of neutron beams from both the local SINQ source and via international collaborations is crucial for Swiss researchers.

From their home base at SINQ, a strong Swiss neutron scattering community developed, which is particularly active and successful (see Sec. 4.1). It continuously promotes technical and scientific developments at SINQ and beyond. Swiss researchers are particularly active in building the new instrumentation at the European Spallation Source ESS in Lund (see Sec. 5.3).

Outreach activities disseminate information on neutron sciences on various levels. Activities include beginners days to introduce young people to science, e.g. for 7th and 8th class pupils and 11th and 12th class students at the gymnasium level. The annual PSI Summer School in Zuoz brings together PhD students and postdocs for one week of intense learning.

Publication of results in research journals is the key measure of scientific success in natural sciences. For a detailed analysis of the publication output of the Swiss neutron community, see Sec. 4.1. The analysis yields a broad distribution of neutron-related research topics over scientific disciplines. The total number and an impressive fraction of publications in high-impact journals demonstrates the overall importance of the research based on neutron beams.

4.3 Prediction of Future Swiss Neutron Community

The beamtime-proposal and bibliometric analyses (Secs 4.1 and 4.2) show:

- Increasing number of proposals by Swiss scientists to SINQ and to international facilities, capped by allocated beamtime through proposal systems
- Increasing spread of scientific fields using neutron beams for their research
- Increasing number of complementary techniques used per article
- Increasing number of authors per article
- 87% increase in published articles from 1999 to 2018
- 108% increase in the number of researchers using neutrons from 1999 to 2018

In addition to these numerical results, several qualitative evolutions are expected:

- The new capabilities at ESS will open fields of science not currently available
- Increased industrial use, among other factors also through creation of ANAXAM

Based on these findings, the following predictions are made for the neutron science community:

- Number of Swiss researchers using neutrons increases by 25% until 2030 and by 40% until 2040
- Swiss demand for neutron beamtime increases by 20% until 2030 and by 30% until 2040
- The domains where use of neutron will grow more than 100% by 2040 include: Life Science, Neutron Imaging, Industry R&D

The Small-Angle Neutron Scattering (SANS-I) instrument of the SINQ at PSI. (Photo: PSI)

5 Neutron Experiment Provision

Producing a beam of neutrons for scientific use requires a large-scale facility where neutrons are liberated from atomic nuclei either by fission or spallation by bombardment from an accelerated proton beam. The first generations of neutron sources were research reactors. Most new sources are based on proton accelerators.

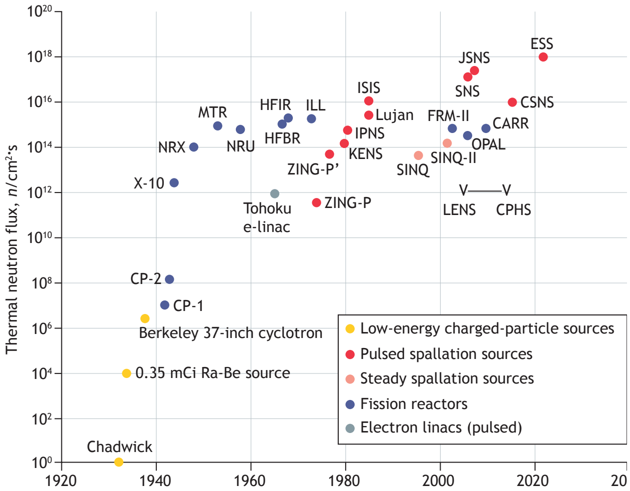


Figure 18. Evolution of fluxes of thermal neutron sources[33]

Figure 18 illustrates the evolution of neutron flux. Reactor-based sources reached their maximum potential with the ILL reactor in Grenoble, France. The three next-generation spallation sources, SNS in US, J PARC (labelled JSNS in Fig. 18) in Japan and ESS (under construction in Sweden) will be the most-intense neutron sources for the foreseeable future.

5.1 Current Landscape

The European neutron landscape was recently surveyed and reported by the Physical Sciences and Engineering Strategy Working group of the European Strategy Forum on Research Infrastructures (ESFRI).[34] We recommend referring to this document for further details, and reproduce here the main findings.

