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Photon Science Roadmap

for Research Infrastructures 2025–2028
by the Swiss Photon Community

Swiss Society for Photon Science

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Content

1 Quo Vadis Lux Maior?

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1.2 Management Summary

In this document the Swiss Society for Photon Science (SSPh) summarizes a survey of the Swiss large-scale infrastructure requirements in the broad field of photon science, both in Switzerland and abroad, for the years 2025–2028. In preparation for the present roadmap, the SSPh has collected the scientific visions and compiled the needs of the photon-science community. For this overview, users of the synchrotron Swiss Light Source (SLS) and the X-ray free-electron laser SwissFEL, the major large-scale facilities in Switzerland, as well as of the European Synchrotron Radiation Facility (ESRF) were contacted directly. The SSPh also approached deans and department heads at all universities in Switzerland and through them the broader scientific community in their respective institutions. Based on analysis of the community response to this outreach, the SSPh distilled recommendations for future strategic planning, with a view to improving access to relevant state-of-the-art research facilities. A draft version of document has been made available to the community and SSPh members, in order to invite wider feedback and input.

The SSPh prioritised the (final) findings and recommendations presented in this roadmap, and distinguished between national and international facilities. In addition, new processes and tools for funding photon-related research were identified. All recommendations aim to support diverse and scientifically excellent research in photon science within an expanding landscape of large-scale facilities.

The recommendations emphasize the need for

- continued support for SLS (SLS 2.0 upgrade) and SwissFEL (Porthos extension),
- continued support for the international facilities European X-ray Free-Electron-Laser (EU-XFEL) and ESRF,
- expanded funding mechanisms for instrumentation that enhance the impact of large-scale facilities, including institution-based photon platforms.

The abridged version of the roadmap (chapter 1) is followed by three chapters on synchrotrons, XFELs and institution-based platforms, in which we provide background, context and justification for these general recommendations. The general recommendations and more specific measures detailed in this roadmap will allow the Swiss photon-science community to maintain its leading status and excel within the international community in the near-to-medium future. It remains crucial, however, to continuously expand our technological capabilities, to react to the changing needs of the community, and to pursue emerging developments in science. Therefore, we suggest to review and update this roadmap regularly.

1.3 Mission Statement

Within the photon science community and beyond, photon sources are central tools in research, indispensable for understanding and controlling matter on all levels of complexity. A substantial part of relevant and important research is done with laboratory-scale instrumentation, where strategies can be quickly adapted; however, in many cases start-of-the-art research requires capabilities beyond those of such sources. Researchers therefore have to work together to develop, operate, and continually upgrade large-scale photon facilities. Moreover, each facility must be justified by a set of scientific goals that are vetted over many years. No single type of facility can accommodate all required photon energies or beam properties, nor the associated experimental infrastructure. As a consequence, there is a need for complementary machines, each with a specific set of parameters and focus. Examples are free electron lasers, synchrotrons, and high-intensity laser facilities, which all have distinct performance parameters and applications.

Currently, Switzerland operates a third-generation synchrotron, the SLS, and an X-ray free-electron laser, SwissFEL, both at the forefront of science. Both facilities are supported by a delocalized network of institution-based laboratories, which help to enhance the scientific productivity and improve efficiency. However, all large-scale facilities are unique and the emission characteristics and instrumentation do vary to cover different needs. In some circumstances, required parameter ranges cannot be covered by Swiss national infrastructure and it is therefore important to have access to European or worldwide facilities via partnerships.

Research at large-scale photon sources often has a strong interdisciplinary character and addresses a broad range of scientific and societal challenges. For example, medical and life sciences, catalysis, energy, environmental sciences, but also material sciences are key disciplines. In the medical sciences, e.g., these facilities are used for improved imaging for diagnosis and therapy, and in the life sciences to determine the structure and function of proteins, enzymes or pharmaceutical drugs. The material sciences address as well major challenges in energy, including energy storage and solar-energy conversion, as well as mobility and information and communication technology. Furthermore, research conducted at large-scale facilities is typically accompanied by major efforts in synthesis, theory or numerical modelling.

Many future innovations and the associated benefits depend directly or indirectly on research pursued at large-scale facilities, particularly in the medical and pharmaceutical sector and in materials research, where future applications rely on materials with novel properties. Moreover, many technical innovations required to realize and continually advance large-scale photon sources bear a large innovation potential for commercial applications and thereby become important innovation boosters. Large-scale facilities also often pioneer new environmentally friendly practices to offset their large footprint.

Due to the many active research programs and diversity of scientific fields, there are natural opportunities for Master and PhD students to pursue and complete their education. Access to cutting-edge facilities with the most advanced instrumentation offer young scientists opportunities to sharpen their research profiles and develop their careers. These scientists will help to maintain Switzerland's position at the forefront of science and innovation for years to come.

In addition, large-scale facilities have an important role in conveying the importance of photon science to the public. Societies that value scientific research understand the need for a high level of funding. Such public perception needs constant nurturing, for example through open days, public events such as Physics on Fridays[1] or Photonics Days[2]. Large-scale facilities often go a step further with permanent installations; for instance, PSI operates iLab[3] and psi forum[4].

Overall, the construction and operation of large-scale photon science facilities is a costly endeavor. However, the benefit to Switzerland and society are manifold and multifaceted: they generate scientific knowledge and breakthroughs; they serve to educate the next generation of highly qualified scientists and engineers; they lead to important advances in information technology and data science, and direct financial return can be found through a broader pursuit of clean energy, or in the life sciences through industrial partnerships with pharmaceutical companies, for instance.

1.4 Findings and Recommendations

All findings and recommendations summarized hereafter are substantiated further in the corresponding chapters. Here, they are grouped in terms of national or international context. Some recommendations relate to what we believe are missing funding instruments that would help large-scale facilities to become even more successful in terms of both ease of access and science output.

National Context

1. Continue to develop and upgrade SLS and SwissFEL to remain internationally competitive. This requires significant funds, beyond those currently available to cover running costs.
2. Make significant additional funds available for entirely new beamlines and for beamline renewal, so that the SLS 2.0 upgraded source characteristics can be fully exploited.
3. Extend the parameter space of SwissFEL by installing a new hard X-ray branch (Porthos) with advanced machine modes, build corresponding beamlines, and complete the beamline portfolio on existing branches.
4. Maintain free access to SLS and SwissFEL based on scientific excellence for all national and international researchers, and preserve equivalent access at other international facilities.
5. Create incentives to help strengthen collaborations between experiment and theory.
6. Intensify the collaboration within the 'Swiss Accelerator Research and Technology' (CHART) initiative for future strategic developments in accelerator-based light sources.

1 https://www.physik.unibe.ch/ueber_uns/aktuell/physik_am_freitag/index_ger.html
2 https://www.epfl.ch/education/phd/edpo-photonics/edpo-news-and-events
3 https://www.psi.ch/en/ilab
4 https://www.psi.ch/en/psiforum

International Context

7. Maintain financial contribution to the ESRF and EU-XFEL facilities.

New Instruments in Swiss Funding Landscape

8. Create a dedicated peer-reviewed funding scheme for complex scientific instrumentation and technology platforms (between 5 and 15 MCHF per project).

Data Management

9. Provide significant resources to acquire, properly archive, process, and ensure open access to the rapidly increasing amount of data generated by large-scale photon sources.
10. Strengthen the involvement in initiatives developing data management and analysis tools as well as machine-learning approaches at the national and international level.

Technology transfer

11. Continue to support and adapt structures (e.g., Park Innovaare, ANAXAM…) for efficient technology transfer to national industries.

1.5 The Status Quo of Swiss Photon Science

1.5.1 National context

Photon science encompasses all research areas that work to generate, manipulate and detect photons or use them to investigate or control complex assemblies of matter. The photon-science community therefore includes physicists, engineers, chemists, biologists, earth scientists and many researchers working in interdisciplinary fields, such as life sciences or environmental sciences. Switzerland has a long tradition in photon science and a well-developed and successful photonics industry. In the past decades, Swiss researchers have often joined forces to tackle greater scientific challenges. Several national centers of competence in research (NCCR) with explicit or implicit focus on photon science – in particular Quantum Photonics, QSIT or MUST – have emerged and have been essential to keep Swiss photon science at the international forefront. In addition, Swiss photon scientists are well connected and part of international networks and collaborations, contributing to many projects supported primarily by European framework programs.

Strong commitments from the NCCR home institutions in terms of financing and allocation of lab space were complemented by structural changes in the associated faculties and research perspectives. These changes have often served to permanently anchor photon science in the corresponding home institutions. For example, NCCR MUST has triggered the foundation of so-called FastLabs at several universities. These technology platforms are intended for interested users with relevant scientific questions that can only be addressed with ultrafast spectroscopy tools. At the same time, NCCR MUST with its FastLab infrastructure had an important role in building and extending the Swiss FEL user community for the SwissFEL, which is a complementary ultrafast X-ray source. In FastLabs, users can test and develop their ideas before submitting a proposal for highly competitive beamtime. Similar successes resulted from NCCR QSIT leading to the foreseen foundation of a joint quantum device lab of ETH Zurich and the Paul Scherrer Institute (PSI).

Substantial investment has been made in two large-scale electron-accelerator-driven photon sources in Switzerland. As previously mentioned, a synchrotron (SLS), producing light across the spectrum from the infrared to the hard X-ray range, and more recently an X-ray free electron laser (SwissFEL), were both built at PSI. More than 570 peer-reviewed publications per year can be linked to experiments at the two light sources. They attract >3,500 user visits per year (before the COVID-19 pandemic), including ~50% from outside of Switzerland. Access to both facilities is granted via a transparent peer-review procedure based solely on scientific excellence and according to international standards. The available beamtime is on average oversubscribed by more than a factor of two. These numbers highlight the importance and relevance of the two photon science facilities not only in the Swiss community but also internationally.

1.5.2 International context

In order to increase the portfolio of complementary photon sources, Switzerland contributes financially to the ESRF as well as to the European XFEL.

ESRF offers a variety of relevant beamlines and Switzerland contributes a share of 4% to the ESRF running costs. Together with Norway, Switzerland operates the Swiss Norwegian Beamlines (SNBL) at ESRF, to which Switzerland contributes 50% of the running costs. In the past, Swiss scientists had an access to ESRF beamlines that was roughly proportional the Swiss financial contribution.

Switzerland is also a partner in the European XFEL consortium and contributes a share of 1.5% to its running costs. In the period 2017–2019 Swiss groups, as PIs, have been granted 3.9% of beamtime, and 15% when considering also experiments with minor Swiss contributions.

1.6 The Next Decade of Photon Science in Switzerland

1.6.1 New large-scale infrastructure

SLS 2.0

The existing SLS synchrotron source will be upgraded to SLS 2.0 between 2023 and 2024, with commissioning expected to begin in 2025. The result will be a diffraction-limited X-ray source with large increases in brightness and spatial coherence and expanded access to the hard X-ray spectral range. New undulators and beamlines will be implemented to capitalize on the unique source characteristics. Key advances are also expected in the speed and spatial resolution of X-ray imaging as well as in available detector technology, enabling novel in-situ and operando studies. Significant additional funding will be needed to upgrade beamlines to fully exploit the new properties of the source.

SwissFEL Porthos

Following the SLS 2.0 upgrade, machine physics and engineering personnel will be available at PSI to construct Porthos, the third branch of SwissFEL envisioned for very hard X-ray emission. Porthos will incorporate the most recent advances in accelerator and undulator technology. In particular, a significant amount of effort will have already been devoted to seeding on the soft X-ray branch Athos to imprint full temporal coherence, and to stabilize the temporal and spectral properties of the source. In combination with the unique, modular undulator design at SwissFEL, new approaches will be explored in X-ray pulse shaping to generate attosecond X-ray pulses and pulse trains with continuously variable time structure, and the capability for multi-color and non-linear X-ray experiments. Once established for soft X-rays, these methods will be adapted for hard X-rays at Porthos, enabling new experiments in the biological, chemical, materials, and physical sciences to address paradigm-shifting scientific challenges.

1.6.2 Institutional platforms

By pooling resources and potentially accessing new funding schemes, additional ultrafast optical laser platforms with performance exceeding that typically available in a university environment should be established for collaborative research. These platforms will attract a strong base of specialized expertise that can be shared with researchers from outside the field of ultrafast science, so that they can develop new research areas. As optical and X-ray experiments provide complementary information, these collaborative efforts will expand the user base of SLS and SwissFEL, broadening the range of scientific challenges to be addressed. Furthermore, vetting new scientific perspectives and refining experimental procedures in a platform environment will lead to more efficient and effective use of precious beamtime at the large-scale X-ray facilities.

1.6.3 Data in Photon Sciences

SwissFEL and SLS 2.0 will present new opportunities for high-resolution imaging at unprecedented frame rates, resulting in dramatic increases in data volume that cannot be handled with existing methods and infrastructure. Whether used for detailed structural determination or for real-time observation of dynamics, simulation and interpretation of large terabyte and petabyte data sets will require a combination of new computational methods, large-scale analytics and high-performance computing. To remain at the forefront of scientific research, and to maximize the return on investments made at the Swiss large-scale facilities, the demand for new hardware and specialized support groups will continue to grow.

Historically, large-scale infrastructures have been at the forefront of innovations in data management. A particularly well known example is the early development of the world wide web at CERN and partner laboratories. It is reasonable to expect similar advances and benefits to society from future developments in handling, archiving and processing large amounts of data. Tangible examples are in image processing, artificial intelligence, and fast and efficient data management. Progress in key aspects of data security or open science will also have substantial impact on society.

In addition, careful data management is essential to ensure that the data are of high quality, traceable, reliable, curated, and reusable. Scientific data are increasingly treated as publications, with their own Data Object Identifiers (DOIs). Funding agencies at the national and European level increasingly request that data be freely accessible according to FAIR (Findable, Accessible, Interoperable and Reusable) principles. Compliance will require new data policies as well as data-storage plans for open access that include metadata, catalogues and e-logbooks. As the core product of photon science, data must be transparent and freely accessible so that they can be mined, exploited, reproduced, and disseminated by third parties. Setting up these systems, needed for a smooth data life cycle management, involves major investments.

1.6.4 International partnerships

Beyond the national initiatives described above, it is important to acknowledge our position in the international photonics community. Currently, Switzerland is a member state of the ESRF and a partner in the European XFEL. In addition to financial support, Switzerland provides crucial scientific and engineering expertise to enable successful construction of large European research infrastructures. An important return on these investments is transfer of knowledge and refinement of tested approaches to the benefit of the future SLS 2.0 upgrade as well as further development of SwissFEL.

Membership also facilitates – and at ESRF is required for – submission of beamtime proposals led by Swiss researchers. This access is crucial as all facilities are oversubscribed and each source is unique. Certain characteristics at ESRF are not available at SLS, moreover the European XFEL is the largest accelerator-driven light source in the world, with clear technical advantages. While beamtime at ESRF is distributed based solely on scientific merit, so far, Swiss researchers have been awarded beamtime at a level commensurate with the Swiss financial contribution. Similarly, as a partner at European XFEL having contributed 1.5% of the running costs, Swiss researchers have been allocated 3.9% of the total available user beamtime. The temporary shutdown of SLS for major upgrades between 2023 and 2024 might trigger an increased need for beamtime at ESRF and similar facilities even beyond 2025. Continued support for European XFEL and ESRF at the current levels is considered to be appropriate and essential.

Recently, Europe has also begun operating the Extreme Light Infrastructure (ELI), a large-scale user facility for optical lasers and the first of its kind. In principle lasers hosted at this facility are larger than any laser that can realistically be supported from within Switzerland. While we have not yet identified significant demand for these sources in the Swiss scientific community, scientific needs and progress at ELI should be closely monitored nonetheless, and partnership and or financial support should be re-evaluated in the future.

1.7 Relationship to Industry

Technology transfer in many areas of photon science has a long-standing tradition in Switzerland. Together with its small and medium-sized enterprises (SMEs) and start-ups, it is amongst the most innovative players in photonics worldwide. There are several professional organizations, including Swissmem with its photonics section[5] or Swissphotonics[6], which support and facilitate technology transfer and ensure that the academic and industrial sectors maintain a close link.

Switzerland is home to a number of important photonics industries. The photonics sector creates a substantial amount of value, with expected annual economic growth rates between 6 and 8%. Currently, the business volume amounts to about 4 billion CHF and the number of employees is close to 10,000.[7] Further growth is expected, as photon science enables other fields to reach their full potential, e.g., image processing, medical technology, communication and information technology, or photovoltaics. Several major trends, such as 'Industry 4.0' or 'Data Science', are based on photon science and applications of photon science, and are expected to have similar societal impact as electronics during the twentieth century.

In many respects, photon science at large-scale facilities, specifically at PSI, adds another dimension to technology transfer, with many benefits to the Swiss society. In general, large-scale facilities often have innovation hubs and joint ventures with industry through which state-of-the-art photon science and technology can create value for society. A specific example is the Park Innovaare complex being built at PSI, where high tech industries can gain access to specialized facilities (e.g., clean room, nano fabrication) and benefit from a unique proximity to the academic and research environment. Benefits arise also from technology transfer to industry involved in the supply chain.

Companies will test their cutting-edge technologies at SLS/SwissFEL or develop such technologies in close contact with scientists and engineers at PSI. Large-scale facilities offer infrastructure to industries which cannot be found anywhere else. To give but one example, pharmaceutical companies often use or even operate entire beamlines at synchrotron facilities for structure determination of, for example, proteins and drugs. Very often, large-scale facilities drive environmentally friendly and sustainable site development, which can serve as a role model for industry. Further benefits are related to human-capital increase for students and early career researchers involved in SLS/SwissFEL projects. Skills acquired in such a unique scientific and technological environment generally translates to a broader career perspective. Finally, another socio-economic benefit arises from public access to PSI or from exploring websites, on-site labs or exhibitions.

Switzerland benefits directly from its excellence in photon science and its innovation potential in photonics industries. Both fields, however, exist in a competitive and

5 https://www.swissmem.ch/de/produkte-dienstleistungen/netzwerke/fachgruppen/photonics.html
6 https://www.swissphotonics.net/home
7 https://www.swissmem.ch/fileadmin/user_upload/Industriesektoren/PHO_Photonics/Broschuere/Swissmem_White_Paper_Photonics_Switzerland.pdf

dynamic international environment and their continued success should be enabled by strategic investments in large-scale infrastructure.

1.8 Impact on Education and Society

Photonics has an impact on virtually every aspect of our life on this planet and the world depends on photonic technologies, for example in communication, in entertainment, in personal and community security, in green energy, in hazard warning, or in the health sector, to name but a few examples.

In Switzerland, the photonics industry serves many of these fields with high-tech solutions and innovations, and employs close to 10,000 highly qualified workers, who often have Bachelor, Master or PhD degrees from one of the Swiss universities. Many of those universities offer special programs in photon sciences to feed the need of the photonics industry for several hundred qualified graduates each year. Their high level of education is foremost ensured by top-level educational programs, but also through internationally competitive large-scale infrastructure. Excellent education paired with research infrastructure of the highest standards provides access to prestigious funding opportunities, such as grants from the European Research Council (ERC), which in turn attracts the most brilliant minds.

In order to spark interest for photonics even at an early age, academic institutions as well as large-scale infrastructures contribute to or organize public outreach events, such as the International Year of Light (2015), Scientifica[8] and many others. They also serve the broader scientific community by organizing international summer schools or internships for students at all levels of education.

1.9 Development of National Infrastructures

Summarizing what has been laid out in the section ‘Next decade of photon science in Switzerland’, national infrastructure should develop along three routes.

First and foremost, it is essential to ensure that SLS and SwissFEL remain at the forefront of machine performance as well as experimental opportunities offered to users. This requires a constant level of financial commitment. For instance, SwissFEL has successfully set into operation the hard X-ray branch Aramis, with two running experimental stations and a third one under construction. The soft X-ray branch Athos has been recently installed and first pilot experiments are scheduled. Scientific and technological knowledge gained during the design and realization of Aramis and Athos, in combination with innovative accelerator concepts, have paved the road to the planning of the third branch at SwissFEL, Porthos, for light at very hard X-ray energies and in ultra-short pulses. The existing SwissFEL building complex already includes appropriate space for Porthos. An extension of the experimental hall to accommodate three additional user stations still has to be realized but is already foreseen in the original building permit issued by the local authorities.

Second, already now we see that large-scale facilities produce enormous amounts of data and this trend will increase even further in the future. All national infrastructures have to be prepared to store and process data, which will likely require new strategies and approaches.

Third, we see that intermediate-size infrastructure, hosted by one or more national institutions, can boost the scientific success of national large-scale infrastructures. Exemplarily, this development is illustrated by the concept of FastLabs, which have been established at the University of Bern and EPFL; a third is foreseen at ETH Zurich.

1.10 Swiss Participation in International Organizations

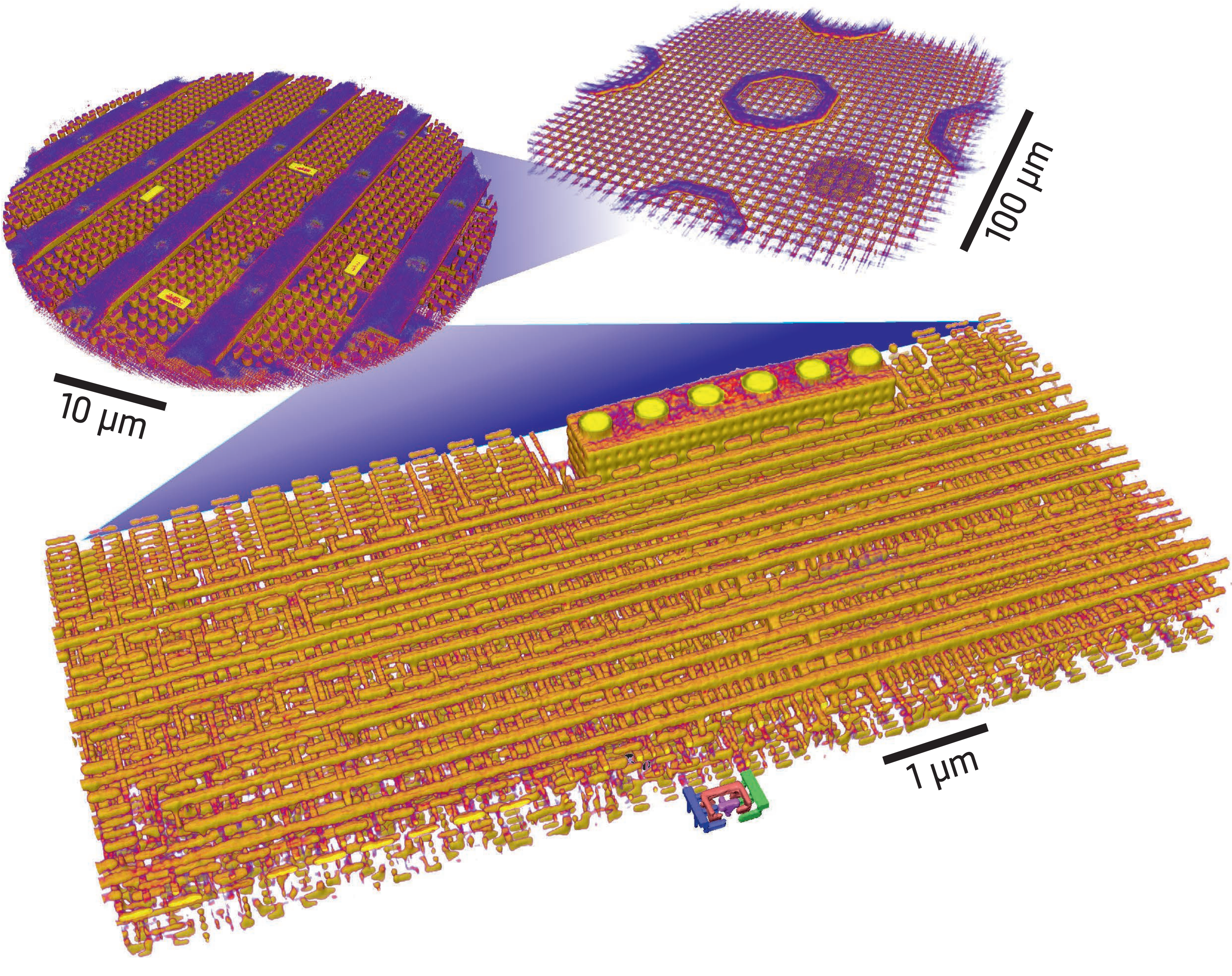
As mentioned previously, Switzerland is an important partner in European large-scale research infrastructures for photon science. These individual facilities are linked and to some extent coordinated by umbrella organizations, which advise them on their long-term perspectives and goals. Switzerland is actively involved in these umbrella organizations, as well as numerous other international collaborations.

