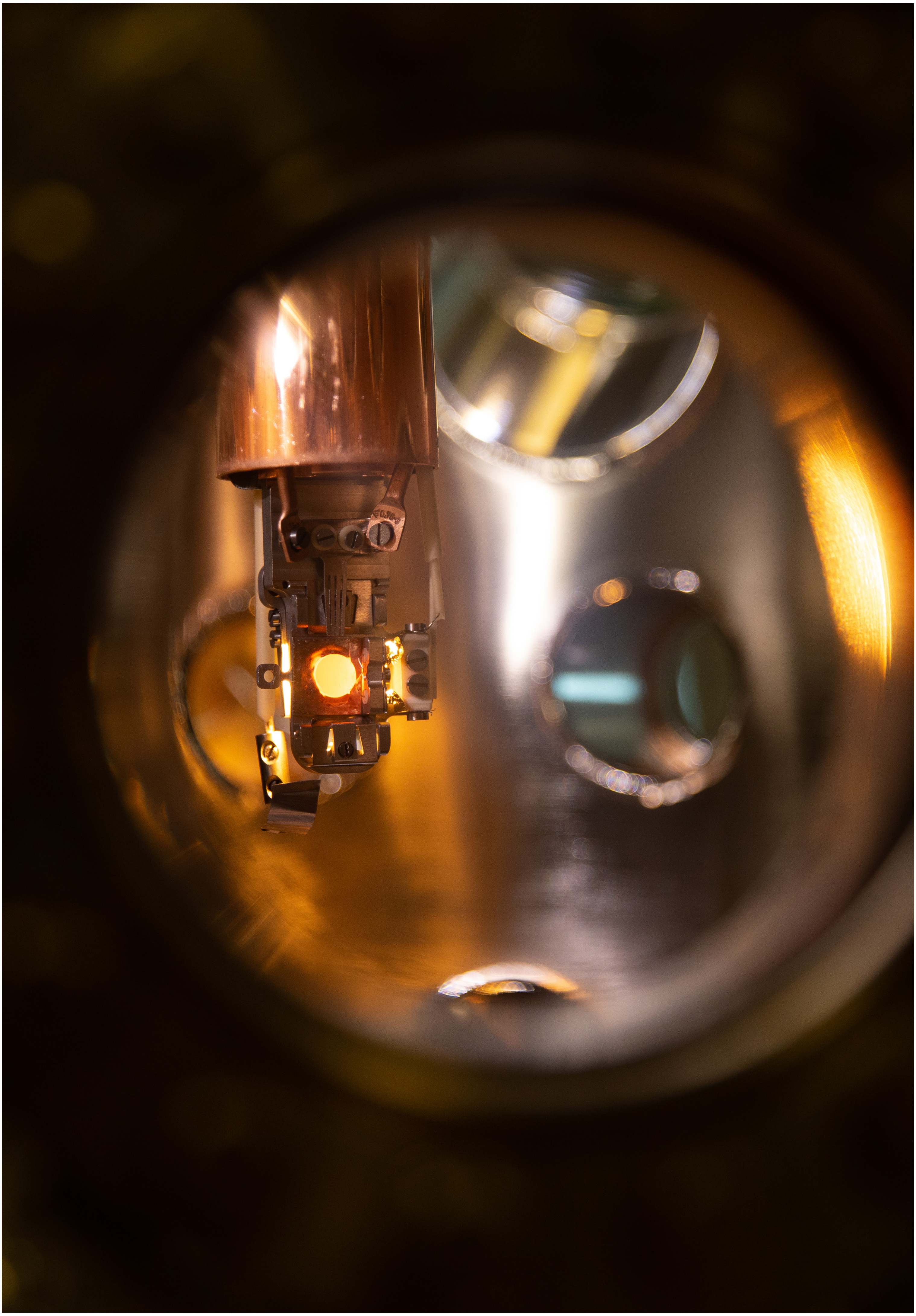
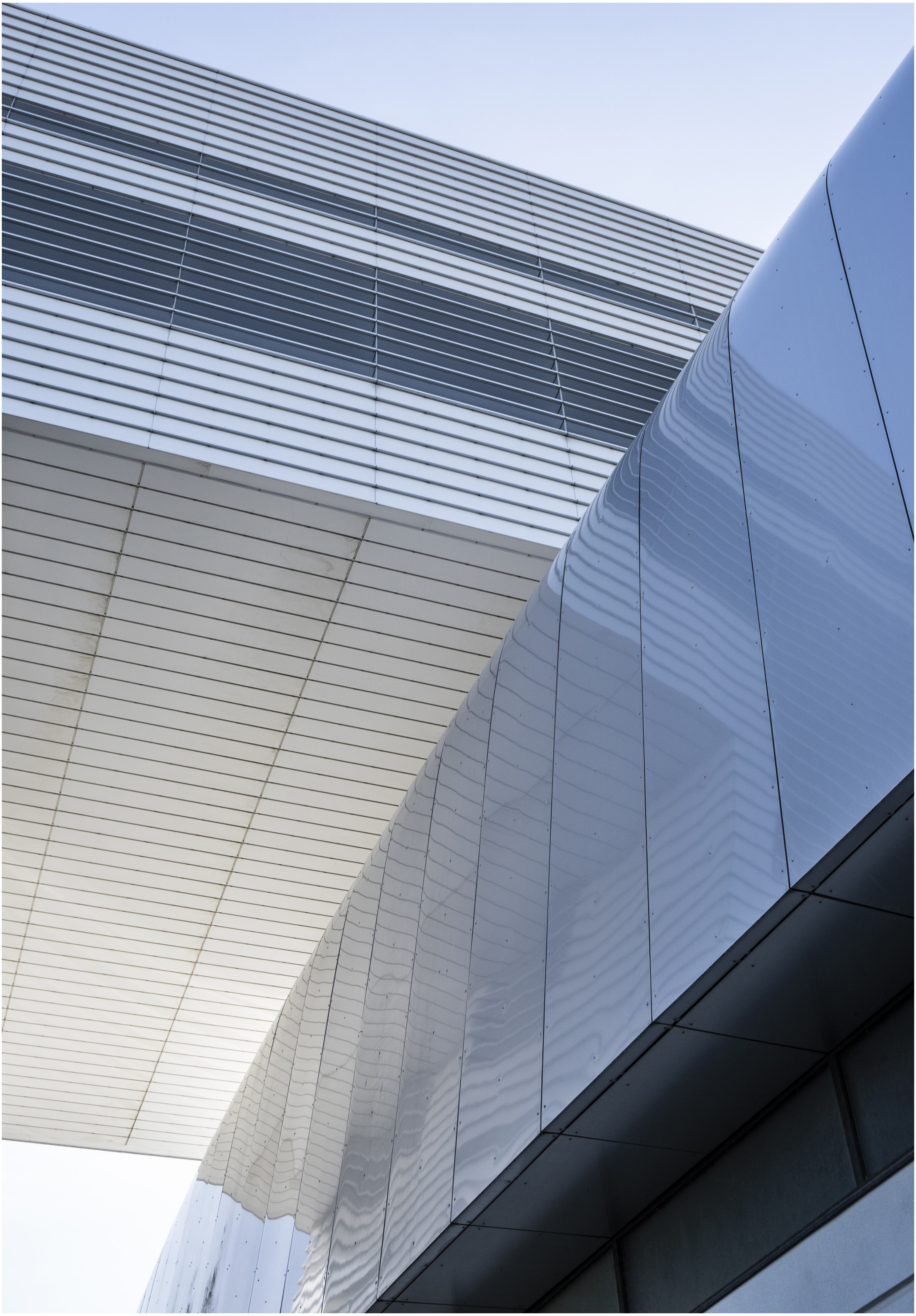
MAX IV
STRATEGIC PLAN
2023–2032



A leading synchrotron
enabling world-class science
for a better future



The mission of MAX IV is to develop and operate world-class accelerator-based light sources, synchrotron beamlines, and related tools for the Swedish as well as the international research communities for science at the highest level of excellence.

We serve academic and industrial communities conducting research and develop methods and techniques in collaboration with them.


Tillträde möjligt
Access possible
Område avsökt
Area searched
Strålnings-fara
Radiation hazard
Laser-fara
Laser hazard
NÖDUPPLÅSNING DÖRR
EMERGENCY DOOR RELEASE

Objectives

An overall goal for MAX IV is to actively target areas resonant with the priorities of the Nordic scientific community and industry, such as developing energy materials and technologies, boosting life and biomedical sciences, and solving environmental challenges. MAX IV also continues and increases its contribution to scientific breakthroughs, targeting quantum materials and device technologies, atomic molecular and optical science, and being a premier and versatile tool to explore new scientific frontiers.

In the next decade, MAX IV aims to operate a minimum of 20 beamlines and to champion our position as the premier light source for Nordic and Baltic users. This will be achieved by devoting ourselves to a steadily growing community, engaging present and new users in the process of developing our scientific program and improving the user experience. Our ambition is to increase the number of users by at least 10% every year beyond 2025. A new open access mode for industry should represent 5% of our total beamtime-related activities.

MAX IV will work in close relationship with user communities, stakeholders, and funders, to significantly expand and upgrade our capabilities, our suite of beamlines and our offering through open calls and proprietary access. By working with researchers and important gateway environments, we will empower these to assume more significant responsibility and contribution to the realisation and operation of beamlines.

This collaborative approach enables us, through our roadmap process, to maintain a prioritised list of beamlines to add to our portfolio of capabilities and ensures that we continue to develop our accelerators and address scientific problems central to the United Nations (UN) sustainable development goals.

Our ambition is to go into the future with the 1.5 GeV ring further developed and a few empty straight sections on the 3 GeV ring. We will have a validated design of a major upgrade of the 3 GeV ring aiming at the diffraction limit for 10 keV photons. The enabling accelerator technologies to reach that goal will be in hand. MAX IV and its suite of beamlines should be fully ready to capitalise on this new leap of ultimate brilliance.