For about 40 years, Europe has held a leading role in the field on neutron science. This position has been due to a powerful combination of multiple low to medium-flux sources across Europe, which served to cultivate local scientific communities, providing a breeding ground for scientific talent and stimulating diverse technical innovation, and a few medium to high flux sources, where state-of-the-art experiments not possible elsewhere in the world can be performed, and which serve as international hot-spots for scientific exchange. The result has been a multi-disciplinary international scientific user community with over 6,000 scientists and engineers from academia, national and international research laboratories and institutes, as well as from industry. Among them these facilities have established a remarkable eco-system of extremely skilled manpower readily available elsewhere for nuclear physics and engineering as well as accelerator expertise.

The past configuration of the European neutron landscape was composed of ten low/medium-flux national sources, three medium-flux sources (FRM II, ISIS and SINQ) and the worldwide highest-flux source, ILL (see Fig. 18).

ILL was built in 1971 as the world's premier neutron source. It is owned and operated by the three founding countries, France, Germany and UK, and 10 partner countries. Switzerland was the second country to become a partner of ILL, and continues a close collaboration both at the scientific and technical-development level. ILL remain the globally leading neutron source with the highest flux and the largest number of operating instruments.

High-flux pulsed spallation sources have been brought online in the US (SNS in 2007) and in Japan (J-PARC in 2010) which have superseded ISIS in the UK as the highest-flux pulsed neutron sources. However, the time-integrated flux of these facilities remains much below that of the ILL. The corresponding pulsed flagship source in Europe, the European Spallation Source (ESS), is under construction in Sweden with expected inauguration in 2023. It will surpass both SNS and J-PARC. ESS is expected to reach full specifications with 20–24 instruments in 2028–2030. ESS is being built as a pan-European international facility with 13 member countries, including Switzerland.

5.2 Future Neutron Landscape

As such, European neutron science stands before an exciting future with hitherto unprecedented experimental

33 https://europeanspallationsource.se/sites/default/files/files/document/2017-09/NGL_CombinedReport_230816_Complete%20document_0209-1.pdf

34 NGL_CombinedReport_230816_Complete document_0209-1.pdf (esfri.eu)

Figure 19. Distribution of neutron sources around the world, showing the strong concentration in Europe.[35]

capabilities at ESS. However, the network of sources with versatile unique instrumentation and scientific specialization faces a challenging time. Of the ten low/medium-flux sources, the two with the strongest user programmes, LLB in Paris and BER2 in Berlin (both of which were frequently used by the Swiss scientific community along with two smaller sources) have already been closed. By 2025, only five neutron sources with international user programmes are expected to remain: ESS, ILL, ISIS, FRM II and SINQ.

It is vital for the Swiss and for the European neutron science communities that these remaining sources are operated and upgraded to provide both top-level capabilities in terms of the most challenging experiments, and sufficient capacity for the many types of investigations that can only be done with neutrons.

In this context, ILL is especially important. Not only is it the highest-flux neutron source in the world. It also has the most operational neutron instruments (about 40), thereby enabling a significant volume of science. ESS aims to reach up to 24 instruments in the foreseeable future. While these instruments will be extremely powerful, other sources will be needed to accommodate the growing usage of neutron probes in ever-diversifying fields of science (see Chapter 3).

There are interesting ongoing efforts to develop so-called high-brilliance sources, which would be cost-effective local sources to replace the closed low-flux sources. As technology progresses, this could alleviate the situation. However, in the intermediate future, the most cost-effective solution to the reduction in joint European neutron science capacity would be to maximize the number of operating instruments at existing sources.

An important challenge to a holistic strategy for neutron science in Europe and worldwide is the sharing of investment and operation costs. National facilities are nationally funded, at times with smaller specific international partnerships, for instance around specific instruments. In general, access to these facilities is solely based on scientific excellence of the proposals. The two international facilities, ILL and ESS, are jointly funded by multiple countries. To ensure that the joint investments in neutron science are as effective as possible, collaboration and coordination is required not only on the technical level, but also on the decision and funding levels.