Switzerland is involved through PSI in the new research consortium that has been established in Europe, the ‘League of European Accelerator-Based Photon Sources’ (LEAPS). LEAPS was founded in 2017 and encompasses all European synchrotron radiation and FEL user research infrastructures, with the goal to reach a new level of cooperation, coordination and integration for addressing future challenges in science, innovation and data management. The LEAPS members have a collective understanding that future technological developments require resources and competences that surpass the capabilities

8 https://www.scientifica.ch

of individual research infrastructures, and that the full spectrum of technological challenges can only be effectively addressed through concerted effort of all LEAPS institutes, as well as in collaboration with industrial partners. The primary goal of LEAPS is to ensure and promote the quality and impact of the fundamental, applied and industrial research carried out at the respective facilities to the greater benefit of European science and society. Switzerland holds several key positions in the LEAPS consortium and was strongly involved in the coordination and preparation of the new LEAPS INNOV proposal for the innovation pilots call INFRAINNOV-04-2020 (funded in early 2021) and other strategic documents for the consortium. The LEAPS INNOV project incorporates an important technical collaboration project on novel insertion devices for higher-brilliance photon beams, which is co-lead by a Swiss member of LEAPS.

Switzerland is also active in Horizon 2020 collaboration projects on the European level in the field of photon science, including 'Convenient Access to Light Sources Open to Innovation, Science and to the World' (CALIPSOplus) and the 'European Open Science Cloud (EOSC) Photon and Neutron Data Services' project (ExPaNDs).


100 µm
10 µm
1 µm

2 Synchrotrons

2.1 Executive Summary

Synchrotron radiation, combined with a series of advanced experimental techniques, provides a versatile means to tackle fundamental scientific questions throughout the natural sciences, and to address societal needs, for example in technology or the medical sciences. Switzerland operates the SLS synchrotron at PSI, which is used extensively by all Swiss universities and the main ETH institutions. The industrial use, amounting to 10% of the allocated beamtime, is also significant. There are several companies that offer different branches of industries proprietary access. The light source has an excellent standing in the international context and has been the source of several important developments, including the ptychography imaging technique or detector technology. It is therefore of great importance that the SLS is kept on the top level, which requires a continuous improvement beyond the currently initiated upgrade program. An upgrade of all beamlines and instrumentation has to be ensured for the optimal use of the improved source characteristics. There exists a clear gap in funding schemes for intermediate-sized projects in the Swiss research landscape. This is a problem for the use of synchrotron radiation, as a process is missing for realizing or initiating the construction of new beamlines or replacement/upgrade of existing ones. Such projects often go beyond the level that SNSF can support, but are clearly too small for the BFI Botschaft. A funding scheme/process is required so that the community can realize such projects, hand in hand with the facility.

The other cornerstone of Swiss use of synchrotron radiation is the access to international synchrotrons, in particular the ESRF (including the SNBL) and other national light sources, which are widely used by the Swiss community. These facilities are complementary to those available at the SLS in terms of energy range and experimental capabilities. It is therefore important to maintain the financial contribution to the ESRF and support access to other facilities through keeping the SLS open to the international user community. The access scheme should remain based on scientific excellence of the proposed projects. A general trend in many fields of natural sciences is to tackle the problems with a multimodal approach, using imaging on all length scales and study the dynamics spectroscopically as well as in real time. It therefore becomes more and more important to cover the relevant experimental techniques on all length, energy and timescales, which for photon sciences requires a coherent approach with lasers, X-ray FELs (XFELs) and synchrotrons, using all the relevant X-ray techniques. One such approach that can be generalized to other disciplines has been suggested in the Chemistry Roadmap in the context of the operando center. Moreover, synchrotron radiation techniques are rapidly developing and the trend to smaller, faster and imageable is creating dramatically larger data sizes, for which new strategies need to be developed, requiring significant financial investments in the near future.

While synchrotrons are costly endeavors, the benefit to Switzerland and society are manifold and multifaceted: they generate scientific knowledge and breakthroughs and educate the next generation of scientists and engineers. In addition, direct financial return comes through the broader pursuit of innovation in areas such as clean energy or in the life sciences through industrial partnerships with pharmaceutical companies, to give but two examples for value creation.

2.2 Findings and Recommendations

SLS

Finding: The SLS is essential for the Swiss and international community. The SLS currently stands out by offering highly stable photon beams, outstanding instrumentation, and excellent user support. As such, the SLS is recognized internationally as a facility offering services of high quality with a significant impact on a broad range of research fields, including important branches of industry.

Recommendation: The SLS should be kept at the top level in comparison to other synchrotron facilities across the world by ensuring that the quality of science and instrumentation can be maintained.

ESRF

Finding: The European Synchrotron Radiation Facility is an important complementarity tool for the Swiss user community, in particular as it offers higher X-ray energies and a broad variety of different experimental techniques compared to the SLS. The allocated beamtime is commensurate with the Swiss financial contribution.

Recommendation: Maintain the contribution to the ESRF facility.

Access

Finding: The Swiss synchrotron user community is very broad and diverse, spanning many research fields, and at the same time very successful and internationally leading in several fields and X-ray techniques. Moreover, the community benefits from intense collaborations with the international community through the use of other national X-ray sources and the international users at the SLS.

Recommendation: Free access to state-of-the-art beamlines must be ensured for all researchers independent of their country of origin. Similarly, a continuous access of Swiss-based scientists to other national X-ray sources must be ensured. Access should be based solely on the criteria of scientific excellence of the projects and include possibilities for long-term, rapid, mail-in and remote access.

Trend

Finding: A general trend in addressing scientific questions is based on a multimodal and in-situ characterization approach. Such approaches are very important for a series of communities, e.g., related to energy research, catalysis, biomedical and environmental research, with a view to combining techniques such as diffraction and scattering, imaging and spectroscopy. In addition, exploring the complex physical interactions in novel materials also requires a wide range of spatial resolution, from nanometer to centimeter, spectral ranges, from meV to tens of keV, and a large dynamic range, from picoseconds to days.

Recommendation: Ensure that the complete space, time and energy range for X-rays is accessible to the Swiss scientific community.

Current SLS Upgrade

Finding: It is essential that the SLS upgrade program will be realized and completed. It is also of high importance that all the beamlines can benefit from the new source characteristics, and that there are sufficient funds available to modify the beamlines and experimental tools accordingly. In addition, it is mandatory that the beamlines and experimental infrastructure are continuously improved so that all beamlines can benefit from the upgrade program and can be kept on a competitive level.

Recommendation: Additional funds should be made available to guarantee that the whole SLS beamline portfolio remains competitive and benefits fully from the SLS 2.0 machine.

Strategic funding instrument

Finding: SLS beamlines enable unique scientific experiments, impossible to realize elsewhere, with innovative methods and cutting-edge instrumentation, allowing Swiss researchers to take a leading role internationally. Strategic refurbishments and improvements of beamline instrumentation is crucial to maintain the Swiss leadership position.

Recommendation: Create a dedicated funding instrument for medium-size scientific instrumentation projects (5–15 MCHF) to support collaborative, science-driven synchrotron beamline upgrade programs.

Operando center

Finding: The Swiss crystallography, chemistry, and materials science community proposes a new center for operando synchrotron studies that combines very different, yet complimentary diffraction and/or spectroscopy beamlines, including the SNBL (ESRF), the project of the Debye (SLS), and parts of other SLS beamlines. The center aims to stimulate developments of complimentary instrumentation dedicated to in-situ and operando diffraction and spectroscopy. It is focused on multi-technique experiments to simultaneously obtain crystal, molecular, atomic and electronic structural information.

Recommendation: Due to the rapidly growing number of synchrotron users from these communities, we support the creation of an Operando Center as proposed by the Chemistry Roadmap.

Data management

Finding: Data handling is becoming an increasingly important issue and should be given careful consideration as large-scale facilities are going to generate enormous amounts of data. This covers a series of challenges and topics, from (common) data formats to open accessibility of data and codes and scripts for data reduction and treatments. Storage capacities that go beyond current forecasts have to be ensured. Ensuring proper data management and backup is crucial, and this requires new strategies. In addition, there is a strong need to develop data-driven methods for beamline operation, which will bring synchrotron tools to even wider user communities and provide them with new capabilities. One example of this is cutting-edge structural biology research, exemplified in developing antivirals for the SARS-CoV-2 coronavirus.

Recommendation: Ensure that the SLS gets sufficient funds and support to cope with this foreseen dramatic increase in data-management complexity and storage capabilities. It is important to create tools to bridge the gap between data processing and analysis for the user community. In addition, regulations imposed from funding bodies, such as open access, should be realizable for the facilities and the users and provide in practice a real benefit to the research community.

2.3 List of Authors

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Marco Stampanoni (ETH Zurich, PSI)
Urs Staub (PSI, board member of the SSPh)

Acknowledgments
The SSPh has delegated this chapter to one of its board members, who invited a group of people that represent different fields using synchrotron radiation – biology, chemistry, crystallography, material sciences and condensed-matter physics – with the goal of simultaneously covering expertise in the most important X-ray techniques, such as diffraction, spectroscopy and imaging, using both soft and hard X-rays. In addition, they are employed at different institutions, from universities and the large institutes of the ETH Domain. Moreover, contacts have been established to X-ray users in the Geoscience, Biology and Chemistry Roadmaps.

To write this chapter on synchrotron radiation, this group of people then reached out to obtain the feedback of many synchrotron users, as explained in the introductory chapter.

The authors thank the user communities for their broad input.

The authors also acknowledge Joanne McCarthy from the ESRF and Stefan Janssen from PSI to support us with user and publication statistical information and the corresponding figures.

We also like to thank Niels Schroeter for supporting us with Figure 11.

2.4 Purpose and Scope

The usage of synchrotron radiation for research has become very popular in the past few decades. The energy range of synchrotron radiation reaches from infrared to hard X-rays, thus opening up a broad variety of applications addressing questions of fundamental, applied or more commercial nature. As a consequence, research based on synchrotron radiation is not a field in itself, but rather represents a variety of experimental techniques applied. Synchrotron radiation is used in many research areas such as physics, crystallography, chemistry, biology and geology and even for age determination in art conservation or archaeology. By definition, a 'synchrotron' is a large-scale facility that is either a stand-alone research laboratory or is integrated into a larger national laboratory. For example, France operates the synchrotron SOLEIL as a separate institution and Switzerland runs the SLS, which is embedded into PSI. For research, the availability of synchrotron radiation is imperative and reflected by the fact that many countries operate one or several synchrotron facilities[9]. Currently the globally largest facilities are the Super Photon ring-8 GeV (SPring-8) in Japan, the Advanced Photon Source (APS) in the US and the ESRF in France. Every synchrotron has a portfolio of so-called beamlines, which run simultaneously and focus on dedicated experimental techniques such as spectroscopy, diffraction and/or imaging techniques. Since industrial research is also conducted using synchrotron radiation, operation of large-scale synchrotron radiation facilities is of interest for the private sector as well. This sector contributes financially to the running cost of the synchrotron and, in return, access to specialized beamlines for private-sector research and development is granted. A similar scenario exists in certain synchrotrons for the public

9 https://en.wikipedia.org/wiki/List_of_synchrotron_radiation_facilities

sector; for instance, in addition to the SLS, Switzerland is engaged in the ESRF by contributing a share of 4% of the running costs and a 50% share of the running costs of the SNBL. Scientists employed at Swiss universities or at related higher-education institutions have therefore access proportional to the Swiss contribution. As is common for fundamental research from the public sector, access to synchrotron radiation is granted through a peer-reviewed proposal system and open to all scientists worldwide. The major European national synchrotron facilities to which Swiss scientist have free access are PETRAIII (Hamburg, Germany), the Diamond Light Source (Harwell, UK), BESSY III at HZB (Berlin, Germany), SOLEIL (Paris, France), ELETTRA (Trieste, Italy), and ALBA (Barcelona, Spain).

Below, a few examples are given of future challenges in research using synchrotron radiation in different research fields.

Biological and medical sciences – In order to understand the working mechanisms of drug-protein interactions on a molecular level, it is important to determine the structure of the proteins involved. Macromolecular structures at near-atomic resolution of medically relevant targets significantly drives computationally guided structure-based drug design. As a consequence, improving drugs in terms of specificity towards their target protein to cure diseases leads to a reduction in unwanted side effects and thus to better drugs. In addition, protein-structure determination of pathogenic origin, e.g., of the spike protein of SARS-CoV-2 viral particles, may serve to improve or design pharmaceutical lead compounds to prevent infection in the first place, or to cure the diseases caused in a more efficient manner.

Condensed-matter physics – Fundamental challenges are mainly twofold: oriented towards advancing our understanding of modern quantum materials, and for developing new materials that possibly offer novel functionalities. In both cases, synchrotron radiation is essential, not only to characterize the atomic, electronic and magnetic structure of new materials, but also to study their interplay and understand their relation to the material functionalities.

One prime example is the case of high-temperature superconductivity, which has both fundamental importance for its physical concept and relevance for energy research. The discovery of superconductivity at ambient conditions would have a tremendous impact on our modern society. As another example in current material research, the development of thin-layered heterostructured materials is highly promising for near-future applications, especially in view of the needs of electronics beyond silicon-based technology. This will potentially open new routes for developing low-power electronic and optoelectronic devices and sensors with a broad range of functionalities. Finally, the understanding and search for materials with non-trivial topological properties have triggered an intense research effort involving fundamental research with electron and photon spectroscopies, and holds great promise for applied research toward the development of future electronic and information-technology devices, and potentially quantum computing. Realizing operando measurements of artificially structured systems and even working devices based on quantum materials is a promising avenue for future research with synchrotron radiation for the hard condensed-matter community in physics.

Crystallography, chemistry and materials science – These communities, which are designing materials to address a number of globally relevant issues – such as climate change, clean water, energy production and storage, advanced manufacturing and other issues coupled to future sustainability – have greatly benefited from the local, competitive, state-of-the-art single and multi-technique beamlines at the SLS and the ESRF. Some of the most extensively used tools include X-ray absorption, total scattering, and X-ray diffraction. Within these user communities there are several future challenges to be met. First, with increasing materials complexity, individual beamlines, equipped with multiple techniques able to simultaneously probe material structures over different time and length scales are advantageous. Second, rapid and regular beamtime access models help to expedite the discovery of structure-function correlations, which are central to materials design and optimization. Similarly, with improved synthetic approaches, such as the use of robotics, materials throughput is growing, simultaneously increasing the need for high-throughput characterization. This combined with brighter sources leads to increasing quantities of data, which necessitates new tools for data storage, processing, and analysis. Also, the community wishes to probe many different aspects of materials. These might range from unveiling reaction mechanisms during synthesis or catalytic cycles to assessing the structural changes of a material under operating conditions. Such work continues to benefit from the high penetration depth of hard X-rays, which permit the study of advanced materials in newly designed devices or cells.

In the current quest to achieve a circular economy, characterization approaches beyond what is available in a single laboratory or beamline will be required. And while synchrotron tools are already an integral part of advanced materials characterization, meeting the existing challenges can help to ensure the continuation of high-impact academic science in Switzerland and improve the rate at which advanced materials are deployed into industry.

Pushing the limits of tomographic microscopy – The advent of third-generation synchrotron facilities such as the SLS have provided a unique probe to X-ray microscopists: a very bright beam with nicely controlled wavefront to shine on tiny samples. Spatial coherence was the key beam property boosting the most significant developments in the field. The simple but phenomenally powerful propagation of a wavefront distorted after passing through a sample has been exploited to generate tomographic (3D) reconstructions with unprecedented spatial and density resolution. Together with high fluxes, coherence-based techniques have pushed tomographic imaging well into the nanometer range, with acquisition speeds up to 100–1000 3D tomograms (volumetric scans) per second. This will allow us to investigate details in a cell or in a microprocessor without taking it apart. This allows also to combine it with in-situ, operando and even in-vivo sample environments, these paradigm-shifting methodological developments enabled comprehensive, multidimensional characterization of realistic systems, with transformative impact on disciplines such as medical, material and chemical sciences.

2.5 The Present Swiss Landscape

The central role is taken by the SLS located at PSI[10].The SLS is a third-generation synchrotron with 16 independent beamlines in parallel user operation, with many beamlines having several experimental stations. Most beamlines and experimental stations are directly accessible for Swiss and international users through the peer-reviewed proposal system, which selects the best proposal based on scientific merit, as it is the standard selection criteria for such large-scale user facilities. There is additional significant use from industry (~10%), with, e.g., the Swiss-based pharmaceutical companies Novartis and Hoffmann-La Roche that contribute significantly to the construction and operation of the beamline PXII. Other companies or users for proprietary research buy beamtime or services either directly or through the SLS Techno Trans AG or Expose GmbH for screening molecules, or through Excelsus Structural Solutions to enhance the selection, development and manufacturing of high-quality (bio) pharmaceutical products. The SLS produced a steady number of publications of approximately six hundred per year (Fig. 1). The ESRF, which is significantly larger publishes about 1800 articles (see Figure 2), and the SNBL more than 100 per year (Figure 3), which shows the importance of synchrotron-based photon science in Switzerland.

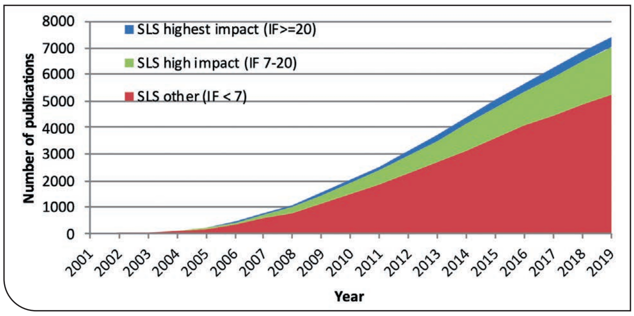

Figure 1: Accumulated number of publications over the years of the SLS since it started in 2001. Orange: publications in journals with the highest impact factors (IFs) IF>= 20, blue IF 7–20, gray IF<7.

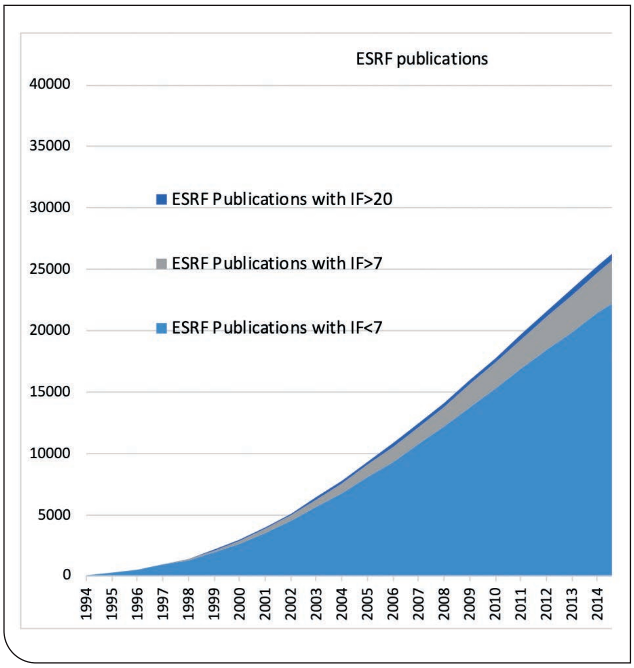

Figure 2: Accumulated number of publications over the years of the ESRF since it started in 1994.

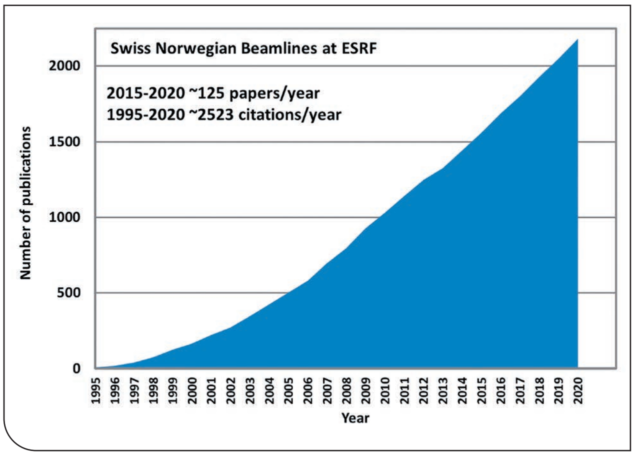

Figure 3: Accumulated number of publications between 1995 and 2020 of the SNBL. The SNBL consists of two beamlines, BM01 and BM31, located at the ESRF in Grenoble, France. The beamlines have a 50% Swiss share.

10 https://www.psi.ch/en/sls

A bit less than half of the total beamtime is allocated through the peer-review process to users (principle investigators only) from Switzerland (see Fig. 4). Within Switzerland, all academic institutions are represented (Fig. 5). Also, many Swiss groups are using beamtime from the ESRF (4% financial contribution, with a similar amount of beamtime allocated that varies though significantly between different fields). In addition to the general share to the ESRF, Switzerland has financed over the years jointly with Norway the Swiss Norwegian Beamlines, which has been beneficial for the Swiss user community (see Fig. 3). This commitment has been terminated by SERI and operation will be covered by ETH Zurich and EPFL, with contributions from the users until 2024. Moreover, many Swiss synchrotron X-ray users use national synchrotron facilities from other countries, mostly within Europe, but also overseas. This is intrinsic for the X-ray synchrotron user community: Main reasons for the use of foreign large-scale X-ray facilities are:

a) Complementary of the infrastructure, in other words experimental techniques that are not available or better-matching characteristics for the proposed experiment.
b) Different priorities in scientific use (defined by the review panel and the source).
c) Existing international collaborations of research projects.
d) Insufficient time available at the national source and its partner, the ESRF.

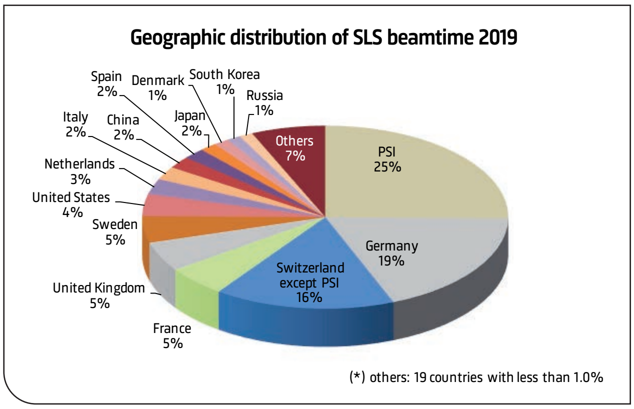

Figure 4: Representation of the geographic distribution of users that have been granted beamtime to the SLS in year 2019.

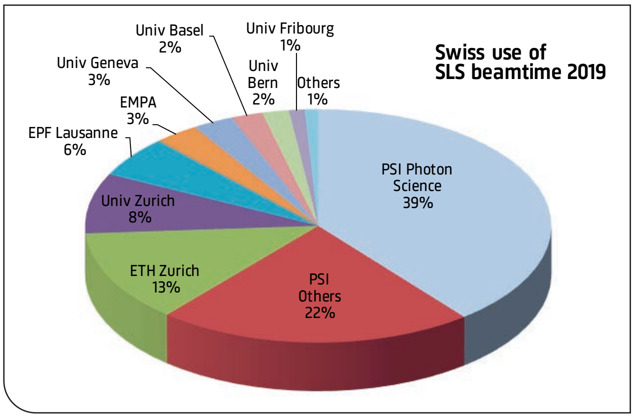

Figure 5: Representation of the geographic distribution of users that are Swiss-based and have been granted beamtime to the SLS in year 2019.

The SLS has an accepted program for upgrading the facility to a diffraction-limited light source, which will provide beams of much higher brightness and coherence. This upgrade program will lead to an effective dark period starting in fall 2023 until the second half of 2024. The major costs will come from the rebuilding of the storage ring and many of the undulators to provide the beam. Though final decisions on the exact details of the projects are currently underway, it is clear that there will be insufficient funds for upgrading all beamlines and building some new key beamlines that optimally use the new beam characteristics. Therefore, not all beamlines will optimally benefit from the new light-source characteristics.

Independent of the upgrade program, one beamline that has recently been funded by the ETH Domain is the Debye beamline for in-situ and operando studies (with a focus on chemistry and material sciences) including X-ray absorption techniques and total scattering methods. Running costs are covered by the ETH Domain until 2024.