The achievements during the next decade will rest on the pillars of optimised science and operation. The high-level Roadmap for developments of optimised science is to achieve

- **Reliable, continuously upgraded, improved and internationally competitive accelerators** with world-leading X-ray brightness and access to ultrafast X-ray pulses, taking advantage of the superior line shape of the energy spectrum of our undulators.
- **Advances in our 2D and 3D soft and hard X-ray imaging capabilities** to the time-resolved realm by exploiting our abilities to generate micron and submicron probes and utilising the unique coherence properties of our X-ray beams.
- **A unique platform for spectroscopies** that fully exploit the brightness from THz to several keV, offering transformational opportunities to probe in-situ and operando surfaces and interfaces.
- **A platform for determining the structure of matter down to atomic length scales** for materials, chemical and life sciences.
- **Opportunities in the form of at least one flagship beamline that will fully exploit the unique coherence properties of the 3 GeV storage ring** for understanding the structure and dynamics of complex systems with X-ray speckle techniques.
- **Strong in-situ and operando science programs** for many research areas, exploiting our ability to generate small, collimated, and intense beams instrumental in measuring time-resolved scattering and diffraction signals of small samples and heterogeneous, imperfect, soft, or weakly scattering matter.

The high-level Roadmap to achieve optimised operation focuses on

- **Optimised user experience** with modern platforms and infrastructures supporting all aspects of our proposals' lifecycle, with steadily increasing user satisfaction.
- **Transitioning from experiments to measurements** to maximise scientific and industrial impact, while adhering to FAIR principles and Open Science.
- **Proactive investment in maintaining our portfolio of beamlines** at state of the art in terms of undulators, optical components, sample environments, X-ray and electron detectors, controls, data reduction, analysis and visualisation tools, and optimising experience with AI-guided and AI-automated experiments.
- **Continued facilitation of opportunities for multimodal and integrative approaches** using multiple X-ray techniques and actively engaging with other methods and supporting infrastructures nationally, especially the ESS and SciLifeLab.
- **Active partnership in national and international scientific projects, training, and outreach activities,** providing an environment that, with the universities, promotes the education and professional training of the next generation of scientists across the nation and beyond. At least 20% of MAX IV personnel should be adjoined to an academic environment.
- **Working practises and organisation of activities that supports world-leading science** and enables MAX IV to achieve our overall vision and mission.

Introduction

MAX IV is committed to supporting and advancing Swedish and international academic and industrial research, especially that which has a societal benefit and leads to a more sustainable future, in concert with the United Nations Sustainable Development Goals (UN SDGs). In collaboration with the Swedish universities, MAX IV also is committed to supporting training and – together with universities – education of the next generation of scientists.

With this document, we set the strategic path for enabling these communities to produce world-leading science with MAX IV and ensure we stay at the scientific forefront. We are extremely grateful to the entire community, especially to the Swedish Universities, and to the funding bodies, governmental, university and private, that have contributed to MAX IV and are invested in its future. We look forward to working closely together as we mobilise for the coming decade.

First of a kind

MAX IV Laboratory is a Swedish national research infrastructure that hosts the world's first 4th generation storage ring. Hosted by Lund University (LU), MAX IV was inaugurated in June 2016 and builds on more than three decades of successful multidisciplinary research at MAX-lab (MAX I-III, 1982–2015)

Our accelerators consist of a 3 GeV storage ring, a 1.5 GeV storage ring, and a 3 GeV linac that serves as a full-energy injector to the rings and as the source for a Short Pulse Facility (SPF). The 3 GeV ring is based on a novel multi-bend achromat (MBA) lattice pioneered by Professor Mikael Eriksson, providing world-leading emittance (0.3 nm rad) in a relatively short circumference of 528 m. This concept has set a standard being emulated all over the world.

A key strategy of the MAX IV design is to focus each accelerator on a specific range of user community needs. The 3 GeV ring is optimised to provide high-brightness, hard X-rays with energy up to a few tens of keV, whereas the 1.5 GeV ring with 96 m circumference, is optimised to meet the needs for softer radiation up to a few keV. While the electron bunches in the rings are made as long as possible to allow reaching the highest transverse brightness, the linear accelerator is equipped with magnetic compressors providing ultrashort electron bunches (<100 fs) which then generate ultrafast X-ray pulses by spontaneous emission. With its high-brightness photocathode gun, the linac is also prepared to drive free-electron lasers. In addition to their low emittance, our accelerators are characterised by highly stable and reliable operation, a 10 Hz repetition rate of the linac, and transparent top-up injection in the rings.

The capabilities of our sixteen beamlines currently available to users can be found at ***https://www.maxiv.lu.se/user-access/find-your-beamline/***.

The user community accesses these beamlines through peer-reviewed applications based on scientific merit and feasibility through a fee-based system based on feasibility and interest. Access is free of charge for users that publish their results in the open literature. Users that wish to keep their results proprietary, typically coming from industry, pay for time used at a cost-recovery rate. Currently about 1000 users per year visit the lab. That number is expected to double in the next few years as more beamline capabilities open to users and MAX IV's attractiveness for excellent science grows.

Financing

The operating costs for 2014–2018 were covered by a joint funding decision from the Swedish Research Council (VR) and LU, with investments in beamlines by the Knut and Alice Wallenberg Foundation (KAW). A second

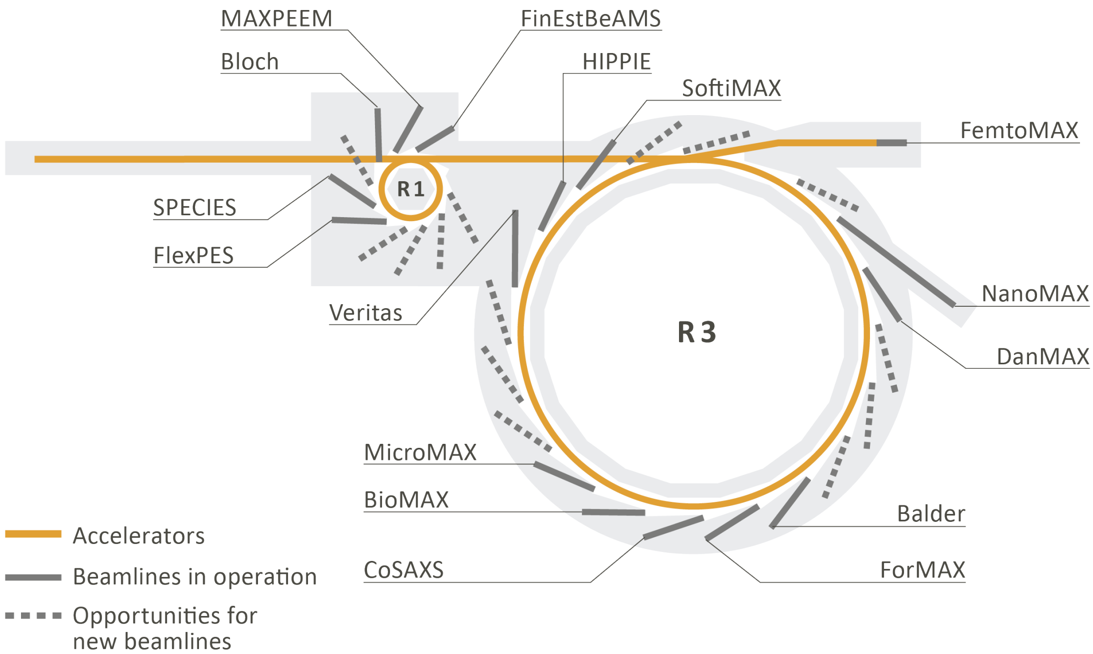


Figure 1: The Linear Accelerator, the 1,5 GeV ring (R1), the 3 GeV ring (R3) of MAX IV Laboratory, and the 16 beamlines in operation spring 2023. Dashed lines indicate sectors available for new beamlines.

funding decision is now in effect, with operating costs and investments in beamlines now principally covered by VR, 14 Swedish universities [1], KAW, the Swedish Innovation Agency (Vinnova), The Council for Sustainable Development (Formas), Energimyndigheten, the Treesearch consortium, the Novo Nordisk Foundation (NNF) in Denmark, The Danish government and three Danish universities [2], and the Academies of Finland and Estonia, among others. From 2021 onwards, the operating cost has increased gradually, reflecting in part the increasing number of beamlines going into operation, but also an increase in overall cost levels. Appendix 2 summarises foreign funding of MAX IV projects and operations.

International context

MAX IV has led the world in the development of a synchrotron with 100-fold greater brightness in the soft to hard X-ray region of the spectrum compared to the previous generation. The European Synchrotron Radiation Facility's Extreme Brilliant Source (EBS) in France and the Sirius source at the Brazilian Synchrotron Light Laboratory were the first to follow the MAX IV track and implement variants of the multibend achromat lattice, and many more are on their way (Fig 2). MAX IV has a unique opportunity to excel in areas of science complementary to those addressed by other synchrotron facilities, and to exploit its exceptional source brightness and coherence, especially while newer 4th-generation facilities are still being built.

Our 16 beamlines in operation from 2023 are in many aspects unique and world-class. This is attributable to the outstanding accelerators at MAX IV, which, for example, enable the best opportunities globally for high-resolution RIXS, nanoprobe beamlines (both for materials and life sciences), serial crystallography, and ARPES. We are currently working towards fuller exploitation of the potential of the coherence of our X-rays by, for example, implementing tomographic imaging.