35 Strategy paper on neutron research in Germany 2020–2045 https://www.fz-juelich.de/jcns/EN/_SharedDocs/Downloads/EN/Strategy_Paper_Neutron_Research_Germany_2020%E2%80%932045.pdf

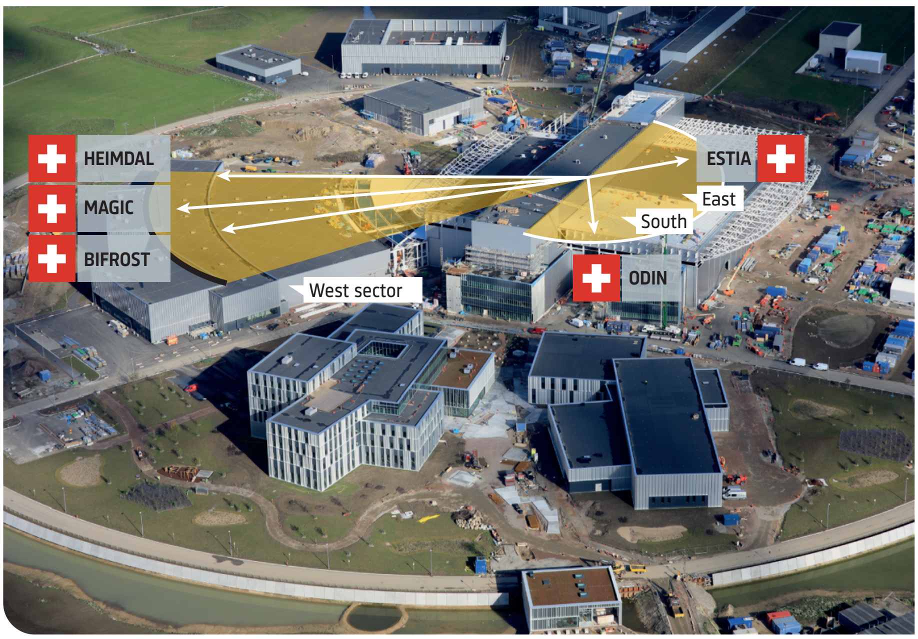
5.3 Swiss Use and Contribution to International Neutron Sources

In context of Europe's leading role, the Swiss neutron science community has a very high standing (Sec. 4.1), just behind the much larger nations, Germany, France and UK in various quantifications of impact. This high-quality position within Europe is largely due to the availability of the high-quality national source SINQ, combined with the access to ILL and other international sources. This enables a strong Swiss neutron science community and also attracts many international user groups, which enriches the scientific community and leads to productive collaborations.

Swiss scientists travel to perform experiments on essentially all the neutron sources in the world, where they obtain beamtime through a peer-review proposal process. The most important international source for the Swiss neutron science community is the ILL in Grenoble, of which Switzerland has been a partner country since 1988. The time-average usage of ILL by Swiss scientists is 4–5%. In the past decade, Swiss membership contributions to ILL has decreased and since 2016 this has resulted in a dramatic reduction in beamtime allocated to Swiss researchers. Many Swiss proposals are accepted by the peer-review committee based on scientific quality, but are ultimately rejected due to national balance adjustment. That means that many promising scientific proposals cannot be carried out, which reduces the scientific return for the investment to ILL. This situation is unfortunate not only for Swiss science, but for the scientific output of ILL as well. A bibliometric analysis in 2015 revealed that 20–25% of high-profile publications from ILL have Swiss co-authors, illustrating the sizeable impact of these detrimental developments. Several efforts, including Swiss membership of a CEA-Grenoble collaborating research group and SERI-financed collaboration measures, have been put in place to improve access to ILL for Swiss users. For the next contract period of Swiss membership to ILL it is very important to restore scientific excellence as a guiding principle for ILL access for European scientists: proposals that are judged among the highest based on scientific excellence should be granted beamtime.

Switzerland is a member of the ESS under construction in Sweden, which will be the world's premier neutron source for decades to come. A speciality of the ESS construction is a very high degree of so-called in-kind financing. In total, Switzerland is investing a total of 155 MCHF and significant intellectual resources in the construction and initial operation phase of ESS. Most of the Swiss in-kind contributions were managed by PSI, contributing additional unique human skills and technical resources to ESS. As a result, PSI is a partner in no less than five of the 15 instruments currently under construction at ESS (see Fig. 20).

ESS is scheduled to become operational in 2023. For the Swiss science community it is imperative to capitalize on this investment by joining the operations phase at a level that matches the potential for Swiss exploitation of ESS.