It is planned to invest in the following years regularly in future optimization of those beamlines not having benefitted optimally from the upgrade, but funds and manpower will be limited without further strengthening the activities. It will therefore be important to have sufficient/additional funds available for the regular refurbishment program for the beamline portfolio.

2.6. Major Successes

Synchrotron-based research is an essential part of many important interdisciplinary national research initiatives such as National Centers of Competence in Research (NCCRs) of the Swiss National Science Foundations (SNSF) or Strategic Focus Areas (SFA) of the ETH Board, European projects within Horizon 2020 (e.g., FET-Open). In addition to these large-scale initiatives, many personal grants have been awarded by the European Research Council (ERC) or Eccellenza grants (by SNSF), for projects on all levels addressing societal needs and challenges. During the past ten years, the use of synchrotron radiation has been central to many research projects proposed within funding schemes supporting career development. In particular, SNSF professorship grants have been delivered, e.g., in the fields of research on quantum materials, for topological materials, for engineering of high-quality artificial functional hetero-structure, for durability of engineering materials and dynamical studies of quantum materials.

In addition to these personal grants, many funded projects (e.g., through SNSF project funding) use in part or are focused on experimental investigations using synchrotron radiation.

Another major success is reflected in the fact that industry directly uses synchrotron radiation. Approximately 10% of the available beamtime at the SLS is sold to industry, and the pharmaceutical industry even paid half of one beamline dedicated to protein crystallography. There are several companies that work closely with PSI and directly offer X-ray tools for different branches of industry. Excelsus Structural Solutions AG offers easy and affordable access to unique synchrotron-based characterization tools at the SLS. The company GratXray AG aims to translate phase-contrast X-ray imaging into medical devices. Expose GmbH provides services and expertise in the field of X-ray protein crystallography for pharmaceutical and biotechnological companies. The technology transfer center ANAXAM is a non-profit organization that provides X-ray analytical methods for companies in the manufacturing business to help industry to improve their manufacturing processes. Finally, LeadXpro AG provides target-exclusive services to customers from the pharmaceutical industry and generates and characterizes drug candidates for partnering with pharmaceutical companies in clinical research, with related therapeutic areas being oncology, inflammation and antibiotics. In addition, there have been spin-off companies such as DECTRIS, which develops and sells X-ray detectors having today more than 100 employees.

Below we give a glimpse of major scientific successes by presenting a few selected examples of some of the large projects and some examples of which type of questions have been addressed in different research fields using synchrotron radiation.

SFA – Personalized Health and Related Technologies (PHRT). The ageing society brings challenges such as an increased demand for tailored implant materials and designed specific drug-delivery systems, with the need of structure understanding on all length scales of the biological system itself, the materials used and the induced changes in the interaction of both. The traditional imaging techniques used in hospitals and state-of-the-art techniques at synchrotrons (and XFELs) should be used complementarily.

Human diseases are studied by combining the expertise in physiology, chemistry and structural biology, where progress is achieved through extended research in macromolecular X-ray crystallography (NCCR Transcure, Fig. 6). New approaches to combat antibiotic-resistant bacteria are established through a transnational interdisciplinary center for antibiotic research, with the aim to find new antibiotics and to develop alternative strategies to combat antibiotic-resistant bacteria by linking basic research directly with clinical research (NCCR AntiResist).

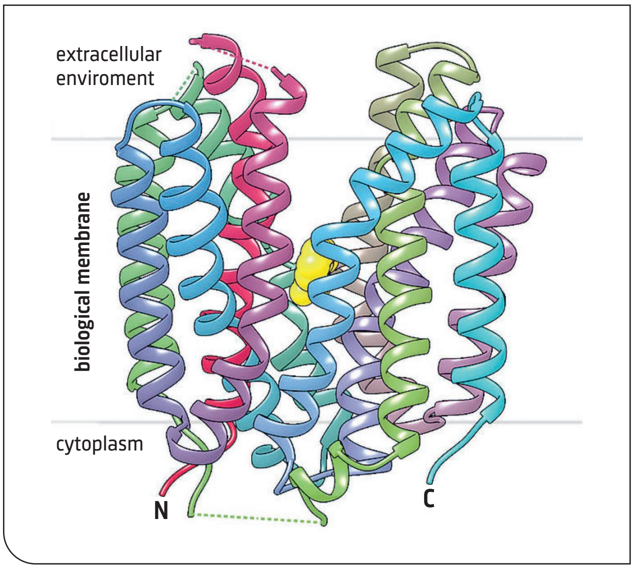

Figure 6: Structure of a membrane protein elucidated by X-ray crystallography. Displayed is the structure of the L-lactate transporter SfMCT in the outward open conformation embedded in the biological membrane.[1]

The NCCR Bio-inspired Materials is an internationally recognized hub for paradigm-shifting research, innovation, and education in the domain of 'smart' materials whose function and design are inspired by nature. It involves synchrotron studies in domains such as imaging, X-ray diffraction and scattering. Inspiration is taken from natural materials to establish design rules and strategies for the creation of macromolecular and nanomaterial-based building blocks and their assembly into complex, hierarchically ordered and responsive materials with new and desirable properties.

Awarded personal Eccellenza and ERC grants are connected with professorship positions, which shape the science landscape of tomorrow and are linked to **the SFA Personal Health and related Technologies (PHRT).** Prominent examples relate to clinical questions raised by colleagues from Swiss hospitals. Materials-based research such as particle-body interactions, drug-delivery systems and the related drug-performance assessment by multiscale analytics are focus areas. X-ray based methods, in a multimodal and multiscale approach including X-ray diffraction and scattering, allow getting novel structural details and insights of hierarchical materials with respect to human bones, muscles, tendons, and soft tissues (Fig. 7).

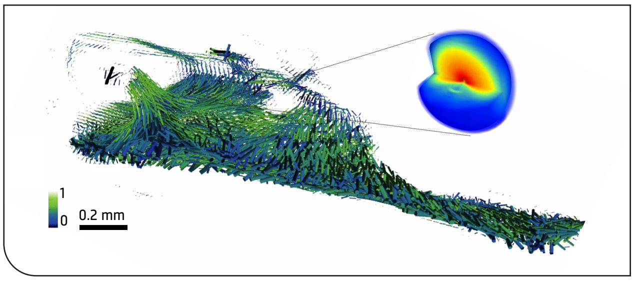

Figure 7: Small-angle X-ray scattering tensor tomography allows the reconstruction of the 3D reciprocal space map in each voxel of macroscopic specimens. Reproduced from Guizar-Sicairos et al. (2020)[2] with permission of the International Union of Crystallography.

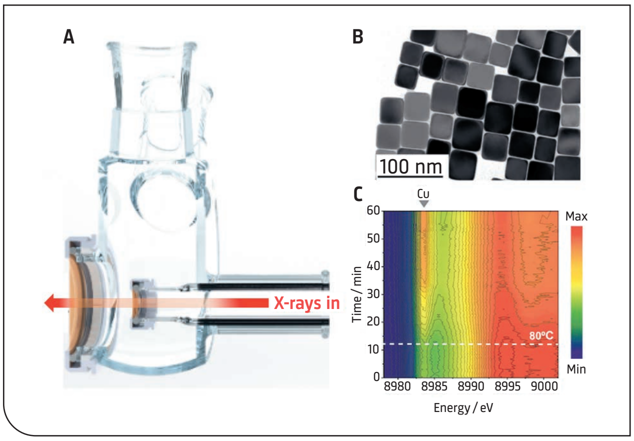

Figure 8: (A) Custom designed in situ X-ray absorption reaction flask used to study the reaction intermediates present during the formation of (B) Cu nanocrystals. (C) Color map of the normalized spectra collected during the heating ramp in the synthesis of Cu nanocubes.[3]

Catalysis research creates the scientific and technological bases for chemical processes and products, and indeed for making the chemical industry in general more sustainable, resource-efficient and CO_2-neutral. In the framework of the NCCR SUCHCAT, the discovery of new catalytic processes will be accelerated and revolutionize the chemical production chain. Other related topics are the creation of multifunctional hybrid platforms based on colloidal nanocrystals to advance CO_2-conversion studies (ERC HYCAT, Fig. 8), the CO_2 capturing and catalysis of materials by atomic-scale design and the related quest for understanding (ERC AMADEUS) and tailoring CO_2 hydrogenation catalysts for selective methanol synthesis via structure-activity relationships across multiple time and length scales (SNSF SINERGIA No. 183495).

Advanced imaging for hard and soft matter. The latest developments in dynamic tomographic microscopy have pushed time resolution well into the sub-second regime, reaching up to hundreds of three-dimensional (3D) datasets per second for selected material systems, while allowing for ever more complex environments to produce realistic sample conditions. On the one hand, this enabled the quantitative investigation of dynamic processes, such as crack propagation in composites,[4] bubble formation in metal foams,[5] and dendrite growth during solidification,[6] to cite a few. These processes all occur within opaque materials – usually hosted in complex conditioning environments – on microscopic length scales and sub-second time scales, making them inaccessible for common characterization methods.

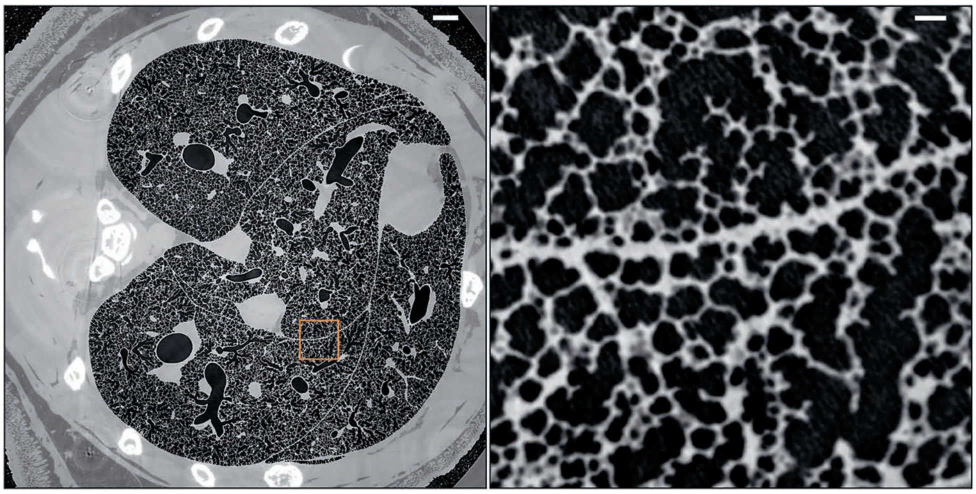

Figure 9: Micrometer-resolution X-ray tomographic full-volume reconstruction of an intact post-mortem juvenile rat lung. The full size of the area on the left is 18.9 × 18.9 mm^2 and on the right 1.5 × 1.5 mm^2. The long thick structure that runs horizontally roughly in the middle of the right panel represents the border between two lobes. Scale bars: 1 mm (left panel), 0.1 mm (right panel). Reconstructed volume: 9095 × 9095 × 7084 $voxels^3$ = 25.0 × 25.0 × 19.5 mm^3, corresponding to a file size of approx. 1.2 TB. Reproduced from Borisova et al. (2020).[7]

On the other hand, high-resolution tomographic acquisitions at sustained speed are particularly powerful for the multiscale investigation of hierarchically structured objects, such as the lung or brain. This approach enabled resolving the entire mouse pulmonary structure from the trachea down to the parenchyma (Fig. 9)[7] or to map the complete microvasculature of a mouse brain.[8] Recent advances in high-speed parallel tomographic reconstruction algorithms have enabled live previews of virtual slices through 3D volumes, paving the road to smart data-acquisition schemes.

SFA – Advanced manufacturing (AM) has now entered our society and is part of our daily life. New manufacturing processes need the development of new analytical tools. X-ray based imaging and diffraction methods are essential to monitor morphology, crystal structure, stress gradients and related changes during manufacturing and in product operation. Great advances have been made in several SFA AM projects. Selective laser melting (SLM), a process category of the AM family, is a powder bed based technique, in which parts are built by selectively fusing the powder particles with a high-power laser source in a layer-by-layer fashion. By tweaking multiple parameters, one can influence the resulting microstructure, and thus the physical properties of the final AM product. By operando X-ray diffraction studies during the laser 3D printing combined with simulations, the SLM process is efficiently optimized. In addition, thanks to the recent development of ultra-fast X-ray detectors (DECTRIS) and improvements at synchrotron beamlines, it is now possible to perform in situ X-ray diffraction and radiography experiments at time scales that are compatible with SLM processing. In Fig. 10, the example of online monitoring of the AM process with respect to crystallographic phase changes is presented.[9]

Condensed-matter physics. A topical challenge of hard condensed-matter physics is to understand and design new quantum materials that cannot be described by simple theoretical frameworks and that display novel physical properties giving rise to rich phase diagrams. This is for instance important for achieving new concepts for qubits needed for quantum computing. To address such questions, there have been several projects in connection with multi-MCHF research projects from industry on quantum computing.

Swiss-based scientists who design new materials displaying specific quantum effects drive the spirit and initiate to uncover hidden quantum properties in known materials, that is, properties that could not be seen by methods employed up to now (ERC-Synergy HERO). Such effects could be used for data processing, transmission and storage in the future and thus become the backbone of future electronics, which need to be faster, smaller and more energy-efficient.

In this framework, a new class of materials, known as topological materials, has become increasingly popular for condensed-matter physics and material science during the past decade. Their peculiar properties turn out to be related to fundamental symmetries of their crystal structure, which can often be predicted by theory. Their discovery relies heavily on the use of synchrotron radiation. In 2019, an international team of physicists involving scientists from PSI and Oxford (UK) discovered a novel quantum material, AlPt, that has new topological properties including chirality.[10] This discovery led to the observation of a new quasiparticle called a Rarita–Schwinger fermion. This might open up new opportunities for novel electronic materials of tomorrow.

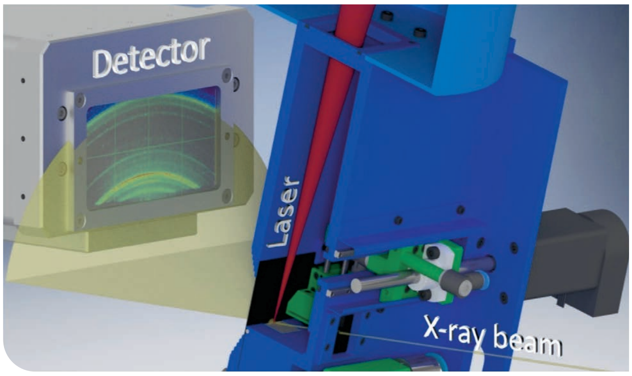

Figure 10: Diffraction geometry during an operando measurement. The X-ray beam enters the printing chamber at the back of the machine, while the laser enters from the top. They both interact with the powder on the build plate. The diffracted X-ray beam forms a diffraction cone that is collected by a high-speed detector in front of the machine. Reproduced from Hocine et al. (2020).[9]

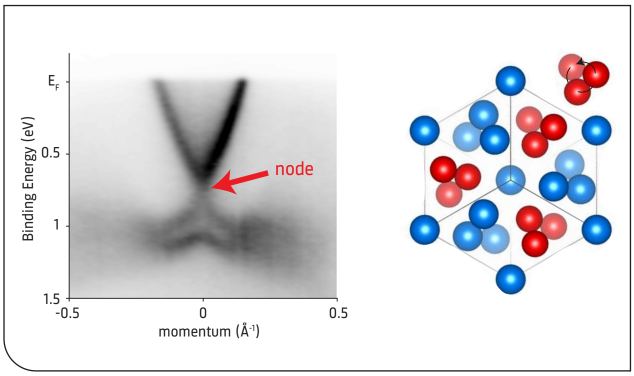

Figure 11: Illustration of how synchrotron radiation can be a powerful probe, in chiral atomic structures such as that of AlPt (left), of the electronic structure (right) using the photoemission technique to reveal in a unique way the presence of topological states. Adapted from Schröter et al. (2020).[10]

2.7 The International Context

Main trends and evolution

The advent of brighter accelerator sources throughout the world creates new opportunities, transforming our understanding of complexity in condensed matter and living organisms across dimensions. Brighter beams coupled to evolving and emerging X-ray imaging techniques provide access to complex and heterogeneous materials as well as to their functionality at a progressively broader range of spatial and temporal scales in a volumetric manner. The focus is increasingly shifting towards more realistic samples and processes probed in-situ and operando under realistic conditions, unravelling time-resolved structural, chemical and electronic information from the macro to the nanometer-scale, where this latter scale in particular is unlocked by coherence-based methods, which are increasingly gaining importance at fourth-generation X-ray sources. The accessible time scales for studying dynamics also cover several orders of magnitude at synchrotrons, where the upper limit is given by the time structure of the probe, and with ultrafast timescales probed on XFELs. This is one of the reasons why most of the European and international synchrotron facilities have started/completed an upgrade program (e.g. at the ESRF) or new sources have very recently been built or are under construction, such as MAX IV in Sweden or the approved High Energy Photon Source (HEPS) in China. These sources approach a diffraction-limiting light source, delivering X-rays with a larger coherent fraction and having much smaller source sizes, to achieve a beam brightness, so that these imaging techniques can be improved by orders of magnitudes, leading to an achievable energy resolution well beyond what is available today in, for instance, spectroscopic techniques such as resonant inelastic X-ray scattering (RIXS).

This comprehensive multidimensional characterization of realistic systems is having a transformative impact on many disciplines and is leading toward new frontiers and discoveries, not only in basic science but also addressing global challenges facing our society today. Most of the X-ray techniques (from scattering to spectroscopy) are exploited in cutting-edge X-ray imaging methods that increasingly address pressing societal challenges and become more and more accessible tools for the industrial research and development sectors. Fields strongly relying on these technologies include energy conversion and storage research, catalysis, the development of environmentally and economically sustainable tailor-made materials, advanced manufacturing technology, (nuclear) waste management and site remediation, and personalized medicine (benefitting for instance from research on the way the human functional units work and new (intracellular) drug-delivery and toxicity studies).

Swiss role

Switzerland, despite its small size, plays a major role and is at the forefront in several of the X-ray techniques such as X-ray scattering, spectroscopies such as soft X-ray RIXS, and X-ray imaging. For example, imaging facilities at accelerator-based photon sources in Switzerland have established themselves among the best worldwide and are actively contributing to the development and optimization of analytical X-ray imaging techniques (e.g., phase contrast, ptychography, and dynamic imaging). Swiss-based X-ray scientists are engaged in worldwide collaborations with the large scientific community in different topics. Also, the interactions with the industrial sector are growing both for technology transfer as well as for X-ray analytics relevant industrial applications. Furthermore, X-ray techniques are more and more strongly intertwined with big data: with one of the ten most powerful high-performance computing facilities in the world, Switzerland is well equipped to face the upcoming challenges in this respect.

This leading role of X-ray science in Switzerland on the international landscape also stems from and is sustained by the high density of technology and innovation on Swiss territory. Its schools, research institutes and competence centers are in top positions in international rankings. The strong synergies of the photon-science community with strong and reliable high-tech, electronic and engineering industrial partners strengthen the competitiveness of Swiss X-ray research internationally.

Collaborations

The recognition of the Swiss X-ray science community worldwide facilitates small and large international collaborations and attracts international scientists to local institutions. Swiss-based scientists using synchrotron-based X-rays are highly competitive in accessing EU funding (see also major successes) and regularly obtain beamtime at other international large-scale X-ray facilities. They are also highly requested in steering committees and boards of existing and emerging facilities as well as in the review of X-ray instrumentation, funding and beamtime-allocation reviewing. Switzerland is also often part of big international photon-science consortia, which in Europe is often steered by the League of European Accelerator based Photon Sources (LEAPS), which represents its science toward the European Union, identifies and promotes collaboration for technical developments (e.g., on undulators or detectors) but also tries to facilitate user-access schemes, support for user travel support (e.g., Calipso) and streamline data formats, to name a few activities. They also create documents on specific topics and a recent landscape analysis, which are giving additional information on the international context of synchrotrons within Europe.[11]

11 https://leaps-initiative.eu/about/leaps-documents

Another important aspect of the international context is the Swiss contribution to the ESRF. The ESRF is not only a much larger facility with many more beamlines, some of which are dedicated to techniques not available at the SLS, but also operates at higher electron-storage energies that facilitates the production of high-energy X-rays. This makes the source strongly complementary to the SLS. The effective beamtime use of Swiss users is close to the share of the Swiss contributions, however, it strongly varies for different fields, but is in the period of 2014 to 2018 particularly strong (above average) in medical, engineering, and instrumentation and methods development applications. This nicely shows the complementarity of the sources as these fields often need higher X-ray energies.

2.8 Synergies with other scientific techniques not based on photons

Synchrotron science is a very diverse field of research. It encompasses not only the technological development of large-scale facilities and instrumentation, but also the advance of methodologies specific to different fields of science and finally the related research within these fields. For this reason, synchrotron science is naturally multidisciplinary.

The competition and synergies are therefore more in the form of other techniques. Below a few of the important complementary techniques and its relation to synchrotron-based photon techniques are given. In general, there are many techniques based in university laboratories, such as standard X-ray diffraction, ultra-violet photoemission or infrared ellipsometry, which exist also at synchrotrons. The difference is mainly in the photon flux, the energy tunability and available spot sizes, which allows more detailed information at the synchrotron compared to the lab-based equipment. The combination of lab and synchrotron experiments enables software and hardware knowledge transfer between lab facilities and synchrotron facilities, in both directions. The preparation of synchrotron experiments often takes place in the X-ray labs for designing in-situ tools and often for proof of concept. The transfer to the synchrotron happens when measurements need high time and spatial resolution or other special requirements. On the other hand, the integration of synchrotron methodologies into the lab procedures lays the foundation for long-term lab-based projects and the know-how transfer to industry and hospitals. The close exchange and feedback loop between lab-based and synchrotron experiments allows for shared tool and software development. The lab-based X-ray equipment remains important to characterize the samples and prepare for more demanding and complex X-ray experiments at the synchrotron.

XFELs: The main advantage of XFELs is that they enable experiments to study dynamics on ultrafast time scales, and also permit the development and applications of nonlinear X-ray methods and measurements that can outrun X-ray damage, which is particularly important for biological applications. See also the chapter on FELs.

Electrons: In the last few decades, X-ray crystallography and Nuclear Magnetic Resonance (NMR) spectroscopy have been the methods of choice to obtain structural information at high resolution of biological molecules. In recent years, technical advances and software developments in single-particle cryo-electron microscopy (cryo-EM) made possible the determination of macromolecules to near-atomic resolution. Nowadays, specimens analyzed by cryo-EM cover a range from large multi-subunit molecular machines to single proteins as small as approximately 65 kDa. Nonetheless, all methods mentioned are complementary and may also be fruitful if combined, e.g., I) for structure elucidation of a large multi-subunit molecular assembly at higher resolution, in which parts of the structure are solved by X-ray crystallography then fitted into the cryo-EM volume of the whole assembly,[11] or II) for the identification of vital ion-binding sites in macromolecular structures obtained by cryo-EM using anomalous X-ray diffraction.[12] In addition, it is worth mentioning that electron diffraction develops heavily into nanomaterials research.

Nuclear Magnetic Resonance spectroscopy: NMR spectroscopy provides valuable atomic-scale structural and dynamics information for biomolecules of moderate size. As mentioned above, in structural biology the combination of complementary methods may have a synergistic effect. Under certain circumstances the combination of synchrotron-based X-ray related techniques such as small angle X-ray scattering (SAXS) or X-ray crystallography (XRC) with NMR has proven to be beneficial.[13, 14] While the combination of SAXS with NMR facilitates the comprehensive characterization of biomacromolecular solutions, the combination of XRC with NMR may lead to the improvement of structures at the atomic level.

Neutrons: Neutron scattering is another large-scale technique that has synergies with methods based on synchrotron radiation, in particular in the field of condensed-matter physics. Neutron-based techniques are very strong in investigating magnetism in complex materials, however typically require larger samples. In comparison, X-rays can be produced with beams orders of magnitudes more intense and can easily get focused and/or collimated to investigate tiny samples so that in-situ processes can be imaged. Synergies exist also in terms of being able to look at fundamental excitations in solids, for which X-rays can more easily access the higher-energetic regime and different types of excitations (charge excitations), whereas neutrons focus mainly on magnetic and lattice excitations at lower energies. For more information on the technique, we refer to the Roadmap on neutron scattering.

μSR: Muon spin rotation is another technique based on a large-scale facility available in Switzerland (at PSI) that is focused on magnetism. Switzerland (PSI) is the leading place for this technique, which has very specialized strengths, such as being a measure of very weak magnetic fields in materials that is e.g. important for superconductors that complement both neutrons and X-rays as well as the laboratory-based NMR spectroscopy.