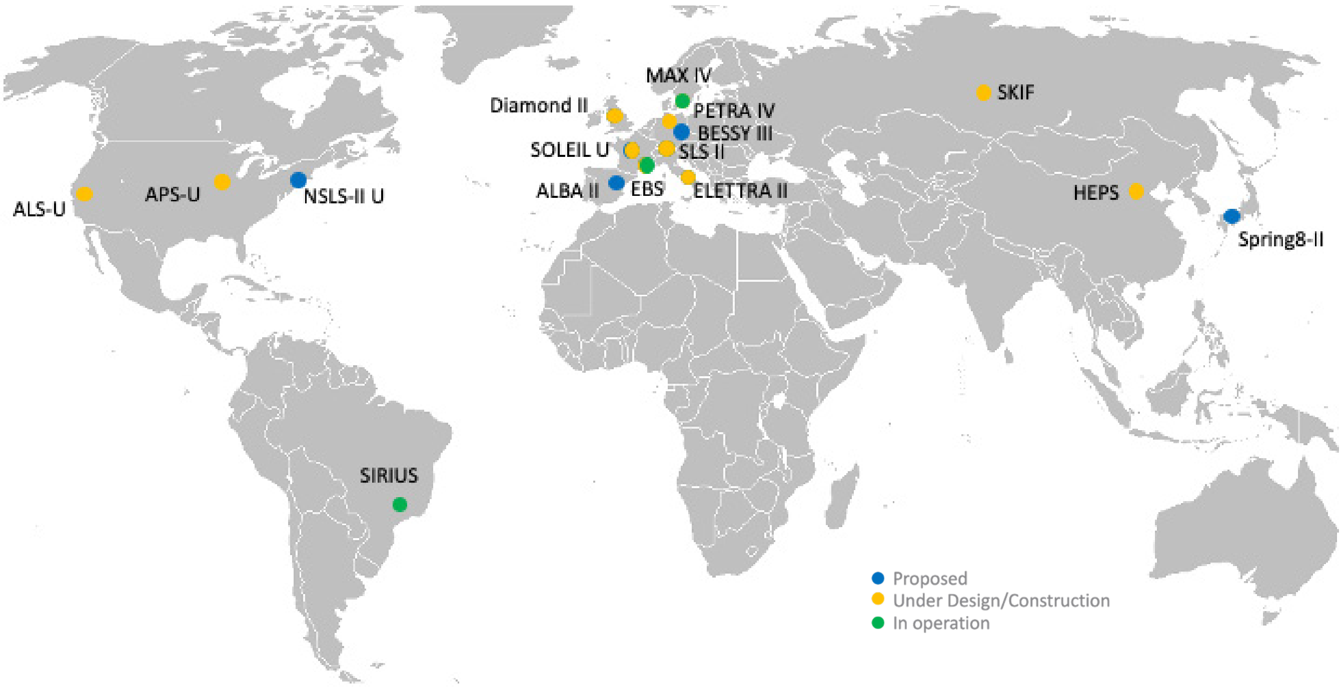


Figure 2: Fourth-generation storage rings using variants of the MBA lattice proposed, under design/construction and in operation around the world in 2023.

MAX IV and its relation to other large infrastructures in Sweden

Sweden has made significant investments in the large-scale research infrastructures that complement and/or advance the usefulness of MAX IV. With, for example, SciLifeLab and the European Spallation Source (ESS) currently under construction in Lund, Sweden is in an outstanding position for research and development. To further increase the impact of these investments, the synergetic opportunities of the facilities need to be fully utilised.

The potential of the colocation of ESS and MAX IV in the Brunnshög area of Lund should be exploited. Scientific complementarity is well documented, and it is in the interest of both facilities that this is realised as opportunities for users. This can be enabled by coordinated experimentation, streamlining of safety processes, common access to sample preparation laboratories and data transfer, analysis, and storage capabilities allowing analysis of X-ray and neutron-based results with similar tools and on a joint platform. Despite differences in the accelerators (superconducting linear proton accelerator at ESS and normal-conducting linear and circular electron accelerators at MAX IV) and neutron vs X-ray instruments, accelerator science and instrumentation development areas of common interest should be identified – these could include underlying cross-cutting techniques such as ultrahigh vacuum, precision mechanics and data acquisition systems.

Similarly, synergies between MAX IV and SciLifeLab regarding, for example, structural biology and bio-imaging need to be exploited. This will require the full support of integrative methods and collaboration on data processing, storage, and analysis.

In addition to scientific complementarity between the infrastructures, there is great potential to explore further synergies regarding user interactions, for example, developing and sharing best practices in managing user projects and data, industrial access, exploring opportunities together in the broad science community, training and education programs and more. The VR financed InfraLife project serves as a common hub between the infrastructures to address these opportunities within the life science area. MAX IV will work for the creation of a permanent platform inspired by InfraLife with a widened scope to coordinate these efforts for the facilities. The coordination and governance of the platform should be close to the facilities' user support organisations.

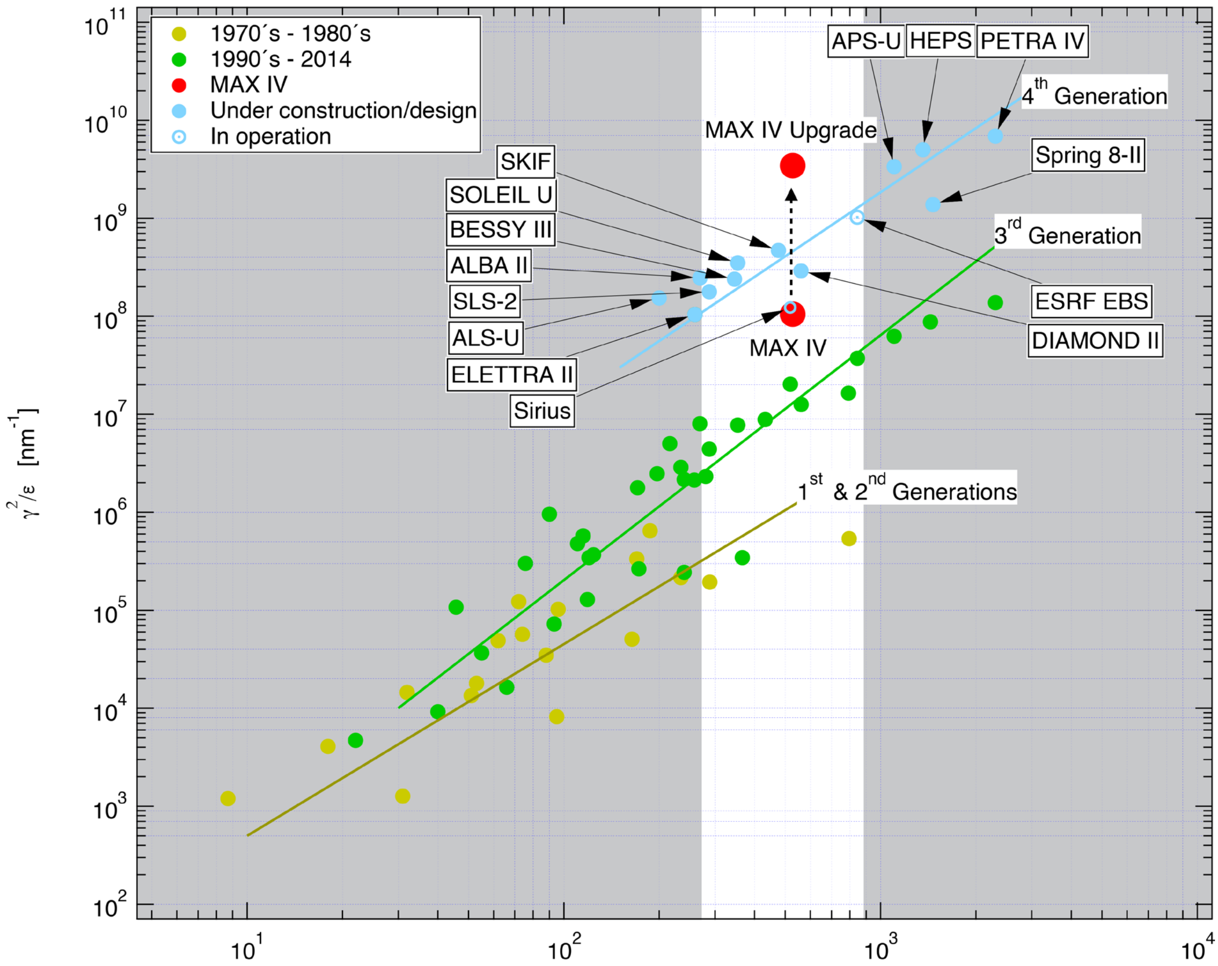


Figure 3: Storage ring performance (defined as the inverse electron beam emittance scaled by the square of electron beam energy) vs circumference for major light sources and generations. The electron beam energy range defines the range of photon energies that can be produced: higher electron energies favour the production of higher energy photons. The larger the circumference, the smaller the emittance and correspondingly the higher the brightness and coherence that can be achieved. The light band comprises the facilities comparable in size to the MAX IV 3 GeV ring. The vertical upward arrow indicates a path with planned upgrades over the next 20 years. These upgrades will allow MAX IV to maintain the edge of the MAX IV 3 GeV ring.

[1] Karlstad University, University of Gothenburg, Karolinska Institutet, KTH Royal Institute of Technology, Karlstad University, Linköping University, Linnæus University, Luleå University of Technology, Lund University, Malmö University, Swedish University of Agricultural Sciences, Stockholm University, Umeå University, and Uppsala University

[2] Aarhus University, University of Copenhagen, and Technical University of Denmark

User Interaction

High-level user support and influence

MAX IV has always engaged present and new users in the process of developing our scientific program and instrumentation. In continuously doing so, as well as improving the conditions under which users do science at MAX IV, we expect the number of users to continue to increase (at least by 10% per year after 2025), and more importantly, the scientific output (for example, measured by publications) of the facility to grow in numbers and quality. With MAX IV providing accelerators and beamlines that create a foundation, it is the users that stand for the scientific output.

Users are engaged in the development of the facility at both governing and operational levels. The user community is represented in most steering and advisory bodies, including the Board, URG (University Reference Group), SAC (Scientific Advisory Panel), and PAC (Program Advisory Panel, which reviews beamtime proposals). MAX IV interacts with user organisations, most notably FASM (The MAX IV Users Association), SSUO (Swedish Synchrotron Users Organisation), and ESUO (European Synchrotron Users Organisation). Users are involved in the regular reviews, commissioned by the SAC, of beamlines in operation. In the operational phase, the user community is involved in developing scientific cases for new instruments, arranging funding, and participating in build-up and operation. This can be adding capabilities to a beamline by, for example, contributing to a new sample environment or detector or developing software for analysis. This can also mean driving and supporting a full beamline project. The current Roadmap process is continuing this user involvement which is fundamental to the continued development of MAX IV.

Supporting users at MAX IV is our priority and translates into many things ranging from developing supportive procedures to providing efficient logistic support for user beamtimes to technical developments. It is an integral part of the strategic development of the facility, and the needs are often specific to certain communities or beamlines, for example, making special sample environments available or developing data analysis tools. Through interaction with beamlines and feedback from users through experimental reports, as well as feedback from SAC and PAC, MAX IV is constantly developing and adjusting these developments.

Increasing user involvement and user access is the main goal of these activities and is specifically supported by developing access modes. Fast access, sample tests, and standard measurement schemes, which are already in place for most beamlines and aim to lower the threshold for new users and emerging science to come to MAX IV. Research addressing global challenges can get access to mission-driven collaborations with EU funding. Currently schemes for circular economy and nanoscience are in place, and upcoming themes include energy materials and health-related topics. The next step in developing user access modes includes long-term proposals that would allow for increased joint developments between MAX IV and user groups. Multimodal access allowing the combination of different methods for one research project, including multi-beamline BAGs (block allocations), will help develop user-driven science and contribute to more efficient use of beamtime.