CH-DK: ESTIA – reflectometer
CH 11.80 MEUR (100%)

DK-CH: BIFROST – spectrometer
CH 4.30 MEUR (35%)

DK-CH: HEIMDAL – multi-scale
CH 4.74 MEUR (35%)

D-CH: ODIN – imaging
CH 3.85 MEUR (35%)

D-F-CH: MAGIC – magnetic diffraction
CH 1.97 MEUR (15%)

Controls, Data, Software, Neutron Optics, Shielding, etc.
Continuous activity in collaboration with ESS and DMSC

Figure 20. Swiss contributions to ESS instruments. Left: arial photo of ESS with location of instruments. Right: list of instruments with Swiss contribution. In total Switzerland is contributing 35 MCHF to ESS instrumentation.

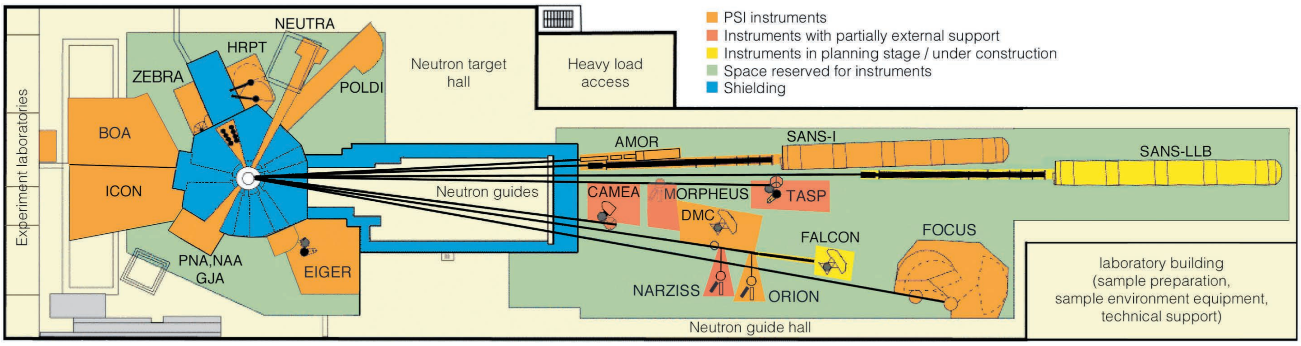


Figure 21. Schematic of the overall SINQ layout. (Source: PSI)

Based on the strong engagement in the construction, and building on 30 years of data from Swiss utilization of ILL, the Swiss demand for beamtime at ESS can be estimated to be at least at the level of Swiss demand for beamtime at the ILL. Among the neutron instruments that will be available early on are three instruments built by Switzerland, or with a large Swiss contribution, respectively: the reflectometer ESTIA, the imaging instrument ODIN and the spectrometer BIFROST. Switzerland will be involved in the early-science programmes of these instruments. Both ESS and Swiss neutron science would benefit from a close collaboration during the commissioning and early operations phase of these instruments, so we recommend that some of the ESS instrument scientists retain Swiss affiliation in addition to their ESS affiliation.

In addition to ILL and in the future ESS, Swiss scientists regularly benefit from access to multiple other neutron sources with complementary instrumentation (e.g., high-resolution spectroscopy and high magnetic fields) in Europe as well as worldwide. This is possible because Switzerland reciprocally grants access for international users to the Swiss neutron source SINQ.

5.4 The Swiss Neutron Source SINQ

Switzerland operates the continuous neutron spallation source SINQ at PSI (Fig. 21). After more than 20 years of operation, it has been undergoing a major upgrade in 2019–2021 with a complete replacement of the neutron guide system and several instruments. When completed in 2021, SINQ will be a state-of-the-art facility with a full suite of neutron scattering instruments.

Particularly competitive instruments include the novel Selene-type reflectometer, and the novel CAMEA-type spectrometer (Fig. 22), both with performance increases of about two orders of magnitude. There will be two modern SANS instruments, and a cold-neutron diffractometer with a large detector for both powder and single-crystal-line studies. From 2022, two more instruments will be upgraded, the engineering diffractometer POLDI and the thermal imaging instrument NEUTRA, and one Laue instrument for tests and internal usage will be added.

It is foreseen that SINQ will provide neutrons for 8 months per year in the next few years. This is an increase of 1–2 months compared to the past 5 years, and allows to offer more beamtime. The continuous maintenance and upgrade efforts of the proton particle accelerator HIPA means that the neutron beam remains of high quality and is extremely attractive to neutron users. In the most recent call in November 2020, SINQ received a record number of proposals for a single call for proposals, underlining the high quality of our facility, the high reputation of SINQ and its staff, and lastly the continuing need for the instruments at SINQ.