Laser spectroscopies: A thriving field of condensed-matter research is now to study the real-time dynamics of atoms and electrons on their relevant timescale (femtoseconds). The necessary pulsed light sources are provided by laser technology and XFELs. The former are nowadays commercially available and typically equip university laboratories (although a few user-oriented facilities do also provide them, see chapter Laser platforms). The latter represent new large-scale facilities that currently emerge across the world and focus on an intense field of development, both for technology and fundamental research. Usually, synchrotron radiation and laser-based techniques are complementary. Before studying the real-time dynamics of materials, it is important to properly understand its static properties, and this is typically done using synchrotron radiation.

Optical/electron imaging: Very exciting is to have the full length scale of atomic two- and three-dimensional real-space information using imaging. Whereas optical imaging is covering large lengths scales, X-rays cover μm-to-nm length scales and electrons with techniques such as scanning tunneling microscopy (STM) or transmission electron microscopy (TEM) nicely complement to the highest, atomic resolution, making microscopy achievable over all relevant length scales.

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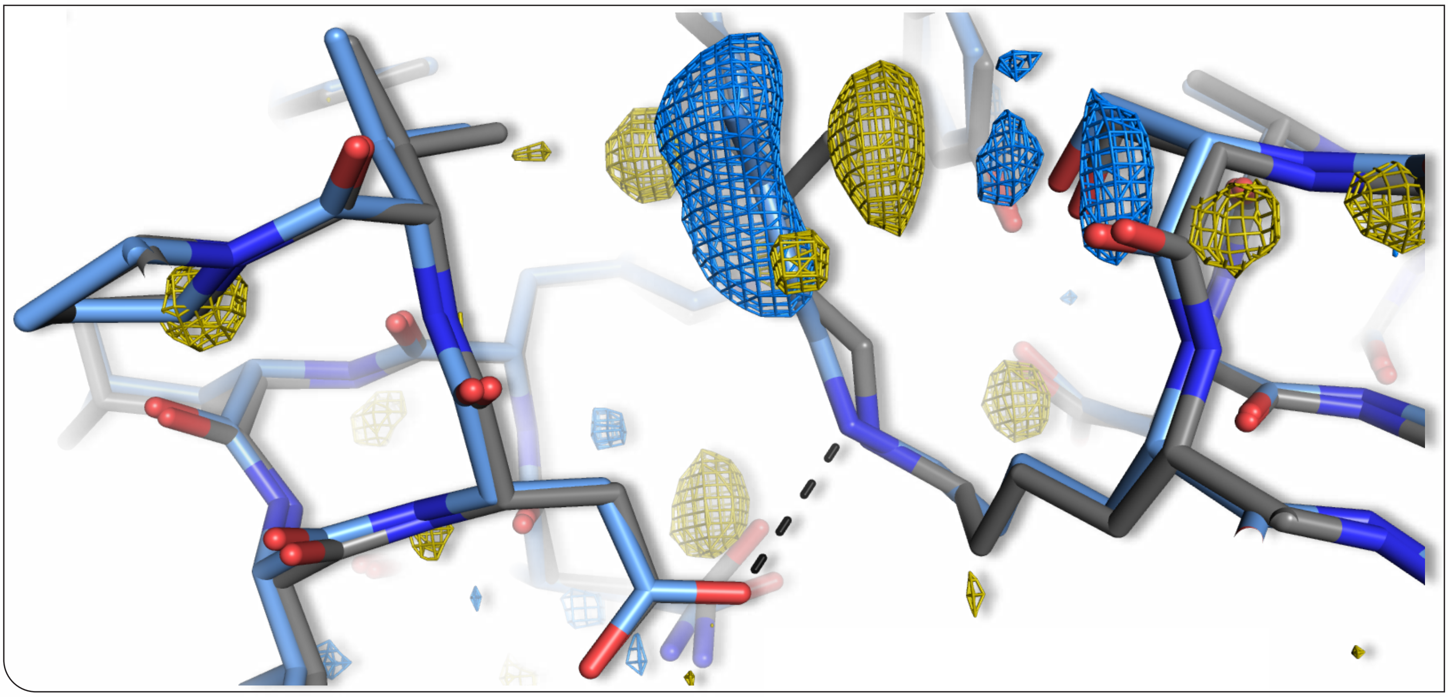

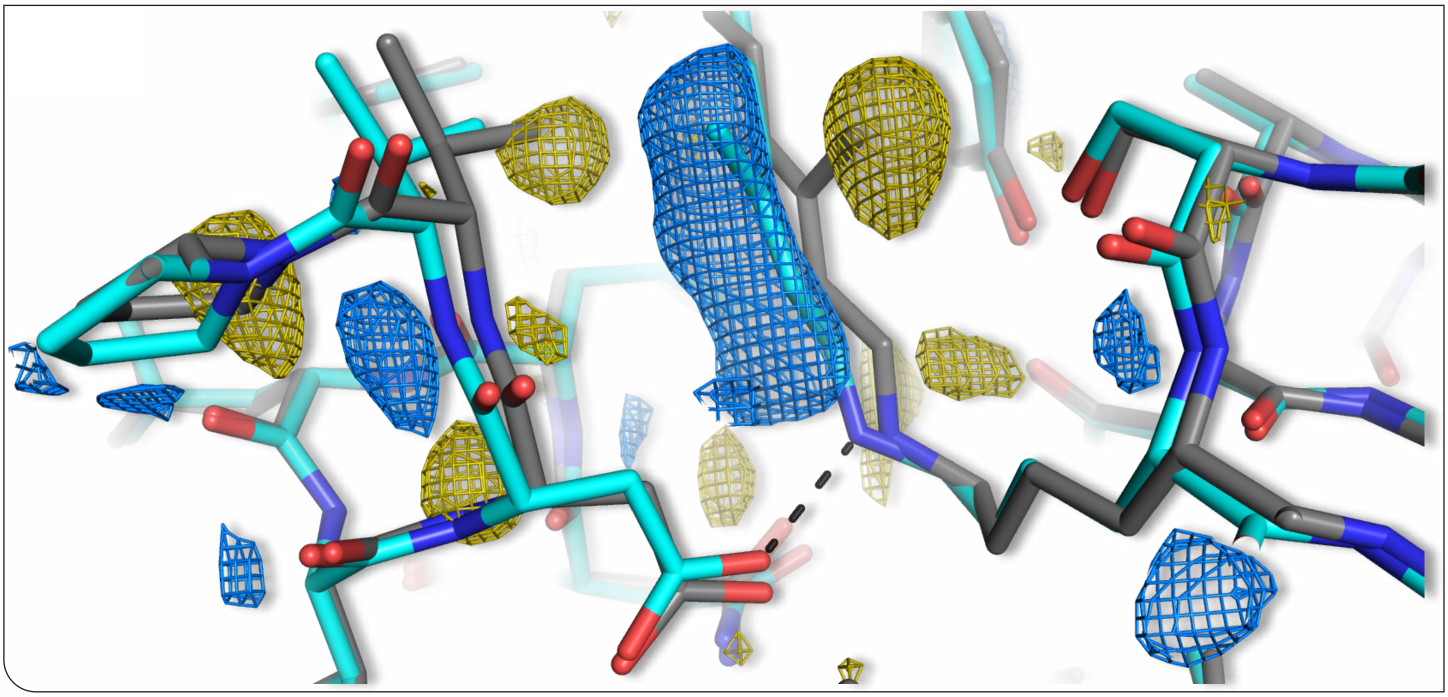

3 Free Electron Lasers

3.1 Executive Summary

Three enduring trends in investigations of structure and function in the natural sciences are 'smaller', 'faster' and 'more complex'. One of the preferred tools of such investigations is electromagnetic radiation – light in a broad sense. Major advances in the investigation of matter with light have been the invention of infrared (IR) and visible lasers, with their capability of bright, ultra-short pulses reaching today the hundreds of attosecond range, and the advent of high-brightness synchrotron X-ray sources (SR). X-ray Free Electron Lasers (FEL) have opened the way to encompass all three above-mentioned trends in a single instrument at much higher photon fluxes.

Switzerland offers the scientific community state-of-the-art infrastructure for the investigation of ultrafast processes such as FastLab (University of Bern) and LACUS (EPFL). With the recently commissioned Swiss Free Electron Laser (SwissFEL) at the Paul Scherrer Institute (PSI), providing femtosecond pulses of soft and hard X-rays, Switzerland strengthens its leadership role as key player in the field.

SwissFEL has successfully set into operation the hard X-ray branch Aramis, with two running experimental stations and a third one being implemented. The soft X-ray branch Athos has been recently installed and first pilot experiments have been scheduled. Scientific and technological knowledge gained during the design and realization of Aramis and Athos in combination with innovative accelerator concepts have paved the road to the planning of the extension of SwissFEL to its third branch, Porthos, covering the range up to very hard X-ray energies and in ultra-short pulses. New opportunities in quantum technologies, quantum chemistry, advanced imaging techniques as well as new routes in time-resolved structural biology and structure-based drug design will be explored.

Swiss academic groups use eight FEL Facilities worldwide on a regular basis, with an excellent scientific output. Switzerland is scientific partner of the European XFEL facility in Hamburg, with a share of 1.5% and a reported usage as PI during the period 2017–2019 as high as 3.9%.

Strategically, Switzerland is working in close collaboration with other European FEL facilities within the context of the 'FELs of Europe' and the 'League of European Accelerator based Photon Sources (LEAPS)' consortia.

Switzerland actively pursues a leadership role in increasing co-operation and coordination of research infrastructures across Europe, making Switzerland an attractive partner in international research-infrastructure projects. This engagement directly benefits Swiss researchers, through ensuring Swiss access to these infrastructures, which often provide complementary techniques to what is available in Switzerland. In this spirit, Switzerland takes a leading role in major European research infrastructure partnerships, such as LEAPS.

3.2 Findings and Recommendations

SwissFEL has fully transitioned to a research facility. It has reached the target repetition rate of 100 Hz as well as the full accelerator electron energy of 6 GeV and a photon energy of 12 keV. The Aramis branch is in user operation, with two experimental stations and the third one is currently being installed. After the pilot phase, the SwissFEL Aramis branch has entered user operations in 2019 with a peer-reviewed proposal process and large international attention. The results of the first SwissFEL experiments have been published in high-profile journals.

Finding 1: The SwissFEL hard X-ray branch Aramis has immediately become a valuable science tool with impact in the biological, chemical, and physical sciences.

The SwissFEL soft X-ray branch Athos is in the installation and commissioning phase and first pilot experiments are planned for 2021. For the SwissFEL Athos branch an innovative accelerator concept has been introduced, dubbed CHIC (interleaved delay chicanes), which enabled new lasing modes such as 'High-Brightness Self-Amplified Spontaneous Emission (HB-SASE)', 'Short-Pulse High-Power (SPHP)' and 'Mode-Locked Lasing (MLL)'. The CHIC concept has already proved very successful in early commissioning experiments and will open up new opportunities not available at other XFELs so far. The endstation concepts are tailored towards exploiting the new lasing modes for novel approaches in non-linear X-ray sciences.

Finding 2: With the Athos soft X-ray branch, SwissFEL has established itself as an innovation driver in novel accelerator schemes, X-ray pulse generation, and ultrafast X-ray science concepts.

There is a strong demand from the scientific community for higher photon energies, enabling higher spatial resolution and reaching K-shell electrons for spectroscopy applications of a critical class of elements. Harder X-rays and the associated longer penetration depth will also enable new approaches for in-situ and operando experiments. Furthermore, novel non-linear X-ray approaches require ultrashort pulses in the attosecond time regime.

Finding 3: New applications that drive XFEL science demand higher photon energies and shorter pulse lengths.

Technical developments increase the flexibility and versatility of the research infrastructure. In particular, superconducting undulator technology can significantly extend the attainable photon energy range compared to existing facilities. Also, the latest generation of high-performance X-ray detectors have led to an exponential increase in data production.

Finding 4: Technological advances enhance the existing infrastructure beyond their initial design envelope. At the same time, they bring new challenges, in particular with respect to data collection, storage, management and curation.

The scientific applications of XFEL facilities broaden and the beamtime use of the Swiss community increases. Swiss academic groups have been using XFEL facilities worldwide very intensively and successfully. The usage of the European XFEL during the period 2017–2019 has been twice as high as the present Swiss share. SwissFEL beamlines are strongly requested and heavily oversubscribed.

Finding 5: There exists a strong demand for XFEL beamtime that can currently not be satisfied.

To cope with the emerging scientific needs for harder and shorter XFEL pulses and supported by the paradigm-shifting accelerator designs and technological advancements introduced at Athos, new schemes aimed at delivering sub-femtosecond X-ray pulses at very high energies are mandatory.

We formulate the following recommendations.

Recommendation 1: The extension of SwissFEL with the installation of a new hard X-ray branch (Porthos) is strongly supported. Through the use of interleaved delay chicanes (CHIC) Porthos will enable advanced machine modes to be implemented in the hard-X-ray regime. This will enable a plethora of first-of-its-kind scientific applications in emerging, high-potential research fields such as time-resolved structural imaging, time-resolved chemistry, quantum materials, advanced imaging as well as novel opportunities at the ultrafast and high-intensity frontier.

Recommendation 2: The collaboration within the 'Swiss Acceleration Research and Technology' (CHART) initiative is crucial and should be further intensified.

Recommendation 3: Switzerland should maintain its EU-XFEL participation.

Recommendation 4: The involvement in initiatives developing data management and analysis tools as well as machine-learning approaches at the national and European level should be further strengthened.

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3.4 Purpose and Scope

The scientific questions addressed by photon sources based on accelerators – synchrotrons and free-electron lasers – should contribute to solving relevant problems our society is facing, from the development of smart and new materials and mitigation of climate change to fundamental aspects in infectious diseases and atomically resolved biochemical structures. Applications cover all kinds of disciplines, from semiconductors for electronics, catalysis for chemical reactions and lead molecules for drug development to research in paleontology and cultural heritage.

The scope of the present document is twofold:

- It provides a concise description of the achievements of SwissFEL's first phase of operation as well as the use of FEL facilities worldwide by Swiss academic groups.

- It presents the case for an extension of SwissFEL, enabling novel scientific applications and FEL modes unique in their art.

3.5 The Swiss Landscape: today and tomorrow

The ability to visualize the structure of matter and the functioning of biological, chemical, and physical processes has been a fundamental driver in scientific investigations and resulting technological innovations. In the past decades, the frontier has moved towards resolving ultrafast processes on the femto- to attosecond time scale, imaging structures with atomic resolution, and following reactions with elemental details.

As of today, Switzerland offers to the scientific community state-of-the-art infrastructure for the investigation of ultrafast processes such as FastLAB (University of Bern) and LACUS (EPFL) in the optical regime. With the SLS at PSI intense synchrotron radiation is provided for the investigation of materials, chemical reactions, and biological structures, including dynamics with timescales from hundreds of picoseconds to minutes. With the recently commissioned Swiss Free-Electron Laser (SwissFEL) at PSI, delivering femtosecond pulses of soft and hard X-rays at a repetition rate of 100 Hz, Switzerland has leveraged opportunities from the ultrafast community and the unique power of X-ray investigations for a broad area of scientific applications.

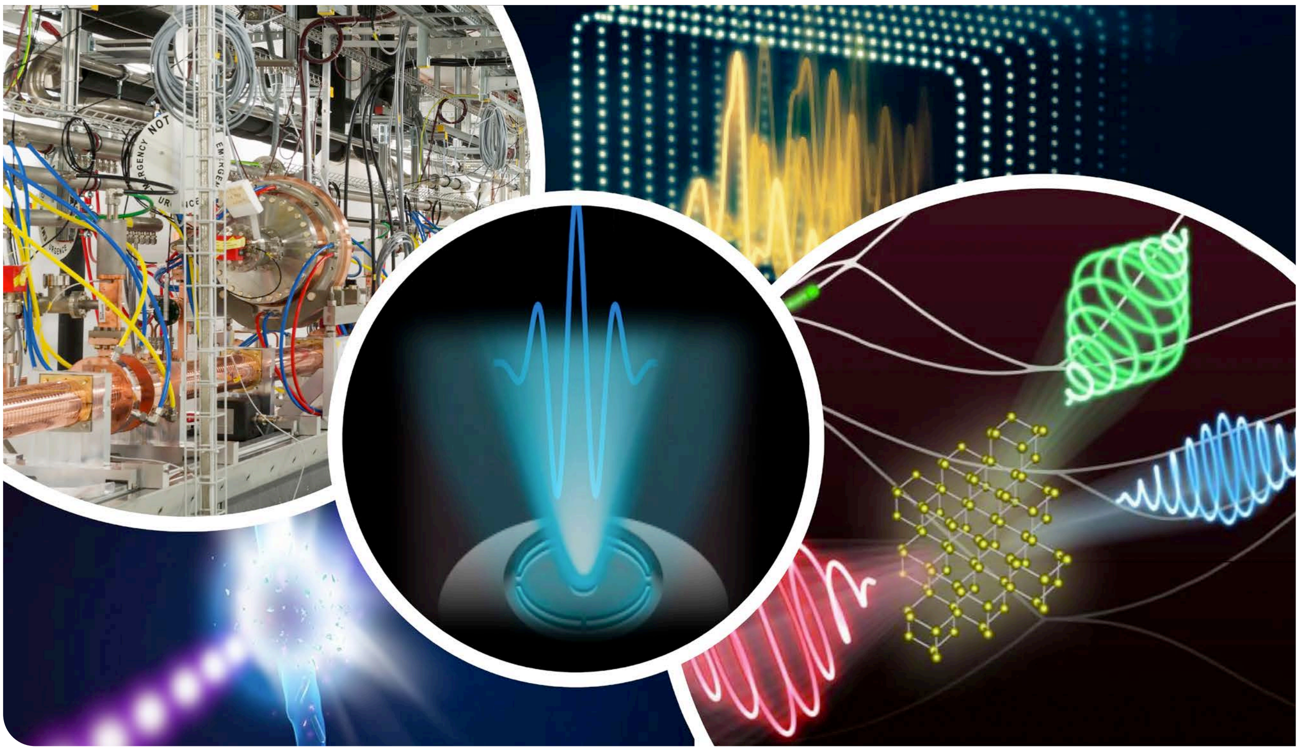

Figure 12: As an advanced waveform generator in the hard X-ray regime, Porthos on SwissFEL will provide ultrashort, very intense X-ray pulses serving a plethora of unique scientific endeavors. Image credits [1]

Such extremely short and very intense X-ray pulses can probe matter in-situ (pulsed magnetic or electric fields) at short distances after stimulation either by photons produced by ‘conventional’ optical lasers or by the FEL itself. This allows, for instance, to make ‘movies’ of what happens on the atomic scale in response to electromagnetic perturbations. There are other comparable facilities in the world (see section ‘The International Context’), but SwissFEL is unique in its flexibility in X-ray pulse generation and experimental-endstation concepts. In particular, for the soft X-ray Athos branch, SwissFEL has innovated concepts for sub-femtosecond operation as well as for the design of its soft X-ray lasing section which, thanks to a unique configuration of undulators alternating with (electron steering) chicanes, it opens up new and unexplored ways for X-ray generation.[30]

The new hard X-ray branch Porthos will enrich the landscape of tomorrow and will enable addressing paradigm-shifting scientific challenges with a world-wide unique hard X-ray undulator line. Porthos will deliver intense (> 1012 photons/pulse), two-color hard (> 20 keV) X-rays and ultrashort (< 1 fs) pulses with very good transversal coherence, and flexible polarization control at a repetition rate of 100 Hz. The targeted beam properties have already cross-fertilized ideas between accelerator physicists and scientists from a diversity of other disciplines, yielding unique scientific proposals to the direct benefit of biological, chemical, materials, and physical sciences as well as new opportunities stemming from the enhanced pulse properties of the Porthos undulator lines.

In the following, some selected examples are briefly presented.

3.5.1 Time-resolved structural biology

The past decade has seen major breakthroughs in modern structural biology with over 165’000 structures of biological macromolecules deposited in the Protein Data Bank to date. Following these successes, many structural biologists now want to go beyond the ‘structure-is-function’ paradigm towards a new frontier: time-resolved structural biology. Biological macromolecules have to undergo sequential structural rearrangements to perform their functions. To capture these dynamic movements and advance the field towards ‘dynamics-are-function’ has been a long-standing dream of structural biologists.

XFELs have proven to be an excellent tool for resolving structural dynamics and provide superior data compared to pioneering experiments using Laue crystallography at synchrotrons.[36] Time-resolved serial crystallography at XFELs is furthermore the only method that allows to resolve atomistic changes in biological macromolecules down to the femtosecond regime.[33, 27, 31] Already the first user run at the SwissFEL provided excellent results on new phasing techniques[6] and time-resolved crystallography in the femtosecond-to-millisecond range.[7] It makes sense to build on these successes when considering the opportunities offered by the new Porthos branch and capitalize on the shorter pulse length and the wider energy range to stay at the forefront of modern structural biology.

The first main difference to Aramis will be a pulse length on the order of a few femtoseconds, to be achieved without compromising beam intensity. This is relevant for one of the key promises of the XFEL technology, i.e., to outrun radiation damage by the ‘diffraction-before-destruction’ principle.[48] Experimental evidence shows that pulses on the order of 50–100 fs provided by Aramis are too long to avoid any radiation-damage effects[22, 10] and that diffraction is self-terminated much earlier.[40] Compression of the available photons into a few femtoseconds by the SPHP mode of Porthos will therefore not only further reduce radiation damage but also provide better data at higher resolution and from smaller crystals because more photons will contribute to the diffraction process. Smaller crystal size is an important advantage for static serial femtosecond crystallography on G protein-coupled receptors and other drug targets.[23] Moreover, small crystals are particularly appealing for time-resolved experiments as the size of crystals is a critical factor determining the achievable time resolution using rapid diffusion of small molecule ligands or co-factors.[29] Today we typically use optical lasers to initiate reactions, which limits the biological systems that we can study to those which can be triggered by light, i.e., either native chromophores such as retinal[7], or synthetic photoswitches.[14] A future implementation of liquid application methods for time-resolved crystallography[18] or similar fixed-target devices that are under development at PSI would allow studying a much wider variety of biological reactions, including enzyme catalysis or the binding of small drug molecules. The Porthos SPHP mode and potentially its radiation-damage-free regime might trigger the revisiting of structure determination by single-particle analysis, something that so far has been the domain of high-repetition-rate facilities like LCLS-II and the EU-XFEL.

In structural biology, the X-ray energy is a critical factor for resolving phase ambiguities via anomalous diffraction measurements. With its extended energy range towards harder X-rays, Porthos will reach the absorption edge of many interesting elements with atomic number larger than 34.[50] The identification and precise location of specific atoms can be crucial to understand protein function. One example is the case when the orientation and position of small molecule ligands needs to be determined in a structure-based drug-design task. Another is the mapping of metal clusters often found as catalytic sites in enzymes. Tracking the position of specific atoms can be particularly important in time-resolved experiments, as it is not always possible to distinguish atoms with similar scattering properties. A time-resolved, anomalous difference map experiment[17] might allow following the exact translocation pathway in light-driven ion transporters that have been recently studied at SwissFEL.[7] One could also envisage to follow the nanochemical synthesis of polyoxometalate clusters in dedicated storage proteins.[41] Such clusters are used in the semiconductor industry because of their diverse and unique chemical and physical properties but require strict synthesis conditions, including high pressure. Time-resolved structural snapshots of how protein enzymes can catalyze such chemical reactions under more ambient conditions could lead to game-changing applications in the chemical industry.

3.5.2 Ultrafast chemistry

The benefits of X-ray techniques for chemical sciences are manifold. In fact, X-ray applications reach from understanding devices under real conditions to fundamental questions in the electronic-to-nuclear coupling on the femto- to attosecond time scale. Chemistry experiments at X-ray sources use a broad range of techniques, generally categorized into spectroscopy and scattering. The increased photon energy of the Porthos undulator will benefit both categories. For spectroscopy, some K-edges of 4d transition metals (Mo, Ag, Pd) will be within reach, providing complementary information to probing the L-edges in the tender X-ray regime available at Aramis. For the higher photon energy regime, the methods developed for time-resolved X-ray spectroscopy measurements, both absorption and emission,[37] can be extended building on the strong expertise available at PSI already.[20] For scattering applications, the higher envisioned photon energy paired with the increase of incident photon energy expected on Porthos will enable methods such as the measurement of pair distribution functions at SwissFEL, which make it possible to obtain atomic resolution in disordered or nanocrystalline materials as well as in molecular systems in the solution phase. In addition to expanding the photon energy range to the K-edges of important elements and higher resolution in scattering experiments, the harder X-rays provided by Porthos will provide new opportunities for in-situ and operando experiments at FEL sources. The higher penetration depth will facilitate the design and implementation of reaction cells for experiments and make this important class of experiments at FELs feasible.