Training and Education

Graduate or undergraduate education is provided by the universities. MAX IV supports these activities, and, where possible and reasonable, promotes them among its network of users. Support can be by supplying material – for example, e-resources – or guest lecturers, and providing hands-on sessions. This is organised through regular Training and Educa-


Elektronenanordnung der 3 äußeren Schalen (vereinfacht):

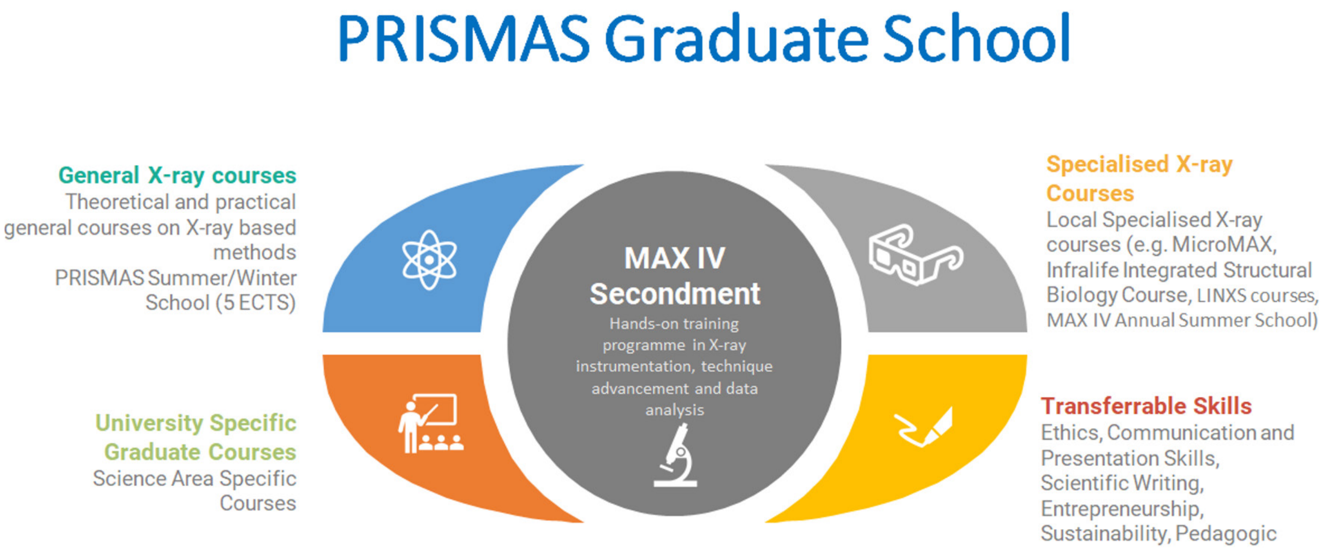


Figure 4: PRISMAS builds an education and training ecosystem in cooperation between universities, MAX IV and other partners.

tion calls and offers access to up to 2% of the total available beamtime for users.

MAX IV, on the other hand, does provide specialised training in specific aspects of synchrotron methods, as well as general introductions of synchrotron methods to a wider academic audience, irrespective of career level, for example, through its summer school program. These are often carried out in collaboration with university researchers, who, in most cases, have extensive knowledge about, and already act as promoters for MAX IV. MAX IV would like to ensure the integration of staff into the academic environment, including the supervision of PhDs and other students at advanced levels.

Finally, the same principles always include non-academic researchers using, or intending to use MAX IV. The latter, for example, from industry R&D or research institutes, however, often have distinctly different training needs that must be addressed accordingly.

PRISMAS, an MCSA Cofund program for 40 joint PhD fellows coordinated by MAX IV, provides a recent successful example of how MAX IV in collaboration with nine partner universities and some 20 affiliated partners from academia and industry, implements its training and education strategy. PRISMAS ensures knowledge and competence transfer from MAX IV to the partner universities, and vice versa, promoting a new generation of synchrotron scientists by providing training and career development, including networking and mobility.

Following the PRISMAS project, MAX IV aims to continue and improve its education program as outlined above, within the available funding frame.

Internationalisation and networks

Geographically, MAX IV is the X-ray user facility of choice for the northern European user community – for countries of the Nordic and Baltic regions. Today, users from the Nordic and Baltic areas including Sweden stand for more than 75% of beamtime proposals. They also contribute to the development and success of the Laboratory with expertise, support, and direct funding.

Relying on strong and long-term collaborations with neighbouring countries [1], MAX IV aims to expand further such interactions to other countries such as Norway, Poland, and the Baltic states to solidify its status as the

Northern European Synchrotron. Such efforts will help MAX IV to unfold its potential and offer partners the possibility to develop their research programs using world-leading X-ray beamlines.

In the slightly larger region, including Northern Germany, four unique research facilities [2] are in relative proximity, with only partly explored potential for scientific, technical, and innovative synergies. EU Interregional projects [3] have already contributed to the strengthening of the interactions between stakeholders in this region. MAX IV is continuously engaged in widening these efforts, according to its needs and in line with Lund University's strategy [4].

MAX IV is an active member of networks bringing together research infrastructures from all over Europe [5], aiming to improve services offered to the user community and to jointly develop large projects on a European level to address societal challenges [6].

These activities always contribute to collaborations with the Swedish user community, as well as existing collaborations on a national level, including the ecosystem at Science Village in Lund. MAX IV seeks to bring the strength of its user community into its international collaboration, mutually offering its users widened access and opportunities, for example, through EU funded projects.

[1] Estonia, Finland and Denmark contributed to construction and operation of FinEstBeAMS, DanMAX and MicroMAX beamlines.

[2] MAX IV, ESS, DESY (hosting Petra III and European XFEL) and Helmholtz-Zentrum Berlin (HZB)

[3] E.g. https://www.halos.lu.se/

[4] https://www.lunduniversity.lu.se/sites/www.lunduniversity.lu.se/files/2021-05/action-plan-for-internationalisation-at-lund-university-2019-2021.pdf

[5] https://leaps-initiative.eu/; https://arie-eu.org/

[6] E.g. https://inext-discovery.eu/, https://nffa.eu/, https://www.leaps-innov.eu/, http://www.calipsoplus.eu/, ect.

Goals in Training and Education

- Support and promote education offerings provided by universities
- Provide specialised training and general introduction of synchrotron methods
- Initiate and coordinate targeted programs such as PRISMAS

Goals for MAX IV's internationalisation and networking

- Expand the existing strong and long-term collaborations in the Nordic and Baltic region
- Continue active participation in European – EU-funded – partnerships
- Include national and local partners in all internationalisation efforts

MAX IV as an enabling organisation

To achieve our mission and scientific objectives, our way of working and organising our activities must match and be excellent. This is one of the key enabling factors for supporting world-class science.

Our ambition is to continue to be on the frontline and, in the future, be able to offer a competitive edge to our users in comparison to other facilities. We are, as an organisation moving into a phase in which we should enable both excellent science but also need to have efficient maintenance and operations in place. This means good support in the user interface but also good support in all aspects important for the smooth operation of MAX IV. Since resources and key competencies are scarce, this means that in parallel, we also need to keep developing the processes and procedures, enabling our operational excellence.

We are striving to achieve

- **An attractive workplace** where we can attract the best scientists, researchers, engineers, and other key personnel and also retain them.
- **Structured working practices,** with clear roles, responsibilities, and processes where we support each other with a collaborative approach and cross-functional way of working.
- **An internal project portfolio which implements our Roadmap,** according to its strategic direction and based on clear prioritisations.
- **A good understanding of our users' needs** both in the near future and also in the longer term, that is, their strategic needs and direction in conjunction with our own, why decisions are taken and what their purpose is.
- **A move into operational excellence** resting on the pillars of user interface support, technical support, and operational support.
- **An efficient use of resources, key competences,** and a programme management approach to our internal project portfolio.
- **A governance structure and leadership that supports our development** into an enabling organisation, while considering a holistic view where decisions are taken from a "best for MAX IV" viewpoint.

MAX IV and Industry

Industry strategy

MAX IV, as a multifaceted research facility at the international cutting edge of technology, is attractive to the private sector for the same reasons that it is to academia. With the world-class tools available at MAX IV, industry can look deep inside the unknown, the "black boxes" crucial to their research and development programs, at an unprecedented level of detail, enabling radical improvements to their materials and processes. These tools give an internationally competitive edge to deliver more attractive and sustainable products leading to increased business revenue.

Today ten out of our 16 beamlines at MAX IV are used by industry. About 2% of the beamtime available to all users is used for experiments through a proprietary access channel, and about 20% is used through collaborative open access with academia. Most beamlines are designed to be versatile, with the potential to impact a broad range of industrial sectors. As MAX IV is still in an early phase of operation, industry has a clear opportunity to participate in and impact MAX IV's future development. MAX IV has an important role in developing national policy relating to industry and in the technology development arena. MAX IV works together with the Swedish Research Council (VR), Vinnova, RISE, and other agencies, including the ESS-MAX IV Joint Office, coordinating industry-relevant initiatives to exploit MAX IV capabilities.

The Industry Relations Office (IRO) focuses on attracting industrial users to MAX IV and encouraging the development of industrial communities, particularly in sectors important to Swedish industries but also to international ones where substantial impact can be made in contributing to the global SDGs. Engaging international industrial users will enhance Sweden's international stature as well as cross-fertilise and strengthen Swedish industry.

The most engaged industrial users of MAX IV today are in the pharmaceutical industry and the paper and pulp industries. By 2030 we expect to have significantly strengthened R&D in these sectors and to have made a significant impact on others such as food and packaging, metals and engineering, life science and MedTech, catalysis and chemical processing, mining, recycling, textiles, automotive and aerospace, and batteries and energy materials sectors. It is a priority for MAX IV to establish an Industry Reference Group (IRG). This will be even more important in view of new access modes, such as a specific call for industrially relevant experiments.

Ambition and strategic goals in relation to industry

The MAX IV strategy toward industry aims to develop industrial research at MAX IV in these sectors, enabling industrial users to reach their SDGs, through the following four ambitions and twelve goals:

1. Broaden the industrial user base of MAX IV

- **Make the relevant industry sectors** across the Nordic and Baltic regions and the rest of Europe fully aware of the research opportunities at MAX IV.
- **Engage the ten most important industry sectors in Sweden** with various initiatives connected to the use of MAX IV.