The reliable neutron provision of SINQ relies on a well-maintained and upgraded proton accelerator, and an optimized SINQ target. Over the past two decades, the SINQ target was optimized for neutron yield per proton, and the proton current has been increased continuously. Further gains could be achieved through an optimization of the neutron moderators close to the target, and from a further increase of the proton current. It is of outmost importance that the accelerator is continuously upgraded and well maintained, with the goal to increase reliability and further increase the proton current.

The existing guide hall points towards the south, and additional instruments could be built by adding a new guide hall towards the north of the SINQ. Currently, there are cold-neutron instruments that take advantage of the neutrons scattered towards the north (the cold-neutron imaging instrument ICON, and BOA, which serves both as a polarized imaging instrument and test instrument for neutron optical concepts). By extending the hall towards the north, it is possible to build a minimum of six new cold-neutron instruments in this area. This is a relatively inexpensive way to increase neutron capacity in Europe, and thus is a

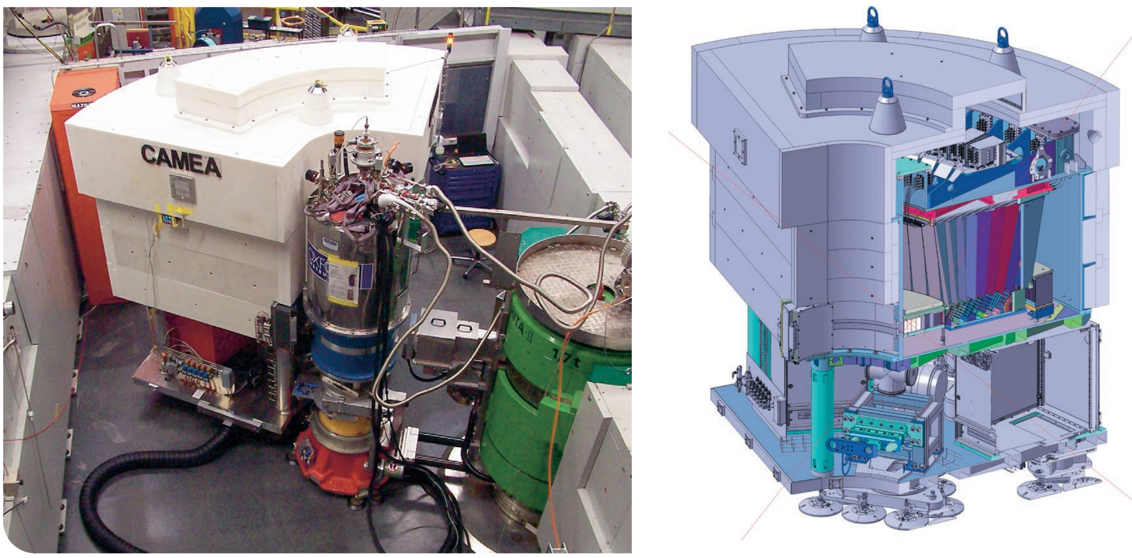


Figure 22. The novel Continuous Angle Multiple Energy Analysis (CAMEA) multiplexing spectrometer at SINQ. (Source: PSI)

unique opportunity for involving European countries that do not operate their own neutron source.

The upgrade or construction of neutron instrumentation often requires considerable funds which are beyond those available through the existing national funding programs of the Swiss National Science Foundation. This makes it often difficult to fund the realization of novel ideas of university- and facility-based groups, although such collaborations yield the most advanced and innovative instrumentation. Many countries have dedicated funding programs designed for innovative instrumentation at national facilities. It would therefore be desirable to have a dedicated funding program for large instrumentation with a cost between 5–15M CHF — a funding instrument that would not only be useful for beam-based user facilities.

SINQ enjoys a number of high-quality institutional collaborations with institutions in other European countries. The longest such agreement exists with DanScatt (the Danish instrument centre for users of synchrotron and neutron sources). Through this collaboration, DanScatt places one post-doc at SINQ, Danish users obtain neutron scattering beamtime, and Danish students are trained at neutron scattering instruments at SINQ.