In the ultrafast regime, the goal to make a 'molecular movie' has been one of the driving forces of FEL science in the last decade, and it has been pursued with a wide range of different techniques and beam parameters.[25] Single-particle X-ray imaging and gas-phase X-ray scattering are two successful examples of great tools to monitor dynamics in the angstrom-femtosecond regime, revealing very rich mechanisms previously only indirectly accessible by spectroscopic methods. These techniques can benefit from the shorter-wavelength X-rays of Porthos, increased time resolution and potentially X-ray pump/X-ray probe opportunities.

Gas-phase X-ray scattering is a growing field focused on understanding the details of the internal dynamics of molecular motion. It has been shown to be capable of visualizing structure dynamics of molecular systems of increasing complexity,[13, 35] but it faces challenges when it comes to the spatial resolution and cross sections when compared to electron diffraction. Extending this technique to harder X-rays (in the range of 20 keV) would increase the spatial resolution of such measurements, opening up the possibility to measure electronic dynamics in excited states, such as transient systems approaching conical intersections. For this purpose, it will also be crucial to utilize short (<10 fs) X-ray pulses to probe the very fast first steps of the excited-state nuclear dynamics and with sub-femtosecond pulses potentially even electron dynamics can be visualized. The foreseen challenges include reduced scattering cross-sections at high photon energies, which can be mitigated by a combination of high pulse energies, development of high-density sample delivery systems and highly sensitive detectors.

Ultrafast hard X-ray scattering can visualize the dynamics inside nanoscale samples with Angstrom resolution. Early applications were targeted at fundamental questions of intense light-matter interaction and non-thermal phase transitions, but there is a growing interest for materials laser processing and advanced manufacturing. Recent wide-angle scattering experiments in the hard X-ray allowed the observation of structural dynamics inside the nanoplasma formed after the laser interaction, by following the evolution of its crystalline structure.[19] This can be extended towards shorter wavelengths and, in particular, shorter X-ray pulse durations to yield higher spatial-temporal resolution. This is especially interesting for the study of clusters with embedded species inside, such that the matrix and dopant dynamics can be monitored independently. For such systems, it would also be interesting to investigate the effect of hard X-ray damage, by using an X-ray pump/X-ray probe scheme, especially for clusters doped with heavy elements that interact more intensely with hard X-rays.

3.5.3 Quantum materials

At shorter wavelengths as provided by Porthos, transmission measurements in solids with thicknesses on the order of 10 µm becomes feasible and larger q-ranges can be accessed. This allows for forward-scattering geometries, so that in turn pulsed magnetic fields up to and possibly even beyond 50 T can be used, in combination with small angle scattering X-ray diffraction (or absorption) probes. This kind of geometry is also appropriate for pump-probe experiments in cases where the pump excitation length is also ≥ 10 µm, which can be the case for THz excitation or for optical excitation of dilute impurities. Another advantage of higher energies is the ability to perform diffuse scattering experiments on solids with sensitivity to several different cuts of multiple Brillouin zones simultaneously, with good q-resolution. This is highly advantageous for experiments that extract information from correlations between structural fluctuations at different q-vectors, with which it is possible to approach new forms of correlation spectroscopy in nonequilibrium states.

Porthos will extend the CHIC-concept to hard X-rays.[30] For example, bandwidth and full polarization control over the X-ray output pulses can offer a route to single-shot, pump-probe X-ray magnetic circular dichroism or time-resolved resonant diffraction studies at tender and hard X-ray edges. While some of this functionality can be achieved in principle using linear polarizations and phase plates in the hard X-ray range, there would be clear advantages, e.g., concerning flexibility and reliability, in developing such capabilities on the source side. Also, for nonlinear applications (where the polarization state can be critical) it might not be possible to implement phase-plate technologies at high X-ray pulse energies. With innovative machine solutions, Porthos might be able to generate timed sequences of X-ray pulses with widely different energies (up to 1 keV). This could then be used for realization of nonlinear X-ray methods such as transient grating spectroscopy, for example to measure momentum-dependent electron-phonon coupling strengths or the q-dependence of ultrafast demagnetization. Access to specific energies in the hard X-ray range can potentially also exploit stimulated emission processes to achieve sensitivity to valence properties.

Finally, combining CHIC techniques with self-seeding at Porthos would bring new capabilities. As shown on the Athos soft X-ray beamline, selective electron bunch degradation and transverse beam shaping in the accelerator, combined with a self-seeded photon emission scheme, yields phase-locked pulse pairs and even pulse trains.[9] When implemented on Porthos, this will allow to generate a fixed phase relation amongst XFEL pulses in the hard X-ray regime, giving Porthos unique control over waveforms in the hard X-ray range. Such phase-locked pulse trains may be a useful basis for new concepts in linear and nonlinear spectroscopies of quantum materials. Although the feasibility of such schemes remains to be investigated with experiments, potential advantages over existing methods include coherent control and readout of quantum states, or highly precise and efficient measurements of electronic transition line-widths.[9] Moreover, the q-range accessible with hard X-rays might allow the investigation of ultrafast charge and spin fluctuations on atomic length scales.

3.5.4 Single-shot ptychography and 3D imaging

Hard X-ray pulses as delivered by Porthos provide the unique opportunity to image ultrafast non-repeatable phenomena with high resolution in complex environments. To capture snapshots of such phenomena, a robust single-shot imaging technique is needed. Over the years several imaging techniques have been proposed. Coherent diffractive imaging (CDI)[49] can suffer from numerical convergence issues and most importantly requires an isolated sample, which often is impractical. In-line holography offers robust reconstruction on extended specimens, but struggles to recover quantitative values for the complex transmissivity, and the resolution is limited by the size of the on-axis focus. Ptychography[44, 47, 46] offers high-resolution imaging without issues regarding quantitativeness and robustness, nor does it require a clean wavefront. However, due to its scanning nature, conventional ptychography is not compatible with single-shot imaging.

Single-shot ptychography has been demonstrated at optical wavelengths, which is easier due to the ready availability of efficient lenses, beam splitters and gratings. For X-rays we propose to angularly split the beam using a grating upstream of the focal point: upon free-space propagation this causes the beams to acquire some degree of spatial separation, therewith achieving the overlapping illumination of different regions of the sample. Downstream of the sample, at the detector position, the beams are completely separated and the diffracted intensities are collected in parallel using a single pixel-array detector. By extracting the separate diffraction intensities and using a phase-retrieval algorithm the complex-valued transmissivity of the specimen can be reconstructed. New algorithms will need to be developed to deal with the overlap of scattering intensities at higher angles in order to improve the resolution which otherwise is bounded by the grating period. This method would also serve as a robust single-shot technique for full wavefield characterization of nano-focused beams.

Dynamics, for example fast domain switching, could be studied by using two-pulse sequential imaging, or by careful tuning of the arrival of different diffraction orders to the sample.

A potential extension to 3D ultrafast imaging would require splitting of the incoming radiation[28] and subsequent recombination at sample position following a scheme dubbed X-ray multi-projection imaging (XMPI). This approach would avoid sample rotation, obtaining 3D information from a single X-ray flash by splitting it into few, angularly resolved beams which illuminate the sample simultaneously. XMPI, when implemented on Porthos, will enable: I) the study in 3D of dynamical processes with pump-probe approaches at temporal resolutions not possible today, II) the acquisition of 3D information on stochastic and non-reproducible samples in diffraction-before-destruction mode, and III) the study of ultrafast phenomena by using the optical setup for split-and-delay experiments. XMPI capabilities are ultimately limited by the number of photons per pulse. Enhancing this number will be crucial therefore for widening the applicability of XMPI, which is expected to address problems coming from the fourth industrial revolution that cannot be addressed with current X-ray imaging techniques and other probes that lack the penetration power of the X-rays. Examples of possible future applications are: I) novel materials characterization such as imaging nucleation in metallic foams, II) performance monitoring of injection devices by observing cavitation formation, and III) microfluidic devices characterization for efficient transport of bioparticles and drug delivery.

3.5.5 Novel opportunities at the ultrafast and high-intensity frontier

The shorter pulses offered by Porthos, reaching into the domain of core-level lifetimes, its higher photon output, and the increased coherence properties will allow envisioning novel concepts for ultrafast X-ray sciences.

Quantum chemical imaging. The development of lasers and novel laser applications is closely coupled with the field of quantum optics. A first application of quantum optics for short-wavelength FELs was a Hanbury Brown Twiss (HBT) experiment at the FLASH facility.[38] With the measurement of higher-order correlations, fundamental statements about the characteristics of the laser source and the degree of coherence could be made. Looking forward, the deviation from linear models and the quantum characteristics of light will become increasingly important in X-ray laser applications and offer new opportunities in quantum coherent imaging.[4]

In principle, interference fringes can be obtained from higher-order correlations even in the complete absence of first-order coherences. This concept has been extended theoretically for imaging applications of arbitrary arrangements of incoherent scatterers and demonstrated for a hole-mask with intense vacuum-ultraviolet FEL pulses.[26]

The principle of quantum imaging can be extended to higher resolution with hard X-ray pulses. It can be further extended to quantum chemical imaging, where the incoherently scattered light associated with deep core-level fluorescence is exploited. With this route, element and even site-specific fluorescence signals can be paired with single-shot imaging approaches, yielding full spatially resolved snapshots of chemical information. Using deep core levels in the hard X-ray regime will enable applications to working devices and operando applications.

Novel nonlinear spectroscopy approaches. For chemical and materials research nonlinear X-ray spectroscopies offer new opportunities with increased sensitivity and highest time resolution. Here the most intense and shortest possible X-ray pulses are required due to reduced Auger decay probabilities. Sample damage at high X-ray intensities – as delivered by FELs and required for X-ray nonlinear spectroscopy – is strongly related to the amount of free electrons released into the system of investigation. At the current SwissFEL energies of up to 12 keV, X-ray photon emission and Auger decay channels are almost equally probable. Increasing X-ray pulse intensities for compensating the typically low nonlinear cross sections increases the risk of material damage but in return low cross sections can be partially balanced with increased interaction lengths, which become favorably possible at higher photon energies. Auger-electron production and multiple ionization are typically the competing processes for any nonlinear X-ray photon-in photon-out spectroscopy.

Higher intensities and better coherence, as demonstrated with the CHIC modes at the SwissFEL Athos branch, are a substantial benefit for exploiting the field of nonlinear X-ray spectroscopies. Temporal coherence and defined phase relations between multiple light-matter interactions enable the investigation of optimal-control schemes that drive matter into the specific quantum states of interest. Exploring multiple X-ray resonances, multi-dimensional X-ray spectroscopies provides insight into electron couplings in chemical systems. Experiments can be performed in solid state, solution (liquid jets) or nanoparticles at atomic length scales. The combination of local and nonlocal transitions allows investigation of quasiparticle behavior (e.g., of phonons or plasmons), electron correlation, ballistic and non-ballistic transport phenomena and the role of coherence. The directed and often background-free stimulated signals in nonlinear X-ray spectroscopies may enable in situ and possibly even in operando investigations. Moreover, with the option of producing phase-locked multiple modes, we envision heterodyne methods in nonlinear spectroscopy or the application of Raman or Ramsey-type spectroscopies in the linear regime in which, for the latter case, phase information is used to retrieve spectral or temporal information from the system of investigation.

Phase-dependent spectroscopies involve correlation methods in the data analysis and signal detection. Often it is not simply the amount of detected photons, but instead the 'quality' of the photon response that becomes crucial for the experiments. Quantum light such as entangled photon pairs can provide novel type of X-rays spectroscopies and enable the development of elaborated methods in the direction of non-destructive X ray imaging (e.g., ghost-imaging) and X-ray spectroscopy techniques. The interest in employing entangled photons as spectroscopic tools was first raised theoretically in the context of two-photon absorption (TPA) spectroscopy in the optical regime that scales linearly with the pump-photon intensity for entangled photons,[52] a fact that could be employed to avoid photo-damage in nonlinear spectroscopies. Nonlinear parametric down conversion of X-ray photons (XPDC) can be used to produce entangled photons either X-ray/X-ray or even X-ray/optical.[42] XPDC is one of the most important processes of nonlinear X-ray optics and has been theoretically and experimentally studied in many works, with realized XPDC conversion-event rates on the order of 0.1 correlations per second at a flux of 1012 photons/s.[5] PDC can find wide scientific applications in, for example, quantum computing, or cryptography. As the cross section of PDC is small, it has been further studied only in a few works without satisfactory development. Comparison between the theory and experiment and the exploration of applications at FELs is therefore promising.

Strong-field interaction phenomena. The investigation of X-ray nonlinear phenomena is of paramount importance for the understanding the interaction dynamics of high-intensity femtosecond XFEL pulses with matter, for fundamental and applied sciences as well as for the development of new X-ray instrumentation and theoretical modelling.

The onset of nonlinear phenomena for tender/hard X-rays is ~10^{19}–10^{20} W/cm^2.[43] In pioneering studies of nonlinear processes, sequential multi-photon absorption/ionization, double core-hole formation, amplified spontaneous emission and inner-shell lasing, saturation absorption, anomalous Compton scattering, highly ionized matter and plasma creation were observed. Other predicted phenomena, such as super-radiance and a number of XRL schemes, have been proposed[51, 2] and could be enabled by ultra-intense sub-femtosecond XFEL pulses. In particular, the sub-femtosecond regime of X-ray nonlinear interaction effects remains to be explored[12] with the development of nonlinear spectroscopies at attosecond timescales.

Photon-electron coincidence spectroscopy has been a longstanding idea that could not be realized so far. The MOSARIX project[15] in the tender X-ray regime is currently under realization and it could be envisaged to extend it to the hard X-ray regime.

Ultra-strong fields could clarify the reaction dynamics in classical electrodynamics and QED and allow the investigation of tunneling ionization and atomic stabilization and potential exploration of the QED nonperturbative regime.

Although the community in Switzerland investigating X-ray nonlinear phenomena is still small, Switzerland can and should take a unique leadership role. In particular, the strong and established theoretical, astrophysics and particle physics communities could in the future become motivated to join this venture.

The possibility of Porthos to reach ultra-intense terawatt–attosecond X-ray pulses[24, 32, 34] could offer unprecedented opportunities to explore a number of fundamental physics questions that have not been accessible so far and pave the way for exploring new frontiers.

3.5.6 Porthos as an advanced waveform generator in the hard X-ray regime

The new hard X-ray branch Porthos will capitalize on the recent SwissFEL advancements in accelerator physics and provide unique operation modes at hard-X-rays, addressing the call to deliver intense (> 10^{12} photons/pulse), hard (> 20 keV) X-rays at ultrashort (<< 1 fs) pulse length with very good transversal coherence, flexible polarization control and with a sustained repetition rate of 100 Hz. Porthos will complete the original design concept of SwissFEL, which included 9 world-class endstations for science, medicine and engineering. A possible layout of SwissFEL with all three beamlines is shown in Figure 13.

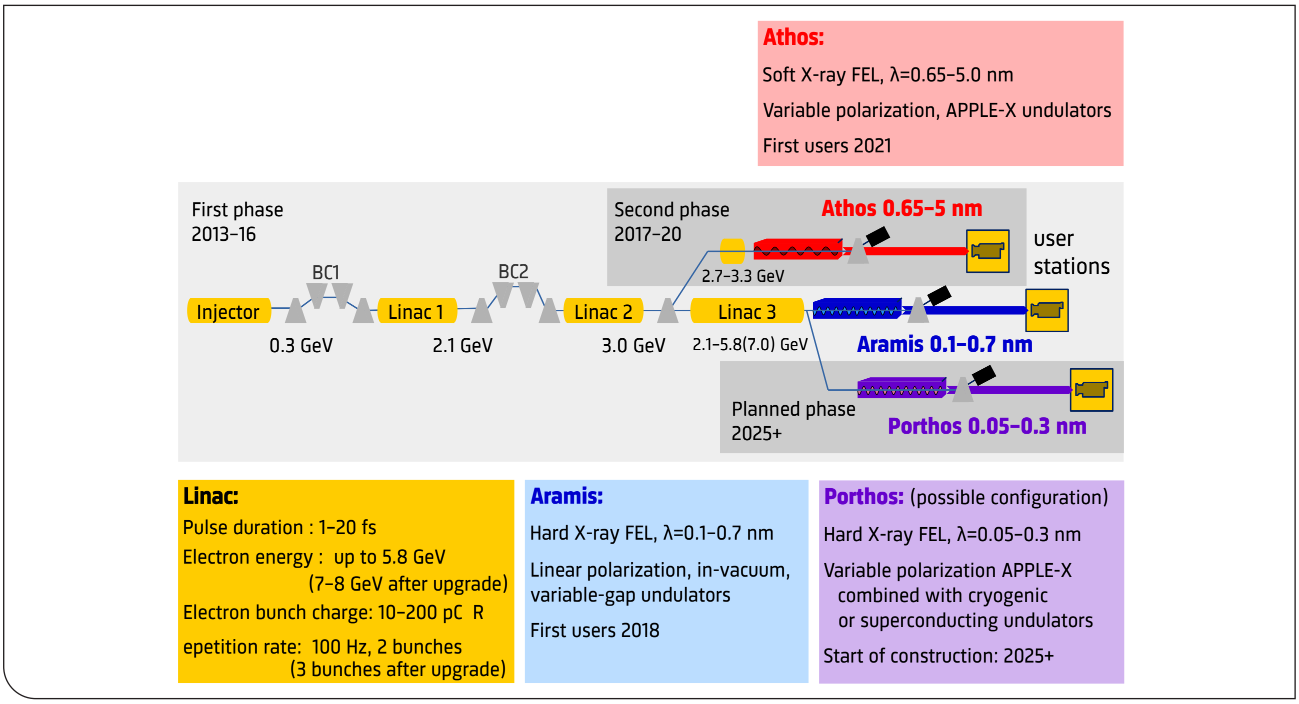

Figure 13: A sketch illustrating the proposed extension of SwissFEL with Porthos, a second hard X-ray branch covering a wavelength range from 0.3 nm down to 0.05 nm. Together with Aramis and Athos, Porthos will accomplish the original design concept of SwissFEL.

Compared to the existing Aramis hard X-ray branch, Porthos will benefit from the following three main accelerator-technological improvements.

Higher reachable photon energy obtained through an increase of electron energy (linac upgrade).

Currently, Aramis relies on a 6-GeV electron beam to reach up to 13 keV photon energy with conventional permanent-magnet undulators (15 mm period nominal K-value of 1.2). The existing accelerator hall provides sufficient space to accommodate additional radiofrequency stations to raise the electron energy up to 7 or even 8 GeV, the maximum allowed by the existing beam dumps. The increased electron energy would immediately raise the reachable photon energy to 18 keV using conventional undulators (as in Aramis), or push it to considerably higher values when considering advanced undulator technology (see below). Depending on how the multibunch operation will be implemented, this 'energy upgrade' might be either installed before or after the Porthos branching point. In the first case the upgrade would be also beneficial to Aramis.

Advanced operation modes with interleaved delaying chicanes (CHIC modes).

Porthos shall feature short magnetic chicanes between undulator modules, enabling the time delay between the electrons and the radiation field to be adjusted precisely, thereby providing precise control of the FEL process beyond the standard SASE operation mode. The additional flexibility granted by CHIC can be harnessed in a number of ways. The most straightforward one consists in a speed-up of the formation microbunches during the FEL process which then reaches saturation with less undulator length (distributed optical klystron mode). A further enhancement of this mode is the so-called high-brightness SASE mode,[39] in which the temporal coherence of the radiation pulse is strengthened to narrow the bandwidth of the spectrum similar to self-seeding methods. More advanced modes enabled by the delaying chicanes include the short-pulse-high-power mode and mode-locked lasing.[45] In the former, the natural limit of FEL saturation power is overcome by allowing the radiation field to tap as yet unspoiled parts of the electron beam in the so-called superradiant regime. This results in extremely short pulses (down to 1 fs or less) with peak powers reaching the TW level. In the mode-locked lasing approach, delays are applied to a periodic modulation of the electron beam, achieved either with an external laser or a beam manipulation in the electron injector, such that the radiation field settles to a global phase for all parts of the beam, thus mode-locking the radiation pulses. The resulting spectrum has a very pronounced modal structure consisting of thin lines. The idea of CHIC to control the FEL process was originally proposed for Athos. First commissioning results look very promising and confirm the expected effect on the saturation length. When implemented on Porthos, CHIC will convert Porthos in an advanced waveform generator in the hard X-ray regime, analogous to Athos for soft X-rays.

Advanced undulator technology.
With both a linac upgrade (increased electron energy) and the CHIC concept, Porthos will significantly outperform Aramis even if the same undulator modules were to be used. A further boost on Porthos performance – in terms of highest achievable X-ray energy but also in operational independence from Aramis – will be achieved by considering undulators with higher magnetic field on axis, which enable a larger tuning range. With recent advances in superconducting undulator technology, undulator strength values of K = 2.5 have become a realistic option for a period length of 10 mm. A shorter period (but higher K-value) with respect to Aramis will result in better overall FEL performance at the same photon energy as well as a considerable extension (+ by 50%) of the photon energy range towards higher values. The installation and operation of superconducting undulators entails significant costs and risks. A realistic mitigation plan would be a hybrid approach, where a conventional undulator line would first provide a robust FEL signal at a sub-harmonic wavelength, with the harmonic target wavelength being amplified by a second undulator line realized with superconducting technology. In fact, the use of harmonic lasing represents an efficient way to extend the photon energy range even further. For instance, instead of tuning directly to, e.g., 24 keV photon energy with a low K value and thus poor performance, the FEL could be tuned first to a sub-harmonic (in this case 8 keV) and the fundamental lasing disrupted with an appropriate configuration of phase shifters, while the initially weak third-harmonic signal can be amplified into high saturation power in the remaining undulator line ('afterburner').

In such a scheme, the first undulator line could consist of APPLE-X type undulators similar to the design being installed in Athos, which may provide full polarization control for photons up to 12 keV energy or higher.

The development of superconducting magnets for future accelerators is one of the central goals of CHART (Swiss Accelerator Research & Technology), an initiative bringing together the leading forces in Swiss accelerator research and development (from CERN, PSI, ETH Zurich, EPFL and the University of Geneva). It is running under the umbrella of the State Secretariat for Education, Research and Innovation (SERI) and the ETH Board. Both large-scale facilities at PSI – SLS and SwissFEL – will benefit from a common technology platform based on CHART.

The existing SwissFEL building complex already includes appropriate space for a second hard-X-ray beamline next to Aramis. An extension of the experimental hall to accommodate Porthos user stations still has to be realized but is already foreseen in the original building permit issued by the local authorities.

Long-term perspective.
As a contribution to the far-reaching goals of SwissFEL (for the periods beyond the present roadmap), the accelerator group of PSI should perform studies and investigations of a branch at longer wavelengths requiring the development of a high-harmonic-generation (HHG) seed laser. Furthermore, a technical assessment of the possibility to operate SwissFEL in a high-repetition-rate mode should be pursued.

These extensions should shape the periods 2028–2032 and 2032–2036 and ensure that SwissFEL stays as a key player in the international scene.

3.6 Major Successes

The SwissFEL accelerator commissioning started in 2017 and already within the same year, the first pilot experiments were fielded. The first call for proposals went out in 2018 with an overwhelming response from the Swiss and international community. The user operations of the hard X-ray Aramis branch started in January of 2019. The build-out of the Athos soft X-ray branch continued in parallel and for this beamline first experiments are scheduled for 2021. The first results from SwissFEL were published[16, 6, 11, 8, 21] with more on the way. Most notably, the list includes a publication from the very first user experiment in January 2019.[16] The impact and value of SwissFEL already becomes rapidly visible to the scientific community.

From the beginning, SwissFEL has been tightly related to the Swiss ultrafast research community. The NCCR MUST (Molecular Ultrafast Science and Technology) launched by the Swiss National Science Foundation (SNSF) in 2010 gathered 26 Swiss research groups working in ultrafast science in an interdisciplinary scheme including chemistry, physics, biology and material science. It has played a major role in facilitating the use of FELs, in strengthening the network activities and in coordinating common research proposals using complementary photon sources.