2. Increase the industrial use of MAX IV

- **Achieve an average of 5% per year of the user beamtime at MAX IV fully proprietary use.** The proprietary fraction will be significantly higher on some beamlines.
- **Allocate up to 5% of the user beamtime at MAX IV to a new open access mode for industry.**
- **Aim to double today's industrial use of MAX IV in collaboration with academia** or other non-industrial institutes through the general user access mode. This will require strategic collaboration and involvement from the Swedish Ministry of Enterprise and Innovation and other national actors.
- **Continuously increase Swedish industry competence in the use of MAX IV** from the basic awareness level to the advanced industrial user level.
- **Increase MAX IV staffing supporting industry by growing organically** in proportion to income, prioritising additional beamline staff and IRO support.
- **Support industrial use of MAX IV from experimental design to data interpretation** through a full range of services tailored to industry needs.

3. Develop MAX IV to support industrial needs

- **Directly involve industry in the development of sample environments** to increase the research capabilities of MAX IV towards industrial use.
- **Incorporate industrial involvement in the planning and funding of new beamline projects** throughout the development of MAX IV.

4. Employ a collaborative approach to industry engagement

- **MAX IV aims to have a strong partnership with ESS on all relevant industry activities,** particularly connected to outreach, education, and strengthening the ecosystem of surrounding stakeholders.
- **MAX IV achieves these ambitions through collaborations on a broad level** with industry, academia, institutes, financing bodies, and other organisations to deliver on industry goals.

Transformative Science

Life and biomedical science

Life and biomedical sciences are one of the most prominent research areas in the Nordic and Baltic regions. There are many well-known world-leading environments for medical research, such as Karolinska Institutet (Sweden), Rikshospitalet (Denmark) and the Oslo Cancer Cluster (Norway). There are also many relevant centres and platforms, e.g., SciLifeLab in Sweden, Biocenter in Finland, and the NNF Centre for protein research in Denmark. All major universities also have substantial research in structural biology. The brightness of MAX IV is particularly attractive for life-science applications; for instance, the flux of our beamlines makes the application of high-throughput crystallography particularly advantageous. Therefore, drug target screening – which was hitherto mainly achieved using biophysical methods – can now be performed with several hundreds of compounds at highly automated beamlines such as BioMAX. This way of screening gives the additional benefit of supplying structural information simultaneously with a confirmed interaction.

The FragMAX fragment screening platform at BioMAX is already used by industry (e.g., Saromics Biostructures, Sprint Biosciences and AstraZeneca) and academia for drug-discovery projects. Prediction of protein folding using artificial intelligence methods through AlphaFold, combined with other breakthroughs, is rapidly changing how integrative structural biology is developing and bridging the gap from the molecular level toward cellular and tissue biology. These fields benefit from multiscale information, as provided by X-ray imaging and microscopy.

These methods, in turn, benefit from the unique properties of our light sources. Spectral as well as spatial Information at the sub-cellular level can be obtained by combining spectroscopy as well as scattering with microscopy. These methods offer 2D/3D information about the chemical makeup and the ultrastructure of tissues, cells, and cellular organelles with a spatial resolution down to tens of nanometres. The coherent flux provided by our 3 GeV storage ring enables imaging with high resolution using coherent diffractive imaging and ptychography methods. These developments will enable further insight into biological mechanisms (cell division, differentiation, transport, pathogen adhesion etc.), diseases & cancer, biomaterials & biomechanics, formulation of medicines including biologics, food and much more.

High-speed 3D computed tomography imaging (e.g., provided by MedMAX) is highly attractive for biomedical research at the micrometre scale. Dedicated 3D imaging beamlines are flagship projects of most third-generation synchrotron upgrade programs (e.g., BM18 at ESRF and TOMCAT at SLS). Pre-clinical studies using 3D imaging will contribute to the knowledge of poorly understood physiological and pathogenic processes and functional anatomy in small animals and tissue samples.

We will also offer unique opportunities to explore the dynamics of the fundamental processes innate to life. Exploiting the high average- and peak brightness as well as short pulses of our sources will open the door to the study of equilibrium dynamics and conformational changes in proteins and other macromolecular ensembles on different time scales, from ultrafast (femtoseconds) to seconds, by Small Angle X-ray Scattering and coherent X-ray scattering methods, imaging, serial crystallography, and spectroscopy.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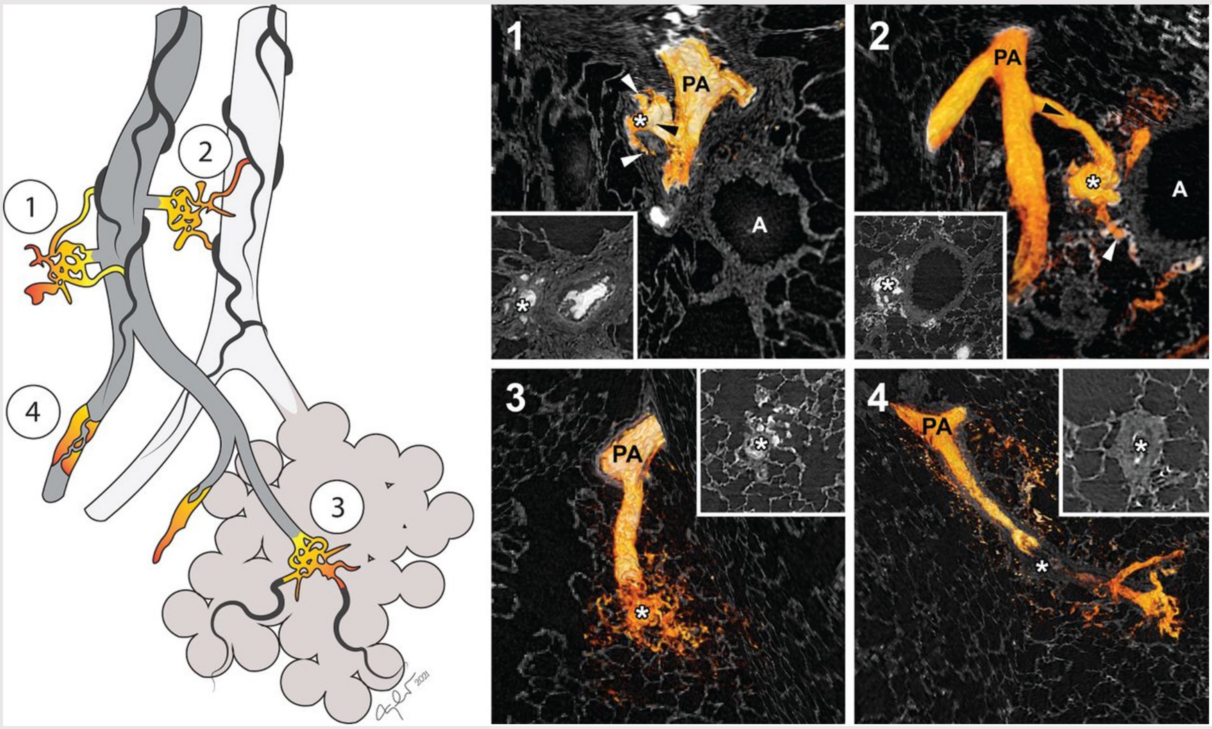


Science Example

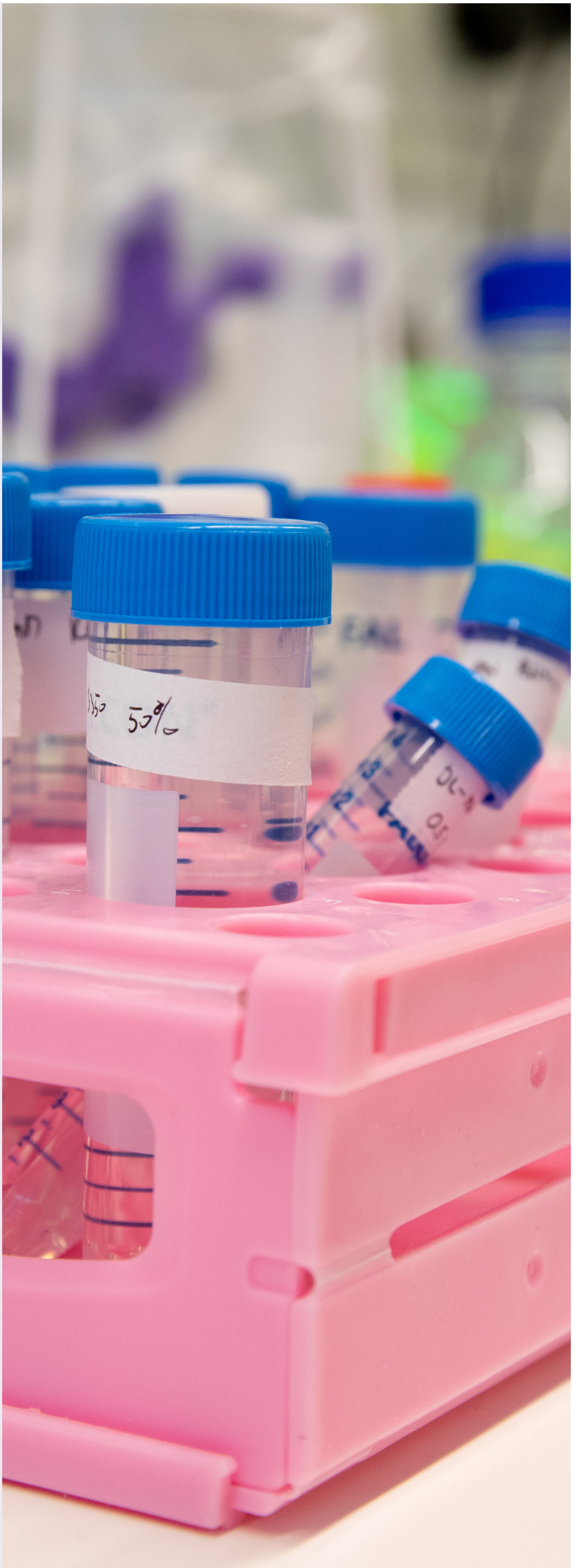
Three-dimensional reconstructions of the four types of plexiform lesions in the rat model visualised by synchrotron tomography imaging at the TomCAT beamline at PSI (Villegen, Switzerland). Plexiform lesions are complex vascular formations originating fromremodelled pulmonary arteries that are a hallmark of severe pulmonary hypertension.