LLB in Saclay is currently transferring their PA20 SANS instrument to PSI, where it will be called SANS-LLB, and half of its beamtime will be made available to French users for the next ten years. IFE from Norway is currently in negotiations to significantly invest in SINQ instrumentation with the goal to provide access to SINQ to Norwegian users. Finally, the Laue instrument FALCON, originally located at HZB in Berlin, will be installed in 2022 at SINQ, and will be made available to in-house users.

5.5. Neutron Science Innovation

SINQ has an important role in the European neutron scattering community. Scientists at SINQ have a long record of innovation of neutron scattering technology. SINQ was the first neutron facility that was based on a supermirror guide system. SwissNeutronics, the market leader in the field of neutron guide systems worldwide, is a spin-off company of SINQ. Over the last 20 years, neutron scientists in Switzerland revolutionized the field of neutron imaging, leading to a strong activity in that area worldwide. More recently, novel neutron scattering techniques, such as the Selene and CAMEA concepts, polarizing analysers, and adaptive neutron optical devices were developed by scientists at SINQ, and some of these are being rapidly adopted at similar facilities elsewhere.

SINQ scientists are involved in five of the first 15 instruments at the European Spallation Source (ESS), employing these innovations. In addition, almost all major neutron facilities are adopting the new concepts that were developed at SINQ, most notably the polarizing analysers, the imaging techniques, and the Selene and CAMEA concepts. SINQ also supports industrial research, and is the worldwide market leader in the use of neutron scattering for R&D work (see Sec. 3.8).

In the next decades, there are several opportunities and challenges: apart from a continuous investment into the development of novel instrumentation, it will be increasingly important to leverage the enhanced measurement capabilities with increasingly sophisticated software to recognize patterns using artificial intelligence and automate the interpretation of measured neutron data using advanced tools, such as first-principle calculations or advanced modelling. This will go hand in hand with an increasing openness of science, where data itself will be published under open data policies.

5.6. Radiopharmaceutical Innovation using Neutrons

Finally, SINQ is also used by groups outside neutron science, for example by the Center for Radiopharmaceutical Sciences (CRS). Together with its partner at ETH Zurich and various Swiss hospitals, CRS plays a central role in the development of innovative radionuclides and radiopharmaceuticals, with the aim of clinical translation in Switzerland. Its bench-to-bedside capacity is based on radiopharmaceutical expertise and know-how in radiochemistry (in collaboration with the Laboratory of Radiochemistry at PSI), preclinical research and Good Manufacturing Practice (GMP). PSI recently made a substantial investment in upgrading its GMP-certified laboratories in order to maintain and extend its capabilities to produce clinical–grade radiopharmaceuticals. A major future focus will be the development of the new opportunities and capacities to develop and produce innovative radionuclides for therapeutic (particularly alpha-emitters) and diagnostic application. To date, Targeted Radionuclide Therapy (TRT) has been performed as a single treatment option. As combination therapies of cancer are now clinical practice, this will also likely be the case for TRT in the future.

Radionuclide production is of strategic importance for nuclear medicine in Switzerland. The proton beam from Injector 2 is essential for radionuclide production using the IP2 target station. CRS/LRC is also fortunate to operate the neutron irradiation stations NIS at SINQ, which has been fundamental in the development of Tb-161, regarded as a most promising therapeutic radionuclide of the future. SINQ is also utilized for the determination of potential radionuclide production routes in preparation of reactor irradiations, as well as for the manufacture of radioactive tracers for benchmark separation experiments.

SCNAT – network of knowledge for the benefit of society

The **Swiss Academy of Sciences (SCNAT)** and its network of 35,000 experts works at regional, national and international level for the future of science and society. It strengthens the awareness for the sciences as a central pillar of cultural and economic development. The breadth of its support makes it a representative partner for politics. The SCNAT links the sciences, provides expertise, promotes the dialogue between science and society, identifies and evaluates scientific developments and lays the foundation for the next generation of natural scientists. It is part of the association of the Swiss Academies of Arts and Sciences..

The **Swiss Neutron Science Society (SNSS/SGN/SSSN)** represents neutron scientists in Switzerland. The goal of the society is the advancement of neutron scattering and other research using neutron sources in Switzerland and in relation to international associations. This includes the support of young scientists, the exchange of scientific ideas, the cultivation of interdisciplinary relations, as well as ensuring optimum access to national and international neutron sources.