In addition to the NCCR, there are multiple SwissFEL-related research and network grants. Funding has been secured through the European Union: one ERC Advanced Grant, one ERC Synergy Grant and one ERC Starting Grant, and through SNSF, with one Ambizione Grant. Some novel capabilities at SwissFEL are driven forward with R'Equip grants, with strong support from and involvement from the wider Swiss academic community;

this includes the Maloja endstation for ultrafast chemical sciences, the SASE–RIXS scheme for condensed-matter physics, pump lasers for time-resolved photobiology, and partial funding of the Cristallina endstation through the CristallinaEXTREME project in collaboration with the University of Zurich.

Three joint professorships have been created with focus on ultrafast science and on the use of FELs; one at ETH Zurich (Institute of Quantum Electronics), one at the EPFL (Laboratory for Ultrafast X-ray Science), and the third at the University of Bern (Institute of Applied Physics).

The pilot and early user-experiment phase at the hard X-ray branch Aramis featured several important advancements in both methodology and in novel Swiss contributions to XFEL science. The first user experiments cover a wide range of scientific disciplines and are often spearheaded by Swiss-based researchers.

In biochemistry, pioneering time–resolved experiments have been performed with the aim of elucidating the behavior of ferric/ferrous heme proteins (Fig. 14)[16, 3] that have an important role in the respiratory function of hemoglobin, and of providing direct molecular insight into the dynamics of active cation transport across biological membranes, i.e., light-driven sodium pumps that convert light into membrane potential and becoming useful optogenetic tools.[11]

Further early SwissFEL achievements include the first resonant tender X-ray diffraction on magnetic and electronic dynamics in a ruthenate, a protein SFX phasing experiment[6] performed at 4.5 keV to enhance the anomalous scattering signal from a GPCR membrane protein, and the first experiment with an X-ray transient grating pump and an optical probe, extending the four-wave mixing technique to hard X-rays.[21] An early example from condensed-matter physics is an investigation of coherent phonon dynamics in a type-II Weyl semimetal, where the X-rays are used to quantify the structural underpinnings of the novel electronic topology of this material.

One important class of experiments that is currently in high demand at XFEL facilities requires the use of phase-stable, long-wavelength pulses to be used in combination with ultrashort pulses of X-rays from the XFEL. The long-wavelength radiation can drive coherent dynamics in condensed-matter systems that are otherwise inaccessible in thermal equilibrium, leading to a host of novel phenomena that so far have been difficult to study with X-ray probes. Commissioning of high-field, quasi single-cycle THz pump capabilities for X-ray diffraction experiments was performed already in 2018. As per 2020, it is possible to apply peak transient THz fields exceeding 600 kV/cm for user experiments at cryogenic temperatures (< 10 K). Similarly, user experiments combining X-rays from the XFEL with intense femtosecond pulses ranging from the mid-infrared to the ultraviolet are now possible at Aramis, alongside new tools to ensure effective time resolution down to 15 fs.[2]

The second branch of SwissFEL (Athos) in the soft X-ray range represents an expansion of the capabilities as well as an increase in user capacity. This is achieved through the parallel operation of both branches with up to 100 Hz repetition rate. The undulator and optics line have been installed and a first experimental station dedicated to ultrafast chemical science and single-shot imaging will enter into operation in 2021.

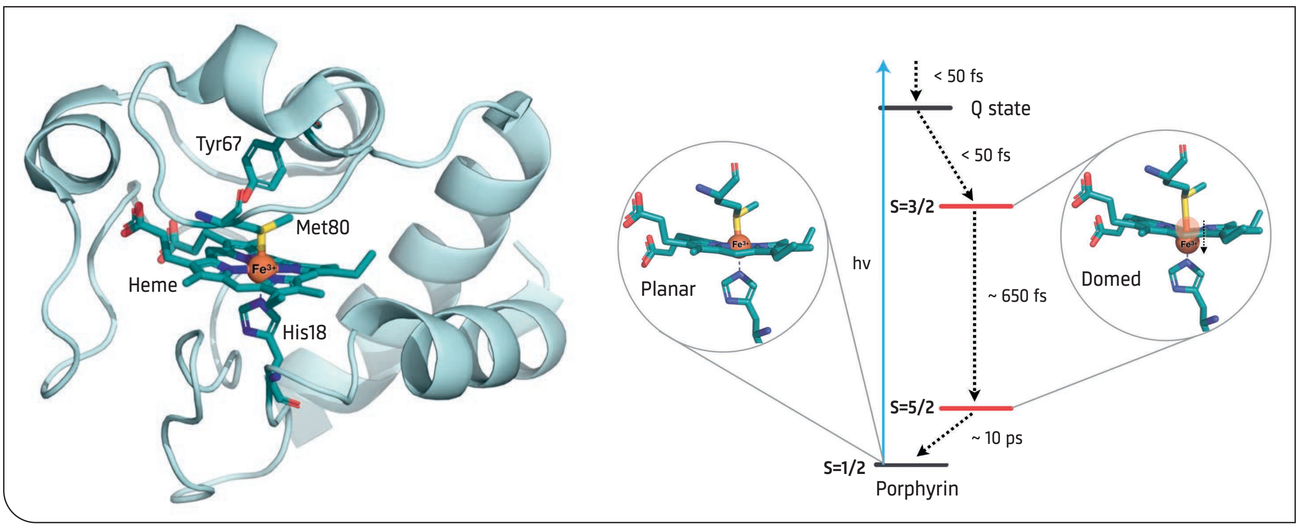

Figure 14: Left: Schematic representation of the ferric heme protein. Right: Schematic representation of the relaxation cascade following UV-visible excitation of ferric Cyt c. From Bacellar et al. (2020)[16].

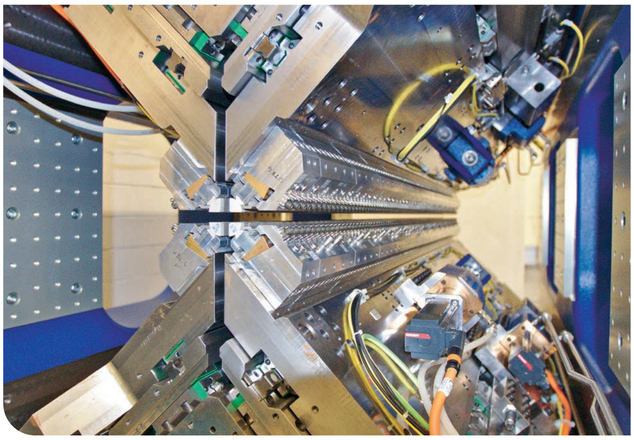

Figure 15: Novel magnet design for Athos, allowing full polarization control of the FEL radiation.

Figure 16: A part of the undulator array for Athos.

The Swiss XFEL community is rapidly growing. In the period 2015–2020 Swiss academic groups have contributed to 200 FEL-related papers. A relative distribution with respect to fields is given in Fig. 17.

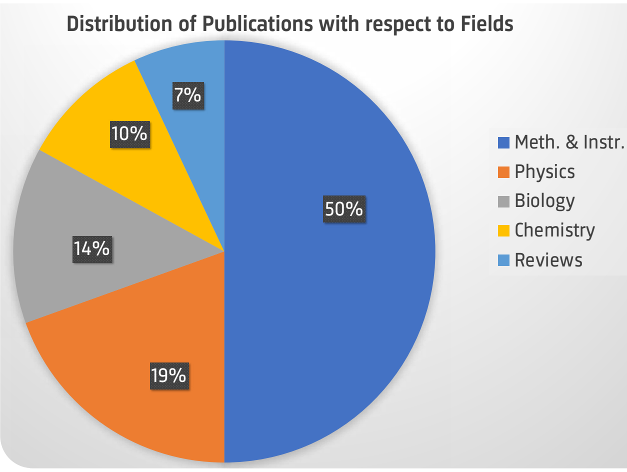

Figure 17: Distribution of FEL-related publications by Swiss groups across research areas.

3.7 The International Context

In 2017 two FEL facilities, SwissFEL and EU-XFEL, providing hard X-ray radiation for user experiments started operation and complement the now-available X-ray spectral regime, previously only available in the USA, Japan and Korea. It is noteworthy that seeding schemes, both for soft and hard X-rays, remain an important area of development for FELs. A list of the presently operating FEL user facilities worldwide is shown in Table 1. It is limited to those facilities used by Swiss academic groups.

It should be noted that SwissFEL is the only nationally funded hard X-ray FEL facility in Europe. SwissFEL as a national facility is a platform for the training of students, doctoral researchers and specialists in research fields within Switzerland and worldwide.

There are two dedicated soft X-ray free electron lasers, FLASH and FERMI, both producing very soft X-rays with fundamental photon energies below 300 eV. This precludes reaching atomic resonances for higher-Z atoms than carbon (284 eV) with the full high-brightness capability of fundamental radiation. Using superconducting accelerator technology, FLASH generates a large number of pulses per second, making it particularly attractive for low-density samples such as gases, aerosols and plasmas. The hard X-ray facilities now operating, LCLS, SACLA, PAL, EU-XFEL and SwissFEL, all include beamlines for producing soft X-rays, with varying degrees of sophistication.

There are a number of projects in Europe under commissioning as well as in the conceptual phase: POLFEL (Poland), MAX IV-FEL (Sweden), TARLA (Turkey), LUNEX (France) and UK XFEL (UK). In addition, two FEL test and development facilities, SPARC (Italy) and CLARA (UK) (see Table 2), serve the further development and testing of FEL schemes, such as sub-fs pulses, seeding or harmonic generation.

A detailed description and the status of the operational FEL facilities can be found on the website of the FELs of Europe collaboration.[12]

Swiss academic groups are at the forefront of research in structural biology, femtochemistry and condensed-matter physics. Due to the complexity of the experiments, the research is pursued in collaborations including a large number of groups (in particular in Structural Biology).

12 https://www.fels-of-europe.eu

Facility	Country	Photon Energy	Repetition Rate	Experimental Stations
FELIX	Netherlands	0.8–400 meV	variable	18
FELBE	Germany	0.5–4 meV	variable	5
FLASH	Germany	14–300 eV	10 × 800 pulses/s	7
FERMI	Italy	15–310 eV	10 Hz	6
LCLS-I	USA	0.4–25 keV	120 Hz	7
LCLS-II	USA	250–7000 eV	up to 929 Hz	3
SACLA	Japan	40–100 eV 4–20 keV	60 Hz 30 Hz	6
PAL	Korea	120–1200 eV	60 Hz	5
EUXFEL	Germany	500–3000 eV 3–25 keV	10 × 2700 pulses/s	6
Swiss FEL	Switzerland	180–2000 eV 4–13 keV	100 Hz	6

Table 1: FEL facilities used by Swiss academic groups

Facility	Country	Start Operation	Electron energy	Wavelength	Pulse properties
CLARA	UK	2022	250 MeV	100–400 nm	< fs to > 1 ps up to 400 Hz
SPARC	Italy	2006	150 MeV	550–800 nm in SASE down to 40 nm in HGHG	30 fs to 10 ps at 10 Hz

Table 2: FEL test and developmental facilities

Switzerland is a partner in the European XFEL with a present share of 1.5%. In the period 2017–2019 Swiss groups have been granted 3.6% of the approved beamtime as PIs. Moreover, Swiss participation as collaborators in proposals led by non-Swiss groups amounts to 15% of the total beamtime granted.

The EU-XFEL has now six experimental stations in operation, located pairwise at three different FEL branches running simultaneously. Due to the presently installed superconducting technology developed decades ago, a special X-ray pulse pattern is used with a combination of macro (10 Hz) and microbunches (4.5 MHz). On the longer term the transformation of the present acceleration scheme towards a continuous wave operation is envisaged. A mixed EU-XFEL- DESY group has started the first discussions on user demands and on the technological challenges. The time frame for a possible upgrade is foreseen to be by the end of this decade.

3.8 Synergies with other Scientific Fields

The technical capabilities and scientific opportunities offered by XFELs are well complementary with those from synchrotron sources and laser-based sources at university laboratories.

There are many examples in chemistry, biology and condensed-matter physics showing the synergies of the use of the above-mentioned facilities to tackle in a holistic way a scientific goal. It is one of the strengths of Switzerland to offer to the community state-of-the art infrastructures: FastLAB (University of Bern), LACUS (EPFL), SLS and SwissFEL (PSI). Furthermore, there is an enhanced use of different experimental methods: X-ray and cryo-electron microscopy in structural biology or photons and neutrons in condensed-matter physics and soft-matter research.

Beyond scientific synergies, it is very important to point out the innovation aspects. Without the experiences gained in construction and operation of SLS, the installation of SwissFEL would simply not have been possible.

With the development of novel pixel detectors for X-rays strongly supported at PSI as a further extension of the pixel detectors for high-energy physics, the amount of data taken at SLS or SwissFEL is approaching the volumes comparable to those in particle-physics experiments. Strategies and technical developments are of common interest between both fields. Swiss groups are engaged in Europe-wide initiatives in data management and analysis, playing an important role in projects such as PANOSC and ExPaNDs.

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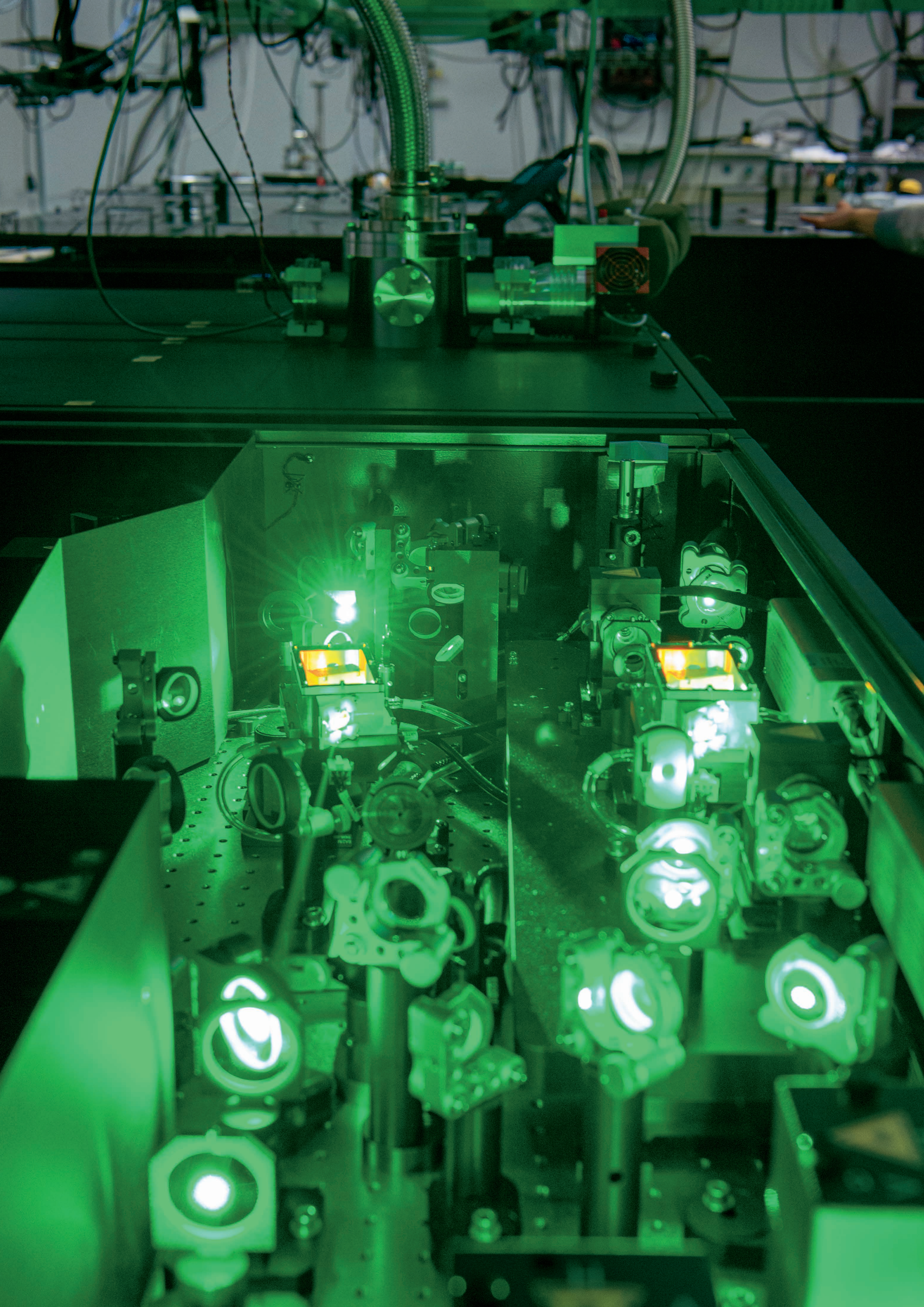

4 Institution-Based Laser Platforms

4.1 Executive Summary

Institution-based platforms bring together different groups in a university or research institute to work on a common goal. These platforms are an efficient way to pool resources and personnel in order to build and develop techniques and scientific projects at the forefront of the field, which would be beyond the reach of any individual PI. Being independent from each particular group, they are a long-term, profitable investment where knowledge and equipment are shared, without the bureaucracy of an external user facility.

In the field of photon science, several such institution-based platforms exist which each focus on different themes. In this roadmap, we use the case of ultrafast science as an example, as it captures well the many advantages of institution-based platforms. It also illustrates their challenges, related in particular to funding. Moreover, ultrafast-science platforms are particularly relevant for the topics addressed in the other chapters of this roadmap.

In Switzerland there are at present two institution-based platforms with a focus on ultrafast science, at different stages of development: LACUS at EPFL, and FastLab Bern at the University of Bern. A third platform, FastLab Zurich, is under discussion at ETH Zurich. Similar solutions have been found abroad, when large investments are necessary which a single group cannot sustain.

Institution-based platforms are essential in the Swiss scientific landscape in that they enable unique technical and scientific developments. These are crucial on their own, to maintain Switzerland's position as a leader in photon science and technology, but they are also a means of creating the community for large-scale facilities such as the SLS and SwissFEL at PSI. In addition to their pioneering role in science and technology, institution-based platforms also promote academic excellence, and provide infrastructure for young scientists at the start of their careers.

Despite their importance, the funding necessary to set up institution-based platforms is quite substantial and remains a major impediment to their development. In the ultrafast-science example we discuss in this chapter, funding came essentially from the institution itself, with some contribution from the SNSF via an NCCR. This limits the impact of such platforms, which currently only the largest institutions are able to afford. We propose a new funding scheme, 'R'Equip Plus', which is independent from the institution, and which would likely benefit other fields of research in Switzerland beyond ultrafast photon science.

4.2 Findings and Recommendations

This chapter examines the characteristics and operation of institution-based photon-science platforms, which involve several research groups within a given institution while providing no significant external user access. Among photon-science fields, ultrafast science is taken as an example. A number of key features emerge, which are summarized in the following, and which prompt a few recommendations.

One big advantage of institution-based platforms is that they enable pooling of financial and personnel resources. This makes it feasible to purchase large-scale equipment at the forefront of technology and to develop unique and versatile setups, which ensure the competitiveness of the platforms at a level that is typically not attainable within a single-PI effort. Dedicated personnel, in turn, guarantees continuity in the maintenance of the equipment, and more generally in the technical and scientific undertakings. It also provides crucial know-how, in addition to the technical capabilities, for the operation of these platforms. Institution-based platforms also benefit from the fact that several groups from different fields work together, which promotes synergies, the interdisciplinary exchange of know-how and the development of innovative solutions.

Finding 1: The pooling of financial and personnel resources at institution-based platforms enables the development of unique and versatile setups while preserving continuity and know-how.

Compared to large-scale facilities with external user access programs, in Switzerland or abroad, institution-based platforms generally have less funding available but they have much more flexibility in modifying the design of the experiments. Added to a more local and more flexible control over user access, this enables, for instance, longer-term experiments and technological developments with custom-tailored solutions, which are challenging to accommodate within the more rigid configuration of a typical user facility. In this sense, institution-based platforms have a crucial role as test-beds for the work performed at large-scale facilities, e.g., in ultrafast science when preparing for experiments at SwissFEL. They enable the development of techniques and the validation of scientific concepts before consuming precious beamtime at those facilities, and help create the community that will make use of them.

Finding 2: Continuous design flexibility together with control over access guarantees the development of long-term innovative solutions at institution-based platforms.

Finding 3: In ultrafast science, institution-based platforms help create the user community for large-scale facilities such as SwissFEL.

Related to their setting within an institution, these platforms offer the possibility for groups who are not experts in photon science to successfully perform sophisticated experiments, making use of the available equipment and know-how, without the bureaucracy, delays and rigid time allocation tied to an application to an external facility. Furthermore, institution-based platforms provide unique training opportunities for graduate students, which not only supports the academic mission of universities but can also serve as a means to attract young scientific talents. Notably, institution-based platforms offer an attractive location for young scientists and junior group leaders to develop their projects. Young investigator grants, such as the ERC Starting Grants or the SNSF Ambizione, Prima and Eccellenza awards, do not generally provide enough funds to set up a high-end laser laboratory, particularly in the field of ultrafast science. Having access to an institution-based platform provides a tremendous boost for innovative projects, and, by relieving or sharing the monetary burden for infrastructure, optimizes national resource allocation.

Finding 4: Institution-based platforms provide non-expert groups with access to technical and scientific know-how.

Finding 5: These platforms provide unique training opportunities for students and optimal settings for young researchers to develop their projects.

Despite their numerous advantages – scientific and academic, as detailed above, and to some extent financial, as resources are more efficiently employed – only two such institution-based platforms exist in Switzerland in the field of photon science. These two platforms have benefitted in part from SNSF funding via the NCCR MUST and R'Equip, but greatly from international grants (three ERC grants funded a great part of LACUS) and from university investments (LACUS also benefited from EPFL funding). Indeed, there is no national funding scheme in Switzerland for 5–15 MCHF investments in equipment. R'Equip grants, the largest equipment grants at the individual-group level, are too limited; larger applications, for significant investments such as those required, e.g., for a large-scale synchrotron facility, are too lengthy and procedural for the amount of funding required. Regarding NCCRs, they are collaborative projects but their goal is not to fund platforms, and the creation of a platform should not require such a large project as an NCCR. An intermediate and agile funding scheme, together with a long-term running budget, would be extremely useful for enabling new institution-based platforms to be created and in further developing the existing ones. Such a 'R'Equip Plus' grant would provide funds to create the platform and would guarantee that funding is available to cover its running costs. In turn, the institution would commit to providing the space and hiring permanent staff members, so as to make the best use of the platform. This commitment from the institution would replace the typical matching-funds requirement. Such a 5–15 MCHF grant would be competitive with the level of funding available to directors in the Max Planck Society in Germany, with the advantage of being independent from a single individual professorship. This guarantees that it would be beneficial not only for the groups directly involved in the platform but also for other groups at the same institution. Groups from other Swiss institutions would also be provided access, via collaborations or via a simplified access procedure. In this scheme, funding for individual groups is mostly preserved but some resources are pooled to create platforms that are technologically advanced, well-managed and efficient while remaining versatile and easily accessible. More broadly, it is likely that such a funding scheme would be beneficial for other areas of photon science as well as for scientific fields beyond photon science, and especially at universities with limited budgets.

Finding 6: Only two institution-based laser platforms exist in Switzerland. They were built with minimal funding from the SNSF.

Recommendation 1: Institution-based laser platforms are ideal as preparation sites for experiments at SwissFEL and XFELs worldwide, from a scientific, technical and personnel point of view, and should therefore be supported.

Recommendation 2: A new equipment funding scheme, 'R'Equip Plus', is needed to cover the 5–15 MCHF investments required to set up and run such platforms. The institution matches this investment by providing the space and permanent staff.

Recommendation 3: Care must be taken that other groups within the institution, as well as non-expert Swiss groups, can access the platform quickly and easily, via a less formal and bureaucratic approach than is used by international consortia such as Laserlab-Europe and LaserNetUS.