The three-dimensional data obtained from synchrotron-based imaging revealed significant plexiform lesion heterogeneity, resulting in a novel classification. This study is an example of the gain in information within microanatomy where spatial information from tomography imaging gave new insights in comparison to 2D-histology. A new hard X-ray beamline for high-speed 3D imaging is essential for these kinds of experiments at MAX IV.

Oscar van der Have, Christian Westöö, Filip Ahrné, Xuefei Tian, Kenzo Ichimura, Till Dreier, Christian Norvik, Maya E. Kumar, Edda Spiekerkoetter, Karin Tran-Lundmark Shunt-type plexiform lesions identified in the Sugen5416/hypoxia rat model of pulmonary arterial hypertension using synchrotron-based phase-contrast micro-CT. European Respiratory Journal, 59, 2102802 (2022); https://doi.org/10.1183/13993003.02802-2021

Area objectives

- **Develop a new hard X-ray beamline for high-speed 3D imaging** with micrometre-scale resolution. In addition to biomedical applications, this beamline will serve the environmental sciences, palaeontology, and other communities.
- **Develop a new beamline for IR spectroscopy on the 1.5 GeV ring.** This will enable the coupling of atomic information with higher-order structural changes of proteins within cells and tissues, giving insight into processes such as stroke, brain trauma, COVID-19, Alzheimer's and Parkinson's disease.
- **Further develop time-resolved 3D functional studies of proteins** at the Balder, CoSAXS and MicroMAX beamlines. This will lead to new insights into protein complex formation, fibrillation and amyloid disease processes, and protein catalysis.
- **Further develop and extend FragMAX for chemical biology approaches.** This will enable an understanding of more complex protein functioning than is currently possible.
- **Extend our capabilities towards biomedical applications** at existing soft and hard X-ray microscopy beamlines such as SoftiMAX and NanoMAX, as well as develop new capabilities, for example, hard XRF imaging at the sub-micrometre scale.
- **Support integrative approaches** offering multiple techniques through the beamtime proposal system and collaboration projects between different beamlines.
- **Strengthen collaborations** with gateway environments providing access to sample preparation, data processing, analysis, and visualisation tools and the structural biology, drug discovery and chemical biology platforms at SciLifeLab and other international platforms providing cryoEM, light microscopy, super-resolution microscopy, and MRI capabilities.



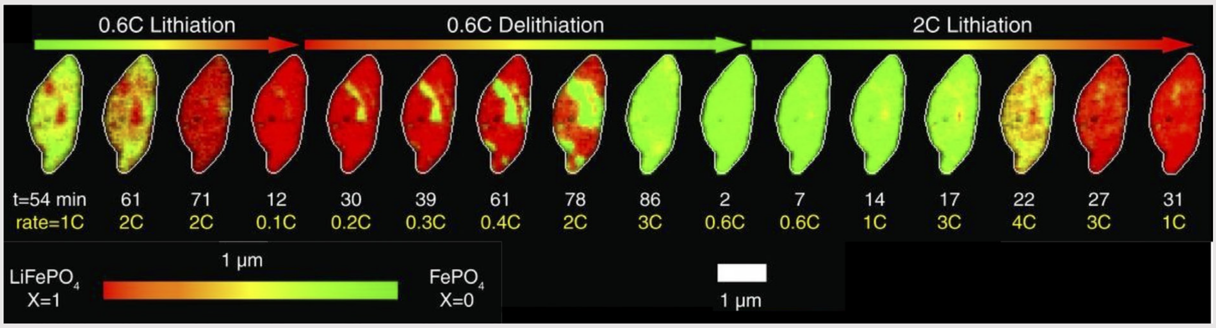
Energy materials and technologies

With the ambition to become the world's first fossil-free society, Sweden is at the international forefront of efforts to transition to a sustainable circular economy. Achievements derive from a long tradition of collaborations between world-leading energy research academic groups across Swedish universities, industry and research organisations. MAX IV is central in supporting academic and industrial users' innovations in energy materials and technologies. Our users benefit from ambient pressure photoemission spectroscopy (APXPS) at HIPPIE and SPECIES to study interfacial processes during battery charge/discharge cycles and the process of atomic layer deposition. Users of FlexPES can study the surface composition of solar cells and battery electrodes via ultra-high vacuum XPS. The photoemission microscope MAXPEEM provides high spatial resolution to investigate surfaces of multicomponent hard materials and special steels. Scattering and diffraction capabilities from the DanMAX and Balder beamlines are, for example, used to study the structure and coordination of active centers in catalysts. The spatial resolution and chemical sensitivity of our SoftiMAX/NanoMAX beamlines allow for mapping composition at different lengths scales of interfaces in multicomponent energy storage or electricity generation devices.

MAX IV has transformational opportunities to capitalise on the advances of modern spectro-micro-tomography techniques and further exploit the small emittance of our 3 GeV storage ring. We aim to expand current material characterisation and screening capabilities with new tender/hard X-ray spectroscopy, imaging, and diffraction beamlines. These new instruments will be the key to accelerating breakthrough discoveries of novel energy-technology-related materials.

There are also untapped and potentially high-impact opportunities to study "complete" operational devices and systems in operation. New experimental platforms at our new hard X-ray imaging and tender/hard X-ray spectroscopy beamlines will be dedicated to reaching this goal. This will open up possibilities to, for example: (i) perform measurements at pressures of several atmospheres, which is crucial to CO_2 conversion, (ii) allow real-time observations of chemical changes at the solid-liquid interfaces in novel batteries, electrocatalysts for hydrogen production, or corrosion-resistant alloys, and (iii) allow following the morphological changes at complex multijunction interfaces critical for the development of highly-efficient multijunction photovoltaic materials.

The availability of ultrafast X-rays from a soft X-ray laser would further benefit energy material research by enabling pump-probe experiments in the femto- to the nano-second time domain. These time scales are critical for investigating charge transfer and charge delocalisation pathways in solar cells or photocatalysts and also for the formation/breaking of chemical bonds during elementary catalytic reactions. Developing an understanding of these processes is central to the discovery of high-efficiency solar cells and selective heterogeneous catalysts.



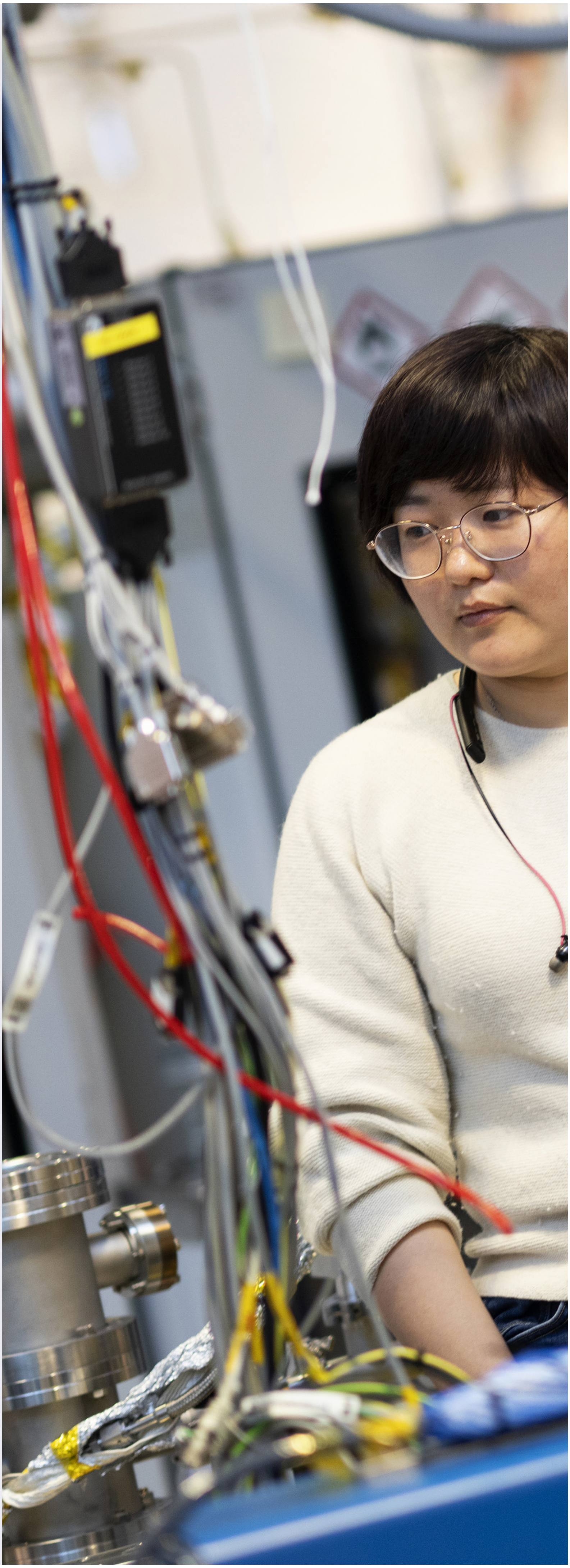
Science Example

Rechargeable batteries lose capacity in part because of physical changes in the electrodes caused by electrochemical cycling. Operando electrochemical X-ray microscopy was used to measure 2D chemical maps of Fe content within a particle of rechargeable battery electrode material, Li_XFePO_4, which undergoes lithiation and delithiation cycles at various (dis)charging rates (1C equals a complete charge within 1 hour). These maps demonstrate the rate of Li^+ insertion and removal from particles in real-time. High cycling rates result in the formation of a solid solution that minimises stress and improves cyclability. However, at slow rates, phase separation occurs within the particle which results in shorter battery life.

Lim, J.; Li, Y.; Alsem, D. H.; So, H.; Lee, S. C.; Bai, P.; Cogswell, D. A.; Liu, X.; Jin, N.; Yu, Y.; Salmon, N. J.; Shapiro, D. A.; Bazant, M. Z.; Tyliszczak, T.; Chueh, W. C. Origin and Hysteresis of Lithium Compositional Spatiodynamics within Battery Primary Particles. Science, 2016, 353, 566–571. https://doi.org/10.1126/science.aaf4914

Area objectives

- **Develop a tender/hard X-ray beamline** for ambient pressure photoemission and X-ray absorption/emission spectroscopies for in vacuum, in situ, and operando studies.
- **Develop a hard X-ray tomography and diffraction microfocus beamline** for fast scanning and tomographic imaging of operando materials/devices.
- **Develop a high-throughput diffraction capability** for material science.
- **Further develop soft X-ray operando spectroscopy** (e.g., RIXS, STXM, APXAS) and photoemission functionalities at the HIPPIE, SPECIES, VERITAS, and SoftiMAX beamlines.
- **Develop access modes and dedicated experimental platforms** to strengthen the Nordic industry's current and future capabilities in close cooperation with important stakeholders in this area, e.g. the Battery 2030+ and WISE initiatives.
- **Provide multimodal experiment capabilities**, where several techniques are used to obtain concurrent or sequential complementary classes of information (e.g., structural, chemical, and electronic).
- **Take an active role in organising nationwide competence and training initiatives** aimed at maximising the efficient use of X-ray-based techniques by academic and industrial users from the Nordic region.



Tackling environmental challenges

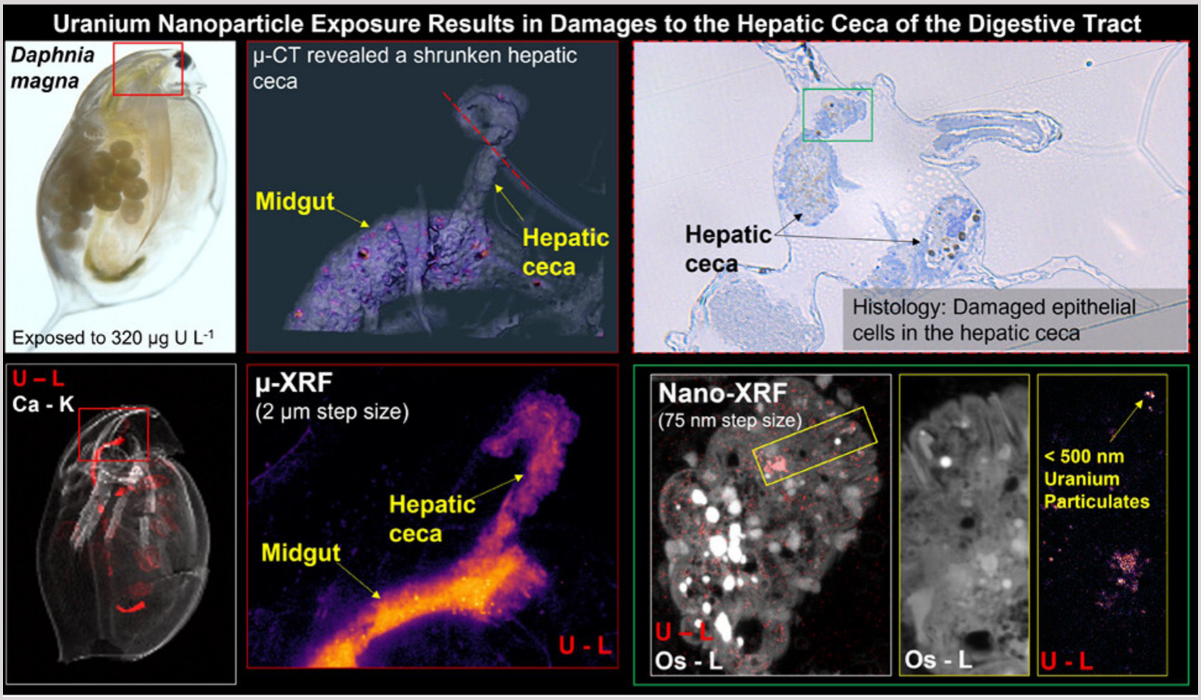
Environmental science is a diverse international research field and a prominent research area within the Swedish and Nordic scientific landscape. Indeed, the annual "Research Barometer" study performed by the Swedish Research Council has for several years consistently shown that this is an area where Swedish universities make a significant contribution to international efforts.

This area not only involves crucial investigations to understand the very complex system of our natural environment and anthropogenic impacts, but it also aims to produce sustainable solutions for the future. Atmospheric science and aerosols, renewable resources, metals, minerals and sustainable materials, food, food production, and soil and water science are areas of paramount importance to ensure our ability to tackle both current and future environmental challenges that threaten our sustainable existence on earth.

To advance research within this field, it is necessary to move away from simple models and instead study real, complex systems. Typically, real samples exhibit heterogeneous structure and chemical composition, and the processes to be investigated occur over many different time and length scales. The research at MAX IV benefits from the exceptional combination of both the high- and low-energy storage rings, each with dedicated beamlines. Balder, ForMAX, and SoftiMAX are prime examples of existing beamlines with a strong environmental community behind them, whilst the flexible endstations at FlexPES and FinEstBeams offer opportunities for atmospheric science-related research. Thus, MAX IV is uniquely positioned to contribute to, for example, finding alternative and novel technical solutions for the development of new materials from renewable bio-based resources, carbon capture and storage using geological reservoirs or construction materials.

Research themes of future significance address: the uptake and distribution of chemicals, nutrients, and pollutants in soil, organisms, or cells; the effect of chemical reactions occurring at the surface of nanoscopic aerosols on large-scale climate change; novel material concepts and new means of materials processing, sustainable use of heterogeneous industrial side streams and bio-based raw materials.

Many X-ray techniques shed light on the complex nature of environmental systems, and often a combination of techniques is required to unravel molecular-scale details of the various relevant processes. To dig deeper into the molecular processes, time-resolved in-situ conditions are necessary to preserve the chemical state of a sample. We aim for a beamline portfolio that covers the range of techniques necessary to provide chemical and structural contrast over different length- and time scales. For example, investigation of the uptake and distribution of chemicals, nutrients and pollutants in soil, organisms or cells for in-situ soil reactions require specialised controlled sample cells in combination with high chemical and spatial resolution. Another important objective is to expand the beamline portfolio with an infrared beamline providing chemical contrast in 1D, 2D and 3D at the nanoscale. To close the gap in both energy and resolution between the nanofocus imaging and bulk spectroscopy beamlines, a new tender-to-hard X-ray micro-focus spectro-microscopy beamline would enable chemical speciation via combined μ-XAS and μ-XRF mapping of larger samples (up to cm). Finally, a dedicated state-of-the-art tomographic imaging beamline, allowing three-dimensional imaging with a large field of view, spatial resolution down to 20 nm, and high temporal resolution (to follow processes in situ), would contribute greatly to this field.



Science Example

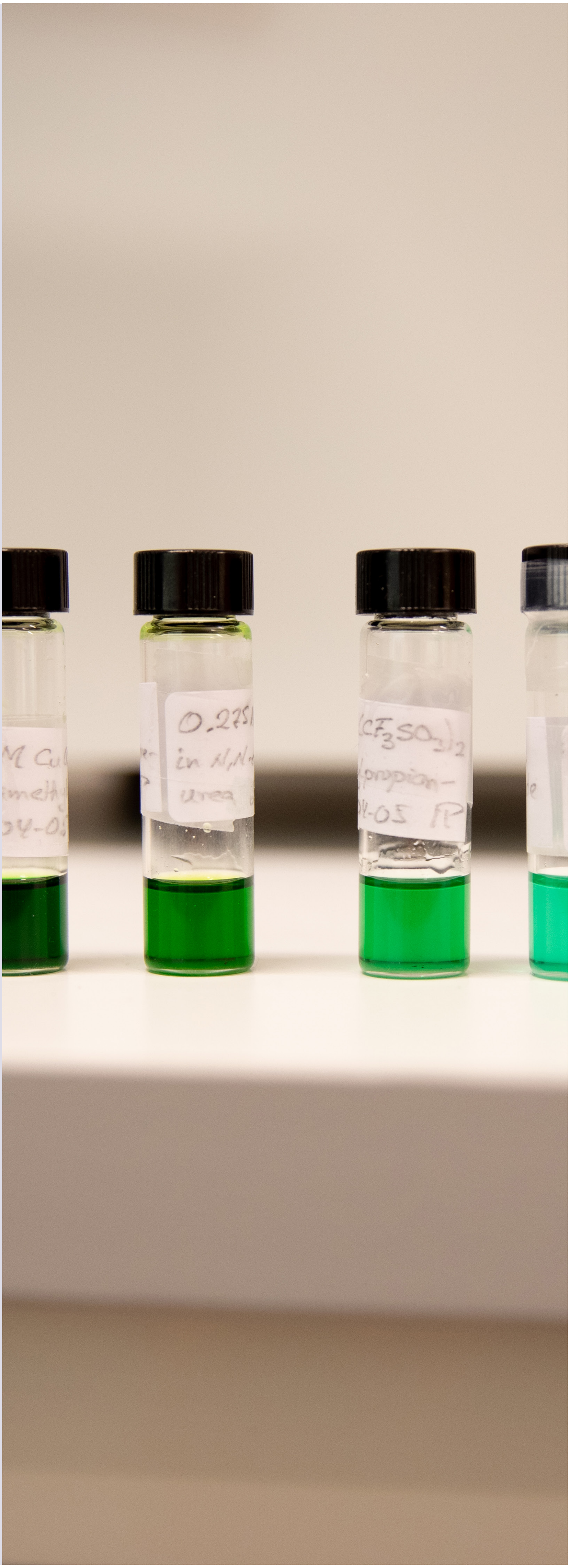
Uranium (U) is released to the environment from a series of naturally occurring U rich minerals and bedrocks such as alum shale and granite, but is also associated with the release from anthropogenic sources, such as U mining and milling industries, nuclear reactor accidents, nuclear weapon detonations, nuclear waste storage, nuclear fuel reprocessing, civilian and military use of depleted U, and, potentially, from the catalyst industry.

Uranium is especially problematic for aquatic ecosystems where it is known to be taken up into the food web and exhibits a chemotoxicity that can lead to acute effects. To find the detailed information of the underlying toxicokinetic mechanisms the aquatic toxicology model organism, the freshwater invertebrate Daphnia magna, a primary consumers of various algae and bacterial species with an important role in nutrient cycling was fed with U nanoparticles (NP) and analysed with X-ray methods. Lind and coworkers could see the biodistribution of internalised U on different length scales by combing different instruments. The microfocused X-ray fluorescence (XRF) U distribution map identified target organs including the digestive tract and hepatic ceca, while in the nanofocused high resolution XRF map was even single U-NP visible inside the hepatic ceca, an organ producing digestive fluids.