4.3 List of Authors

Editorial board
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Acknowledgments
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4.4 Purpose and Scope

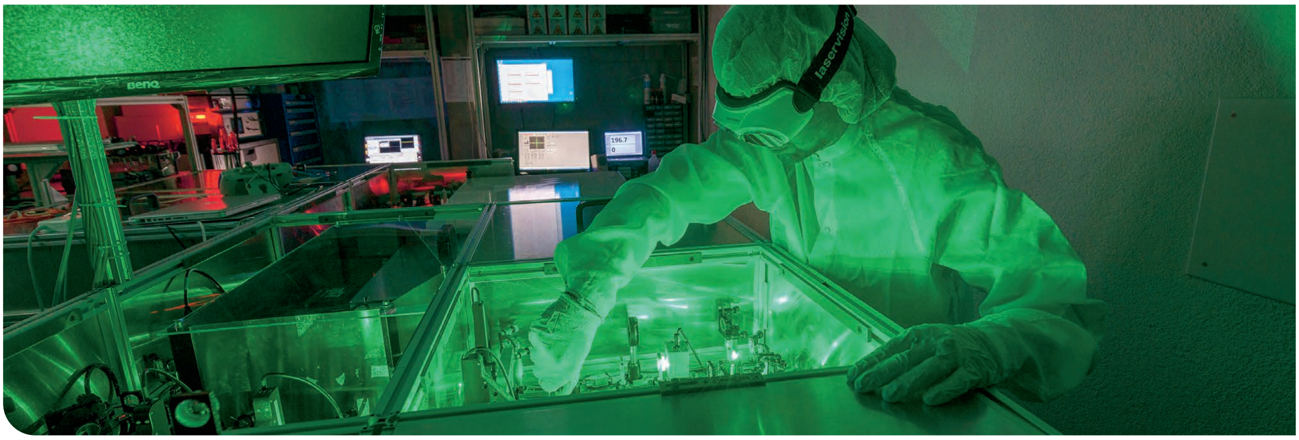
This chapter deals with institution-based photon-science platforms, meaning laser-based laboratories and experimental equipment that are shared by different research groups in the context of a university or research institute, either jointly funded by all of them or with their own independent funding. These are neither facilities, generally open to outside users, nor conventional laboratories, which are clearly associated with one group. Several such institution-based platforms exist and have evolved differently in different contexts.

We use the particular case of ultrafast photon science as an example to discuss institution-based platforms in general. Other fields of photon science could be addressed in this discussion but the arguments would be redundant and we therefore chose not to list them all here.

Institution-based platforms enable a trade-off between the large investment that is required to set up novel and versatile laser-based experiments and the delays and inconvenience of relying on fully user-access facilities. Furthermore, they allow research groups that do not have a focus on laser-based experiments or that do not own a high-performance laser system to benefit from the know-how and capabilities already available at their institution.

Attosecond science, time- and angle-resolved photoemission spectroscopy, liquid-phase core-level spectroscopies (absorption and photoelectron), time-resolved near-field imaging, and time-resolved electron diffraction and microscopy are a few examples of techniques which can greatly benefit our understanding of, e.g., fundamental physical and chemical processes, materials and nanoscale dynamics, but which involve costs that most groups cannot support on their own as well as a level of expertise that restricts the number of teams that can set them up.

The purpose of this chapter is to examine 1) the platforms of this type that exist in Switzerland, what they offer, which scientific fields they serve and how they are organized, in particular by comparison with the international landscape; 2) how these platforms interface with other facilities and tools available for Swiss scientists; and 3) how existing and foreseeable platforms should evolve during the coming decade in order to best serve the Swiss scientific community.



Ultrafast laser physics experiment, ETHZ. (Photo provided by Lukas Gallmann)

4.5 The Present Swiss Landscape

The two Swiss platforms that are included in the general scope of this chapter are at different stages of development and operation. The Lausanne Center for Ultrafast Science (LACUS) is an interdisciplinary center for ultrafast science and technology, formally created in 2015 and with an official start dating back to 2016. FastLab Bern at the University of Bern was established in 2015 during the second phase of NCCR MUST, and a dedicated laboratory was introduced later that year.

Each of these platforms has its specific technical and scientific focus, which makes them generally complementary in the Swiss landscape, although some experimental overlap is present, in line with the fact that they serve different communities at different universities.

4.5.1 LACUS

LACUS is located at the Ecole Polytechnique Fédérale de Lausanne (EPFL) and relies on a tight collaboration between several groups from the fields of chemistry and physics.[13] The Laboratory of Ultrafast spectroscopy (LSU), the Laboratory of Electronic Spectroscopy (LSE), the Laboratory for Ultrafast Microscopy and Electron Scattering (LUMES), the Photochemical Dynamics Group (GDP) and the Laboratory of Quantum Nano-Optics (LQNO) are key players in the technical and scientific development of the setups. New teams are now joining LACUS to further develop and use the Harmonium facility, namely the Laboratory for Quantum Magnetism (LQM), the Laboratory for Ultrafast X-ray Science (LUXS, jointly associated with PSI) and the group for Spin-Orbit Interaction Spectroscopy (SOIS). Finally, the group recently formed at EPFL by Prof. Christian Rüegg (Director of PSI since 2020) will also integrate into the LACUS platform. This gathering of research groups guarantees that sufficient human resources and funding for consumables are available to maintain the experiments. LACUS has also benefited from successful R'Equip proposals for upgrades. At this stage, LACUS has no permanent staff to ensure its operation. It therefore fully relies on research assistants and postdocs with fixed-term contracts. Funding mechanisms to further support LACUS with running costs and permanent personnel are under active discussion at the time of writing.

LACUS currently consists of three core laboratories: Harmonium and LOUVRE, both within the LSU, and LUMES. The Harmonium facility delivers femtosecond extreme ultraviolet (EUV) light pulses between 15 and 110 eV with a duration below 100 fs. These pulses are used for static and time-resolved photoelectron spectroscopy, as well as EUV absorption spectroscopy, directly measuring the electronic structure of matter. Two endstations are dedicated to solids (LSE/LSU) and to molecules and/or nanoparticles in the liquid phase (LSU). An upgrade to the photoemission facility is ongoing at the time of writing, consisting in the integration of a new advanced high-repetition laser source delivering 200 fs pulses in the energy range between 8 and 30 eV in a 5–10 meV monochromatized beam. The upgrade will allow both static and pump-probe ARPES experiments at high energy resolution and on very small samples. Another upgrade consists in an additional pump laser synchronized to the Harmonium source.

The LOUVRE laboratory is dedicated to deep-ultraviolet (250–380 nm) one- and two-dimensional optical spectroscopy and circular dichroism spectroscopy of molecular systems and wide band-gap metal oxides (LSU). It also includes an arm with an experimental chamber dedicated to ultrafast electron diffraction both in reflection and transmission geometry (LUMES).

The LUMES laboratories are equipped with a state-of-the-art ultrafast electron microscope with femtosecond and nanosecond laser sources spanning the wavelength range from 18 microns to 400 nm. This instrument also features the only imaging spectrometer for energy-filtered imaging connected to a direct electron detector in the world. Other state-of-the-art ultrafast optical spectrometers for research on magnetic materials are currently under development.

The strong interdisciplinarity provided by LACUS, spanning from chemistry and biology to solid-state material research, fostered scientific collaborations across Switzerland and resulted in four pilot external user beamtimes in the past two years (J. Osterwalder, UZH; C. Monney, UNIFR; J. Chang, UZH; J. Helbing, UZH) and in international projects through the joint Max-Planck-EPFL center (R. Ernstorfer, FHI Berlin). Since January 2020, and as a member of Laserlab-Europe, LACUS has gained the status of Access Provider and welcomes researchers from Europe who wish to conduct experiments, in particular in the fields of chemistry, condensed-matter physics and materials science.

13 https://www.epfl.ch/research/domains/lacus

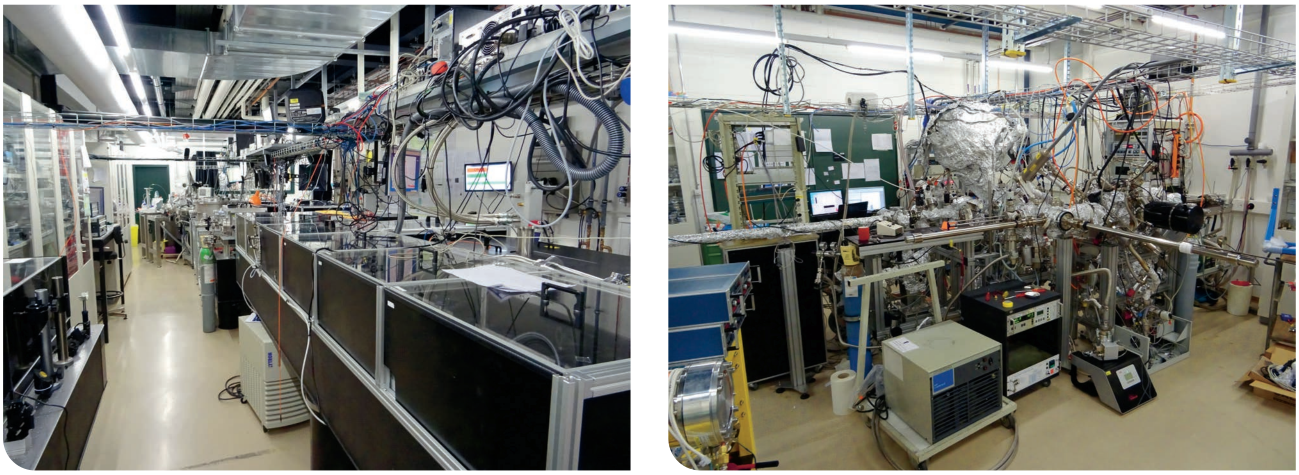


Figure 18: Left: Harmonium laboratory at LACUS. Right: ARPES setup. (Photos Alain Herzog, EPFL)

4.5.2 FastLab at the University of Bern

FastLab in Bern allows research groups from all faculties of the University of Bern to benefit from an internationally competitive, sustainable and cost-efficient development of cutting-edge laser technology to help address fundamental questions and to promote new areas of science and technology.[14] At present, the main users are from the Department of Chemistry of the University of Bern with two joint PhD students. In the past, two joint postdocs with PSI have made extensive use of the platform. Moreover, FastLab supports young researchers at the University of Bern (e.g., ERC grantees or SNSF Eccellenza, Ambizione or Prima awardees) in their academic career by providing them access to expensive equipment and instrumentation that would otherwise be out of reach. FastLab supports access to novel laser technologies for non-laser expert groups to address their scientific questions. The platform employs one permanent staff member.

The laboratory associated with FastLab Bern consists of a femtosecond system, which pumps a number of different synchronized light sources. They include optical parametric amplifiers in the visible and near-infrared frequency ranges as well as white light generation in the range from 400 to 1200 nm. The main applications are broadband Fluorescence Upconversion Spectroscopy (FLUPS) and transient absorption spectroscopy.

External user experiments, partially funded by NCCR MUST, were performed in the context of international collaborations with groups in Germany (N. Ernsting, MBI Berlin; F. Lino and T.-K. Choi, EU-XFEL), Italy (A. Scrotino, U. Palermo) and the UK (A. Vlcek, Queen Mary University of London).

4.6 Major Successes

Several of the groups involved in LACUS and FastLab Bern were driving forces in successfully applying for and running the NCCR MUST, which has in turn provided significant resources for these two platforms. In particular, LACUS has benefitted, over the 2017–2020 period, from the fact that two of its members are part of the NCCR MUST, which provided funding not only for equipment but also for personnel, via five NCCR MUST postdoctoral fellowships. FastLab Bern is mostly funded by the NCCR MUST, through one of its participating groups.

4.6.1 LACUS

In addition to EPFL and NCCR MUST contributions, an ERC Advanced grant and two SNSF R'Equip grants have helped start LACUS (the Harmonium and LOUVRE Laboratories). The LOUVRE Laboratory secured further funding from the ERC (a Starting and a Consolidator Grant), Google (one grant), Lockheed Martin (one grant), the Howard University Washington (one grant), the SNSF (one R'Equip Grant, one SPARK Grant and one ANR/

14 https://www.iap.unibe.ch/research/laser_physics/fastlab/index_eng.html

DFG/SNSF Grant) and the ELI-ALPS Research Institute. Together, these funding sources have covered the 2 MCHF necessary to set up and operate the Harmonium facility, and the 1 MCHF necessary for the LOUVRE laboratory.

In addition to the funding aspect, several awards and prizes have been awarded to PIs, postdoctoral researchers and PhD students affiliated with LACUS. Furthermore, four new groups from EPFL have recently joined the original five core-groups. The new members are now part of the platform and will be intense users of its facilities. One other aspect of the success of LACUS is the academic output, with up to four PhD thesis defended per year since 2016, in addition to several Bachelor's and Master's level projects.

Since 2016, 21 papers have been published emanating from LACUS. A few key publications are referenced here, as examples of the research performed at this platform, ranging from ultrafast photoelectron spectroscopic studies of liquids[1] and ultrafast circular dichroism of chemical and biological[2] samples (cf. Fig. 19) to 2D deep-UV spectroscopy and ARPES studies of solid-state systems of fundamental and technological relevance[3–6] (cf. Fig. 20).

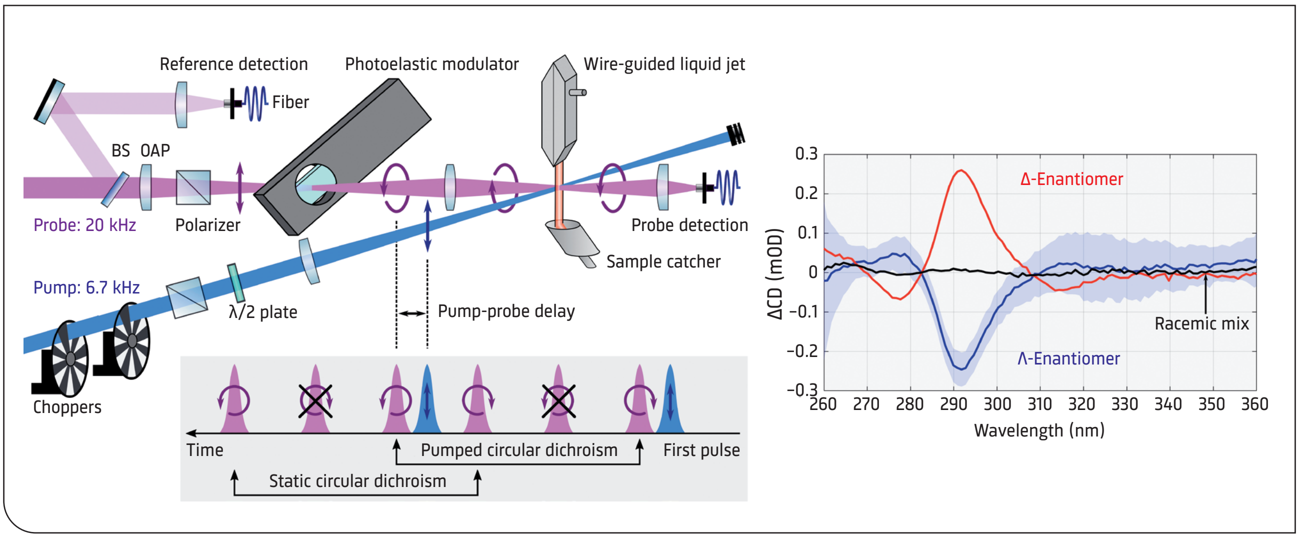


Figure 19: Left: schematic of the time resolved circular dichroism setup.
Right: time resolved circular dichroism spectrum of two enantiomers of $(Ru(bpy)_3)^{2+}$ and the corresponding racemic sample in 0.4 mM aqueous solution, photoexcited with a 400 nm pulse at 50 ps pump–probe delay. Reproduced from Oppermann et al. (2019)[2].

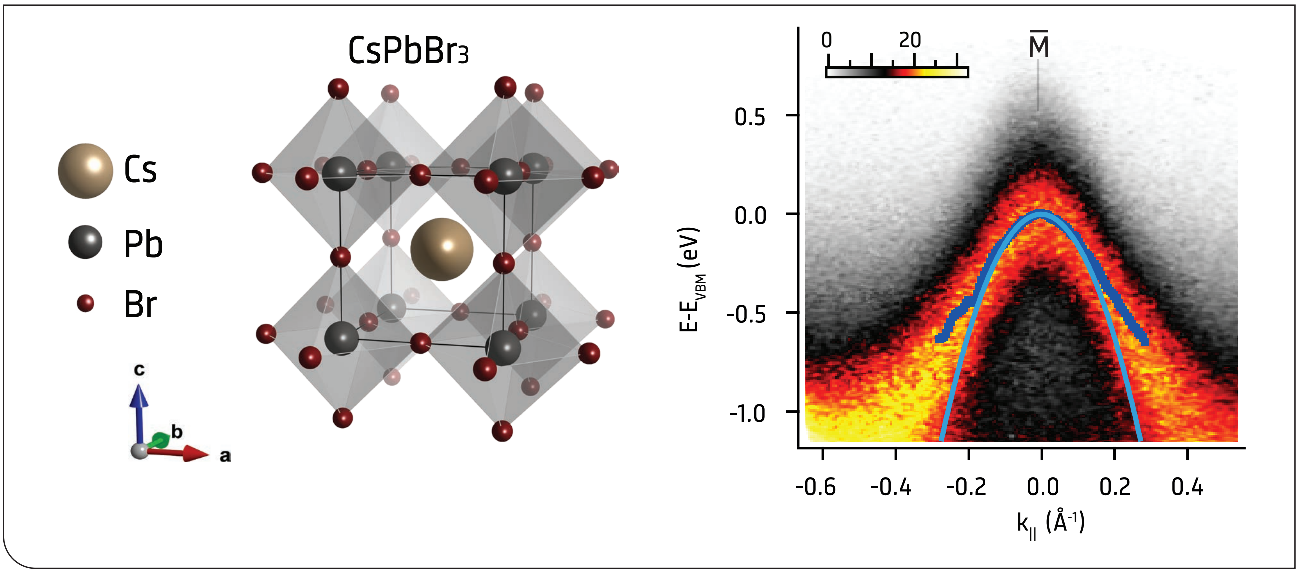


Figure 20: Left: cubic perovskite structure of the $CsPbBr_3$ perovskite.
Right: ARPES intensity showing the valence band maximum, which reveals the formation of large polarons with a hole effective mass of 0.26 +/− 0.02 times the electron mass. Reproduced from Puppin et al. (2020).[4]

4.6.2 FastLab at the University of Bern

FastLab Bern is mostly funded by the NCCR MUST, which has covered the 2 MCHF necessary to establish and operate the platform to date. In 2019, a high-fidelity FLUPS apparatus was transferred from the Max Born Institute in Berlin, providing the users of FastLab Bern with the opportunity to perform state of the art time resolved broadband fluorescence measurements. In addition to equipment costs, joint PhD student positions with the University of Palermo and with PSI were funded via an ERC Starting Grant, the Canadian FQRNT and NSERC and the SNSF.

The scientific impact of FastLab Bern is further increased by its support of postdoctoral researchers and junior scientists who receive prestigious grants such as ERC Starting Grants, SNSF Eccellenza Fellowships, and SNSF Ambizione or Prima Grants. Since operation began, in 2015, several fruitful collaborations have also been established with local groups from the Department of Chemistry of the University of Bern, as well as with groups from abroad. It is planned that two additional groups from the University of Bern will join the FastLab platform in the near future.

The research performed at FastLab Bern ranges from ultrafast methods development[7] and optimization to studies of chemically[8] and physically[9] relevant systems (cf. Figs. 21 and 22). It has led to nine publications so far, of which a few key references are included here.

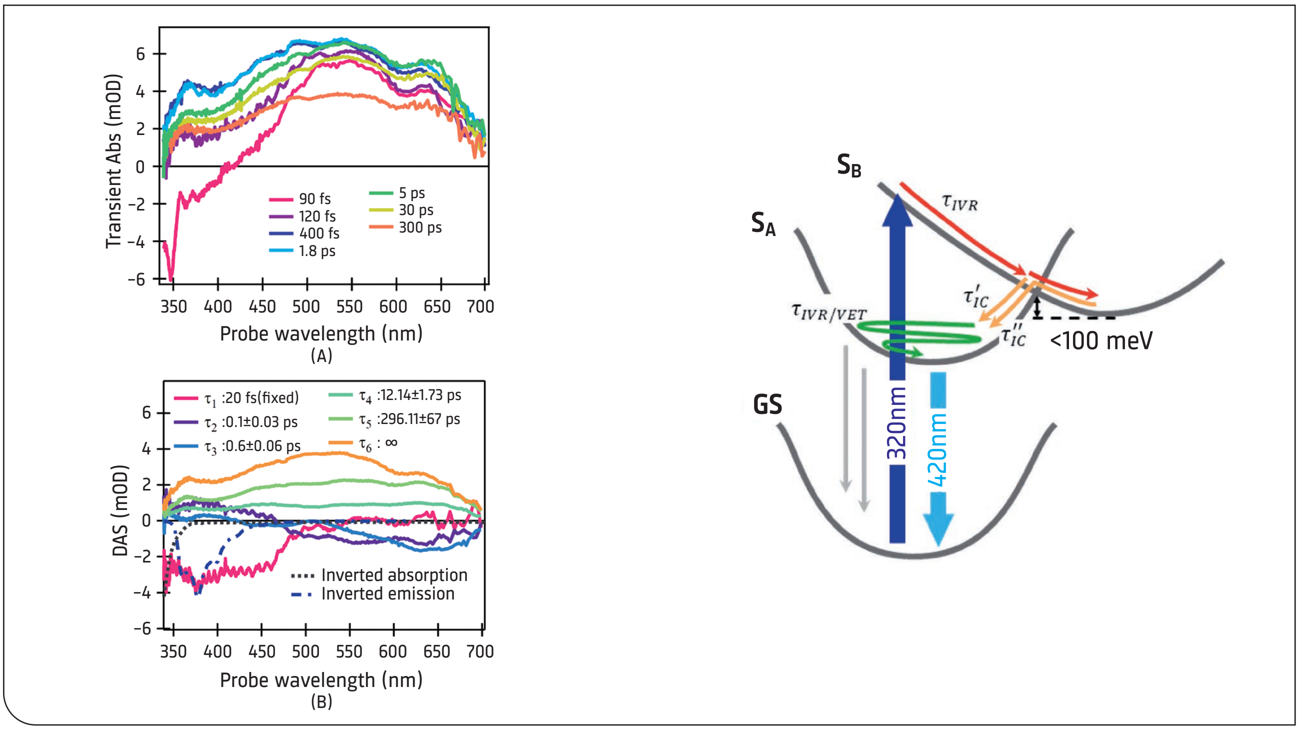


Figure 21: Left: time-resolved UV-vis transient absorption spectroscopy of a phenanthrene monomer, showing (A) the spectra following photoexcitation at 320 nm and (B) the characteristic lifetimes and decay associated with the spectra. Right: photocycle derived from the data on the left. Reproduced from Nazari et al. (2019).[7]

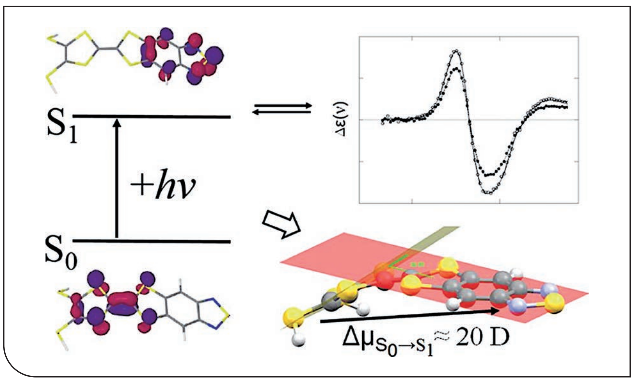


Figure 22: Photoexcitation from the HOMO to the LUMO in tetrathiafulvalene-benzothiadiazole donor-acceptor molecules (left) leads to intramolecular charge transfer (bottom right) and to a change in dipole moment, detected as a change in sample absorption (top right). Reprinted (adapted) with permission from Rohwer et al. (2018).[8] Copyright 2018 American Chemical Society.

4.7 The International Context

As described above, this chapter discusses institution-based laser platforms which provide limited external user access, taking ultrafast science as an example in the much broader field of photon science. In this section, the Swiss case is compared with its international counterparts. However, given that these platforms are internal to the universities it is not trivial to identify them, so that a caveat must be added in that the overview of the international context presented here is not exhaustive.

Two programs exist, in Europe and in North America, which aim at bringing visibility to different platforms and at providing a structure that facilitates visits from external users. Laserlab-Europe was created in 2004 as a network of laser laboratories, which now includes 35 institutions.[15] User access to the laboratories is evaluated based on research proposals. Financial support is provided by the EU's Horizon 2020 program, both for improvement of the member laboratories and for travel and accommodation of the users. Laserlab-Europe AISBL was created in 2018, an international non-profit association which brings together 43 leading laser research infrastructures in 21 European countries, as a means to complement the EU-funded project with a longer-term perspective. Swiss researchers make up 2–3% of the users of Laserlab-Europe facilities outside of Switzerland. In 2020, one swiss laser laboratory (LACUS, at EPFL) joined Laserlab-Europe as a member.

LaserNetUS is a network of 10 laser laboratories in North America, created in 2018 and funded by the USA Department of Energy (DOE).[16] The DOE funds are used to support the participating laboratories. User access, at the users' expense, is managed via a research proposal system. The LaserNetUS program is currently up for renewal.

Both Laserlab-Europe and LaserNetUS connect laboratories of different sizes, including some run at a single group level, large-scale user facilities, and several institution-based platforms, as discussed in this chapter. Such consortia are beneficial not only because they promote the exchange of ideas and people but also because they provide a source of funding for the member laboratories, which is in some cases essential for their maintenance. In those cases, allocating time for external users' access is a means to support internal activities.

LaserNetUS is relatively new and its impact is still difficult to evaluate. Laserlab-Europe, on the other hand, has led to a long list of projects and publications. It is a very successful program, its impact being made clear by the fact that it is the longest running European network, recently renewed for the fourth time for another 4-year term.

A current list of sources is included as an appendix, which provides an overview of the international context. A corresponding map is shown on Fig. 23. They deserve a couple of comments. (a) Laser facilities, such as LOA and CELIA in France and RAL in the UK, provide user access via conventional external user applications. They are not institution-based platforms and therefore fall outside the scope of this chapter. Being nationally funded, they require no financial support from abroad, namely from Switzerland. (b) Institution-based laser platforms in

Figure 23: Map of light sources providing user access, excluding synchrotrons and X-ray FELs (cf. table in the appendix for more details).

15 https://www.laserlab-europe.eu
16 https://www.lasernetus.org

North America mostly focus on high energy systems. This is a type of research which does not, at present, exist in Switzerland on a laboratory scale. It could, however, benefit from the recommendations made in this chapter.

4.8 Synergies with other Scientific Fields

Institution-based platforms complement large-scale user facilities in terms of science and technology, as well as cost, resources and accessibility.

Different radiation wavelengths provide a different piece of the puzzle in the investigation of the physical properties of a novel material, the different stages of a chemical reaction or the dynamics of a particular biological process. There are, therefore, inherent synergies between the science that is produced in laser laboratories, with wavelengths typically between the THz and the (extreme-) UV range, and the experiments performed in large-scale short-wavelength X-ray facilities, namely synchrotrons and XFELs for static and time-resolved experiments, respectively. This inherent complementarity has a clear manifestation in that several members of the institution-based platforms we discuss in this chapter have long-time collaborations or dual appointments with PSI, which hosts a synchrotron, the SLS, and an X-ray Free-Electron Laser, SwissFEL. This is the case for two groups that are members of LACUS and one group that is a member of FastLab Bern.

In particular regarding time-resolved measurements, which the advent of XFELs has recently made available at X-ray wavelengths with sufficient photon flux, laser-based experiments are very often used as a first step to test the sample and validate an idea, which is then developed fully at an XFEL. This is a resource- and cost-efficient way to prepare a measurement or to develop an experimental approach so as to make the most of the scarce beamtime available at large-scale facilities. In this sense, laboratory-based sources produce, to some extent, the community for the larger facilities. Conversely, laser-based experiments are often needed to complement a picture, which time-constrained measurements at an XFEL cannot fully resolve.

Aside from scientific and technical synergies, there are innovative aspects to be considered. Novel developments, such as for instance the capability to reliably generate an intense laser pulse at a particular wavelength, pushed by laboratory-based sources, and in particular by institution-based platforms where innovation is a goal by design, can lead to technological improvements at an XFEL facility or synchrotron. The same is, of course, also true in reverse.

4.9 References

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4.10 Appendix

The list below presents the light sources which provide user access via a structured process (facilities) or on a smaller scale (platforms). Synchrotron and X-ray FELs, which form the basis of the two other chapters of the roadmap, are left out of this list.

EUROPE

Name	Technical focus	Institutions involved	Scientific fields	Outside user involvement (%)	Part of a network?	Website	Type
AttoLab	Spectroscopy Ultrafast dynamics	Paris-Saclay University	Chemistry Physics	–	–	http://attolab.fr/index.php	Platform
CALT	Quantum Optics, High intensity laser physics (HIL), Spectroscopy	Institute of Physics (IFZg) in Zagreb	Physics Chemistry Biology	Under construction	Laserlab-Europe	http://calt.ifs.hr/en	Platform/ Facility
CELIA	Ultrafast lasers HIL Spectroscopy	Université de Bordeaux	Physics Engineering	100%	Laserlab-Europe	https://www.celia.u-bordeaux.fr/en/home	Facility
CLF	Spectroscopy HIL Imaging	Central Laser Facility	Physics Chemistry Biology	100%	Laserlab-Europe	https://www.clf.stfc.ac.uk/Pages/home.aspx	Facility
CLL	Spectroscopy	University of Coimbra	Chemistry Biology	Partial	Laserlab-Europe	https://www.uc.pt/en/uid/laserlab/facilities/transient-absorption	Platform/ Facility
CLPU	HIL	Centro de Láseres Pulsados	Physics	100%	Laserlab-Europe	https://www.clpu.es	Facility
CLUR	Spectroscopy Ultrafast lasers	University of Madrid	Chemistry Engineering	–	Laserlab-Europe	https://www.ucm.es/ulc	Platform/ Facility
COLA	Spectroscopy Ultrafast dynamics	Université de Bordeaux	Physics Chemistry Nano-technology	Partial (also industry)	–	https://www.loma.cnrs.fr/plateforme-cola	Platform/ Facility
CUSBO	Spectroscopy Imaging	Politecnico of Milan	Physics Chemistry Biology	Partial	Laserlab-Europe	https://www.fisi.polimi.it/en/research/european_facility/cusbo	Platform/ Facility
FELIX	FEL	Radboud University	Physics Chemistry Laser technology	100%	Laserlab-Europe	https://www.ru.nl/felix	Facility
GSI	HIL	Helmholtz Center Darmstadt	Biomedical Chemistry Physics	100%	Laserlab-Europe	https://www.gsi.de/start/aktuelles.htm	Facility
HIJ	HIL Ultrafast lasers	Helmholtz Institute Jena	Laser Technology Physics	Partial	Laserlab-Europe	https://www.hi-jena.de/en	Institute/ Facility
HZDR	FEL HIL	Helmholtz Center Dresden Rossendorf	Physics Medical Technology	Partial	Laserlab-Europe	https://www.hzdr.de/db/Cms?pNid=145	Institute/ Facility

HiLASE	Ultrafast lasers	Institute of physics, Czech academy of science	Science Industry transfer	Partial	Laserlab-Europe	https://www.hilase.cz/en	Institute/ Facility
ICFO	Spectroscopy Imaging Quantum optics Photonics	The Institute of Photonic Sciences	Physics Chemistry Photonics	Partial	Laserlab-Europe	http://www.icfo.eu	Institute/ Facility
IEP	Spectroscopy Ultrafast dynamics Photoemission	Technical University Graz	Physics	Partial	Laserlab-Europe	https://www.tugraz.at/en/institutes/iep/home	Institute/ Facility
ILC	Spectroscopy Imaging	University of Bratislava	Physics Chemistry Biomedical	Partial	Laserlab-Europe	http://www.ilc.sk/en/vyskum/laboratoria	Platform/ Facility
ISMO	Spectroscopy Imaging	Université Paris-Saclay	Physics Chemistry Biology	Partial	Laserlab-Europe	http://www.ismo.u-psud.fr/?lang=en	Institute/ Facility
INFLPR	HIL	National Institute for Laser, Plasma and Radiation Physics	Physics	Partial	Laserlab-Europe	http://www.inflpr.ro/en	Institute/ Facility
IPHT	Photonics	Leibniz Institute of Photonic Technology	Biology Medicine	Partial	Laserlab-Europe	https://www.leibniz-ipht.de/en/institute/photonics-for-life.html	Institute/ Facility
IPPLM	HIL	Institute of Plasma Physics and Laser Microfusion	Physics	Partial	Laserlab-Europe	https://www.ifpilm.pl/en	Institute/ Facility
IST	HIL	Universidade Técnica de Lisboa	Physics	Partial	Laserlab-Europe	https://www.ipfn.tecnico.ulisboa.pt/research	Institute/ Facility
Laserlab Amsterdam	Spectroscopy Photonics	Vrije University Amsterdam	Chemistry Biology Physics	Partial	Laserlab-Europe	http://www.laserlab.vu.nl/en/index.aspx	Platform/ Facility
Laserlab DK	Ultrafast lasers Imaging Quantum optics Technology	Aarhus University Technical University of Denmark University of Copenhagen Bispebjerg Hospital University of Southern Denmark Aalborg University	Physics Chemistry Biomedical	Partial	Laserlab-Europe	http://laserlab.dk/about	Platform/ Facility
LENS	Spectroscopy	University of Florence	Physics	Partial	Laserlab-Europe	http://www.lens.unifi.it	Institute/ Facility
LIDYL	HIL Spectroscopy	CEA/Saclay	Physics Chemistry	Partial	Laserlab-Europe	http://iramis.cea.fr/LIDYL/en/index.php	Facility
LLC	Spectroscopy Imaging	Lund University	Physics Chemistry	Partial	Laserlab-Europe	http://www-llc.fysik.lth.se	Institute/ Facility
LL-NSC	Spectroscopy Imaging	University of Jyväskylä (JYU)	Biology Chemistry	Partial	Laserlab-Europe	https://www.jyu.fi/science/en/nanoscience-center	Institute/ Facility

LOA	Ultrafast lasers Spectroscopy	CNRS – Ecole Polytechnique (EP) – ENSTA-Paristech	Physics	Partial	Laserlab-Europe	https://loa.ensta-paristech.fr/?lang=EN	Institute/ Facility
Lord Porter Ultrafast Laser Spectroscopy Laboratory	Ultrafast dynamics Spectroscopy	University of Sheffield	Chemistry Physics Biology Academic/ teaching	Partial, ~10%	–	https://www.sheffield.ac.uk/laser-spectroscopy	Platform/ Facility
LP3	Ultrafast lasers	CNRS Université d'Aix-Marseille	Physics Engineering Biology	Partial	Laserlab-Europe	http://www.lp3.univ-mrs.fr	Institute/ Facility
LULI	HIL	École Polytechnique, Palaiseau	Physics	Partial	Laserlab-Europe	https://portail.polytechnique.edu/luli/en	Institute/ Facility
MBI	Ultrafast lasers Spectroscopy	Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy	Physics	Partial	Laserlab-Europe	https://mbi-berlin.de/homepage	Institute/ Facility
MPQ	Ultrafast lasers Spectroscopy	Max Planck Institute for Quantum Optics	Physics Chemistry	Partial	Laserlab-Europe	https://www.mpq.mpg.de	Institute/ Facility
MUT-IOE	Defence	Military University of Technology Warsaw	Photonics	Partial	Laserlab-Europe	http://www.ioe.wat.edu.pl	Institute/ Facility
ORION	HIL Defence	Atomic Weapons Establishment	Physics	Partial, 15%	Laserlab-Europe	https://awe.co.uk/what-we-do/nuclear-warheads-lifecycle/science/understanding-plasma-physics/orion	Industry/ Facility
PALS	HIL Ultrafast laser	Prague Asterix Laser System	Physics	Partial	Laserlab-Europe	http://www.pals.cas.cz	Platform/ Facility
Sofia University	Ultrafast lasers Spectroscopy	Sofia University	Physics	Partial	Laserlab-Europe	http://quantum.phys.uni-sofia.bg/index-en.html	Platform/ Facility
STRATH	Quantum optics Photonics	University of Strathclyde	Physics	Partial	Laserlab-Europe	https://www.strath.ac.uk/science/physics	Platform/ Facility
ULF-FORTH	Spectroscopy	Institute of Electronic Structure and Laser	Physics Chemistry Photonics	Partial	Laserlab-Europe	https://www.iesl.forth.gr	Institute/ Facility
ULLC	Spectroscopy	University of Latvia	Physics Photonics	Partial	Laserlab-Europe	http://www.lasercentre.lv	Platform/ Facility
USZ	–	University Szegend	Physics	Partial	Laserlab-Europe	http://www.physx.u-szeged.hu/angol/fizika.php?ID=23	Platform/ Facility
VU LRC	HIL Spectroscopy Ultrafast lasers	Vilnius University	Physics Material Science Biophotonics	Partial	Laserlab-Europe	https://www.ff.vu.lt/ltc	Institute/ Facility
WIGNER	Ultrafast lasers Spectroscopy Quantum optics	Wigner Research Center for Physics	Physics Material Science	Partial	Laserlab-Europe	https://wigner.hu/en	Institute/ Facility

NORTH AMERICA

Name	Technical focus	Institutions involved	Scientific fields	Outside user involvement (%)	Part of a network?	Website	Type
Advanced Beam Laboratory	High energy lasers Particle acceleration	Colorado State University	Physics	Partial	LaserNetUS	https://projects-web.engr.colostate.edu/accelerator/index.php https://www.lasernetus.org/facility/advanced-beam-laboratory	Platform/Facility
ALLS	High energy lasers Ultrafast dynamics Imaging Spectroscopy UED Attosecond Particle acceleration	Université du Québec (INRS)	Physics Chemistry Engineering Biology Medical Material science	Partial, 40% (also industrial users)	LaserNetUS	http://inf.emt.inrs.ca/?q=en/ALLS	Platform/Facility
BELLA	High energy lasers Laser plasma acceleration	Lawrence Berkeley National Laboratory	Physics	Partial, 15%	LaserNetUS	https://bella.lbl.gov	Platform/Facility
CUOS (resuming operation in 2023)	High energy lasers Particle acceleration	University of Michigan	Engineering Physics Astrophysics Material science	Partial, 60% (after 2023)	LaserNetUS	https://cuos.engin.umich.edu	Platform/Facility
ELL	High energy lasers Particle acceleration Ultrafast dynamics	University of Nebraska – Lincoln	Chemistry Medical Engineering Physics	Partial	LaserNetUS	https://www.unl.edu/diocles/home	Platform/Facility
JASLab	Attosecond HHG Imaging Spectroscopy	University of Ottawa (NRC Canada)	Physics Chemistry	None	–	https://www.attoscience.ca	Platform
JLF	High energy lasers Laser plasma acceleration	Lawrence Livermore National Laboratory	Physics	~100%	LaserNet US	https://jlf.llnl.gov	Facility
KLS	Ultrafast dynamics HHG Attosecond	Kansas State University	Physics Engineering Academic/teaching	Partial, ~10%	–	https://jrm.phys.ksu.edu/lasers.html	Platform/Facility
Lasir	Ultrafast dynamics Spectroscopy Imaging Microscopy	University of British Columbia Simon Fraser University	Chemistry Physics Life sciences Engineering	Partial, ~10%	–	https://lasir.ca	Platform/Facility
MEC	High energy lasers Warm dense matter	LCLS/SLAC	Physics	~100%	LaserNetUS	https://lcls.slac.stanford.edu/instruments/mec	Facility

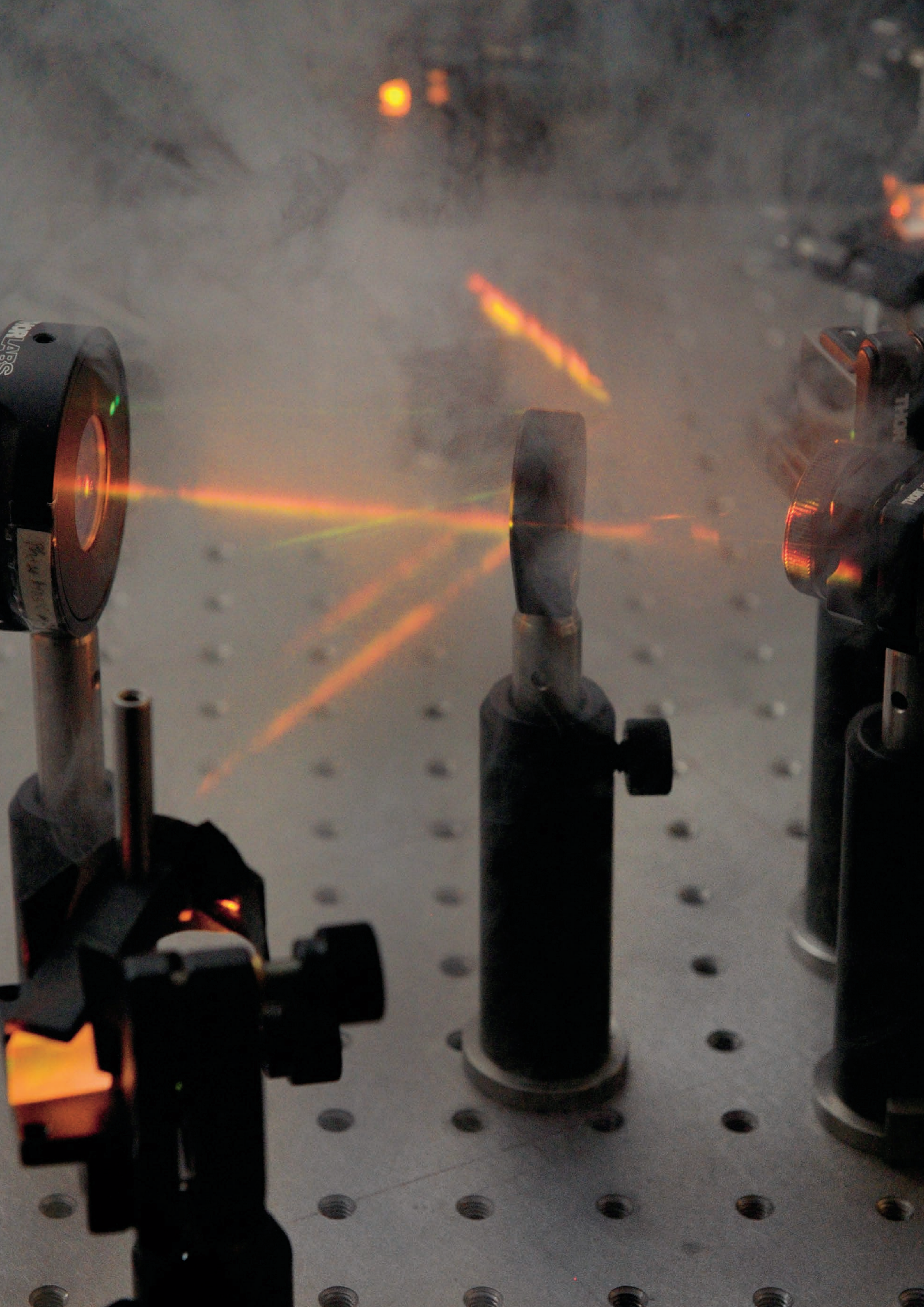
NeXUS	Attosecond XUV, soft X-rays Ultrafast dynamics ARPES STM	Ohio State University	Physics Chemistry	100%	–	https://nsf-nexus.osu.edu	Facility
OMEGA EP	High energy lasers	University of Rochester	Physics Material science Laser technology	100%	LaserNetUS	https://www.lle.rochester.edu/index.php/omega-laser-facility-2	Facility
Scarlet Laser Facility	High power lasers	Ohio State University	Physics Engineering	Partial, ~50%	LaserNetUS	https://hedp.osu.edu/facilities/scarlet	Platform/Facility
Texas Petawatt Laser	High energy lasers Particle acceleration HHG Warm dense matter	University of Texas at Austin	Physics Engineering	Partial, >70%	LaserNetUS	http://texaspetawatt.ph.utexas.edu	Platform/Facility
UFL @ ASU Core facility	Ultrafast dynamics Spectroscopy Imaging Microscopy	Arizona State University	Chemistry Physics Biology Material Science	Partial, <10% (other universities and industry)	–	https://cores.research.asu.edu/ultrafast-laser-facility/about	Partial/Facility

ASIA AND AUSTRALIA

Name	Technical focus	Institutions involved	Scientific fields	Outside user involvement (%)	Part of a network?	Website	Type
Australian Attosecond Science Facility	Attosecond Quantum photonics	Griffith University	Physics Quantum biophysics	–	–	https://www.griffith.edu.au/centre-quantum-dynamics/our-centre	Platform
CASTECH	Attosecond Imaging Spectroscopy	POSTECH Max Planck Institute (MPC-AS)	Chemistry Physics Nanotechnology Laser science	–	–	http://lsl.postech.ac.kr	Platform
Institute of Physics	High energy lasers Attosecond	Chinese Academy of Sciences, Beijing	Laser technology	Partial	–	http://ultralaser.iphy.ac.cn	Platform/Facility
Laser and Synchrotron Research Center	Spectroscopy Imaging Microscopy Ultrafast lasers	The University of Tokyo	Physics	–	–	http://www.issp.u-tokyo.ac.jp/maincontents/organization/lasor_en.html	Platform

List of Abbreviations

SSPh	Swiss Society for Photon Science
SLS	Swiss Light Source
SwissFEL	Swiss Free Electron Laser
ESRF	European Synchrotron Radiation Facility
EU-XFEL	European X-ray Free Electron Laser
XFEL	X-ray Free Electron Laser
CHART	Swiss Accelerator Research and Technology
NCCR	National Centers of Competence in Research
ETH Zurich	Eidgenössische Technische Hochschule Zürich
EPFL	École polytechnique fédérale de Lausanne
EMPA	Eidgenössische Materialprüfungs- und Forschungsanstalt
PSI	Paul Scherrer Institute
SNBL	Swiss Norwegian Beam Line
CERN	Conseil Européen pour la Recherche Nucléaire
DOI	Data Object Identifier
FAIR	Findable, Accessible, Interoperable and Reusable
ELI	Extreme Light Infrastructure
SME	Small and Medium Sized enterprises
ERC	European Research Council
LEAPS	League of European Accelerator-Based Photon Sources
CALIPSOplus	Convenient Access to Light Sources Open to Innovation, Science and to the World
ExPaNDs	European Open Science Cloud Photon and Neutron Data Services
SNSF	Swiss National Science Foundation
BFI	Botschaft zur Förderung von Bildung, Forschung und Innovation
SOLEIL	Optimized Light Source of Intermediate Energy to LURE (France)
LURE	Laboratoire d'Utilisation du Rayonnement Électromagnétique (France)
SPring-8	Super Photon ring-8 GeV (Japan)
APS	Advanced Photon Source (US)
PETRA	Positron-Elektron-Tandem-Ring-Anlage (Germany)
BESSY	Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung (Germany)
HZB	Helmholtz Zentrum Berlin (Germany)
ELETTRA	Sincrotrone Trieste (Italy)
ALBA	Third-generation synchrotron light source facility located in Barcelona (Spain)
SFA	Strategic Focus Area
PHRT	Personalized Health and Related Technologies
AM	Advanced Manufacturing
SLM	Selective Laser Melting
MAX	Swedish Synchrotron Facility (Sweden)
HEPS	High Energy Photon Source (China)
RIXS	Resonant Inelastic X-ray Scattering
cryo-EM	Cryo-Electron Microscopy
NMR	Nuclear Magnetic Resonance
STM	Scanning Tunneling Microscopy
TEM	Transmission Electron Microscopy
SASE	Self-Amplified Spontaneous Emission
CHIC	Interleaved Delay Chicanes
LCLS	Linac Coherent Light Source (US)
CDI	Coherent Diffraction Imaging
XMPI	X-ray multi-projection imaging
XPDC	X-ray Parametric Down Conversion
FLASH	XUV and soft X-ray free-electron laser (Germany)
FERMI	Free Electron Laser Radiation for Multidisciplinary Investigations (Italy)
FELBE	Free Electron Laser at the Forschungszentrum Rossendorf (Germany)
SACLA	Japanese Free Electron Laser
PAL	Pohang Accelerator Laboratory (host of South Korean Free Electron Laser)
POLFEL	Polish Free Electron Laser
TARLA	Turkish Free Electron Laser
LUNEX	French Free Electron Laser
UK XFEL	British Free Electron Laser
CLARA	British Free Electron Laser
SPARC	Italian Free Electron Laser
PI	Principal Investigator
LACUS	Lausanne Center for Ultrafast Science
UZH	University of Zurich
UNIFR	University of Fribourg
FHI	Fritz Haber Institute
ARPES	Angle-resolved Photoemission Spectroscopy
FLUPS	Fluorescence Upconversion Spectroscopy
NSERC	National Science and Engineering Research Canada
DOE	Department of Energy
LOA	Laboratoire d'Optique Appliquée
CELIA	Centre Lasers Intenses et Applications
RAL	Rutherford Appleton Laboratories



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