Byrnes I., Rossbach L. M., et al. Synchrotron XRF and Histological Analyses Identify Damage to Digestive Tract of Uranium NP-Exposed Daphnia magna. Environ. Sci. Technol. Article ASAP (2023). https://doi.org/10.1021/acs.est.2c07174

Area objectives

- **Develop a new beamline for tender-to-hard X-ray micro-focus spectro-microscopy,** dedicated to spatially resolved X-ray fluorescence (XRF) and X-ray absorption spectroscopy (XAS). This will allow the study of larger specimens (cm) with micron resolution, and, for example, enable us to look directly at nutrient cycling to understand changes in phosphorus speciation and micro-distribution in forest soils.
- **Develop a new beamline for IR spectroscopy.** This enables for example mapping of microplastics in aqueous and terrestrial environments by distinct molecular fingerprints.
- **Develop a new hard X-ray beamline for 4D tomographic imaging,** with a large field of view and the possibility of nano-tomography, will provide means to study, for example, the assembly of bio-based nanoparticles into new functional materials.
- **Develop specialised sample environments,** together with our user community, that replicate realistic conditions.
- **Support integrative approaches offering multiple techniques** through the beamtime proposal system and collaboration projects between different beamlines.
- **Collaborate with our user community and higher education institutions to provide training and education.** This involves outreach to new users lacking formal training in synchrotron use whose research has great potential to benefit from integrative X-ray methods.



Quantum materials and device technologies

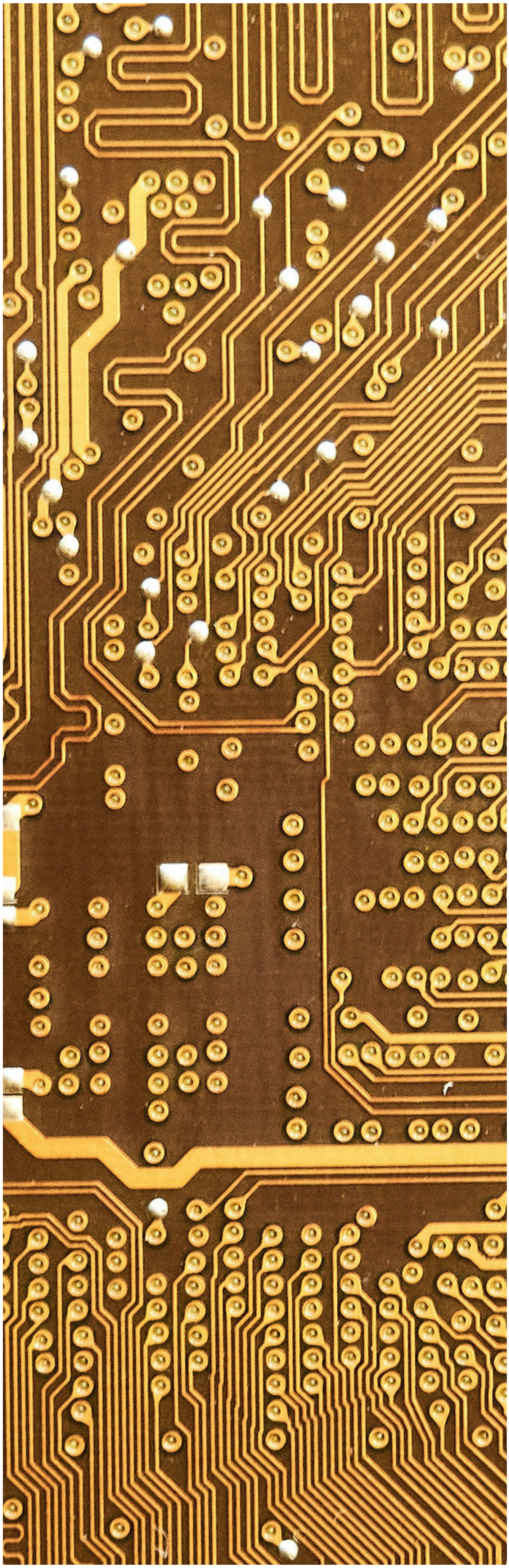
Quantum materials and devices, many based on combinations of semiconductors and/or novel materials, are highly active research areas that have the potential to radically transform our technological landscape. Sweden and the Nordic region comprise many well-established initiatives directed to this effort, the Wallenberg Centre for Quantum Technology (WACQT), the Danish NATO Centre for Quantum Technology, the Microsoft Quantum Materials Laboratory in Copenhagen, the Norwegian Centre for Quantum Technology and InstituteQ in Finland. In Sweden, this also connects to a diverse set of activities, some connected to the MyFab nodes and initiatives such as the Wallenberg initiative materials science for sustainability (WISE).

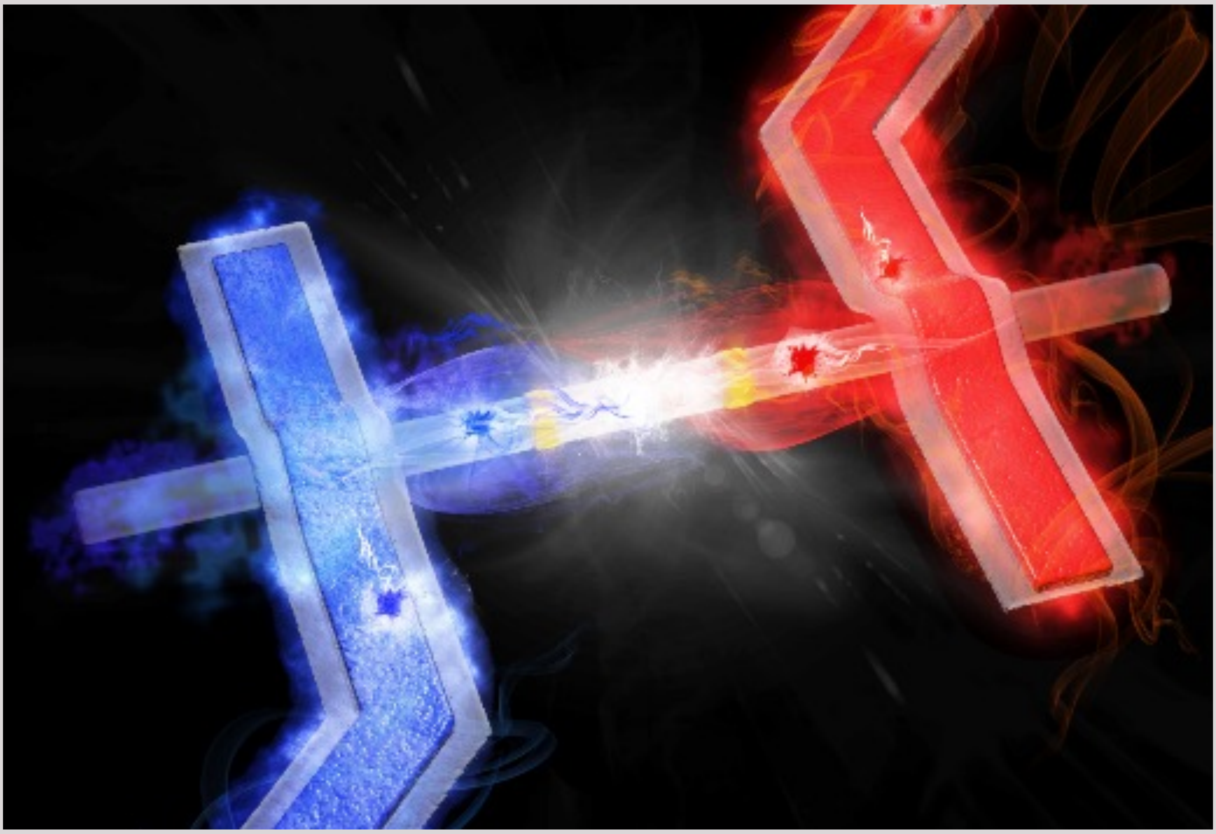
The sensitivity and specificity of synchrotron X-ray techniques are ideally suited to investigate many of the intrinsic properties of quantum materials . X-ray spectroscopy, as well as coherent and incoherent X-ray scattering/diffraction, and imaging, allow probing the equilibrium, out-of-equilibrium, and stimulated structure and dynamics of matter at relevant spatial and temporal scales. The broad photon energy range (10 eV to 10s of keV) and the high brightness of our accelerators ensure that several of our beamlines are already actively contributing to this field. In the UV/soft X-ray regime, our Bloch beamline, with its 10-micron incident beam size and its large photon flux and energy resolution, contributes to understanding the delicate interplay between spin-orbit coupling and strong electronic correlations such as intertwined charge density waves. In the hard X-ray regime, scanning nanobeam diffraction microscopy performed at the NanoMAX beamline has been instrumental in revealing the dominant role of atomic and nanoscale structural defects in the orientation and pinning of magnetic domains in spintronic materials.

MAX IV is uniquely positioned to strengthen its contribution to quantum materials and device research by pushing the current boundaries of spectroscopy, coherent and incoherent X-ray scattering, diffraction, and imaging capabilities. For example, a nano-focus ARPES beamline will ideally respond to the research needs of communities studying out-of-equilibrium quantum materials, e.g., to investigate the influence of strain, gating, and current injection. Furthermore, soft- and hard X-ray microscopies based on nanometric-sized beam scanning and ptychographic approaches will strengthen the investigations of the crystalline, compositional, and morphological heterogeneities in 2- and 3-dimensions. There are untapped opportunities to study the dynamics of topological magnetic systems like skyrmions and spin-ice structures by developing X-ray Photon Correlation Spectroscopy and X-ray dichroism approaches. These capabilities are and will be relevant for a vast spectrum of device technology research, from traditional ones close to industrial implementation and relevance all the way to future technologies and concepts.

The coupling of X-rays carrying Orbital Angular Momentum to matter is of growing international interest at light sources. Fourth-generation light sources like MAX IV are also uniquely positioned to provide OAM beams with a wavelength in the X-ray range. These could open new opportunities to explore systems exhibiting spin-orbit coupling but also for spintronics and orbitronics applications.

Furthermore, an ultrafast source of X-rays would allow studying the ultrafast dynamics and out-of-equilibrium response of quantum materials by allowing time-resolved pump-probe ARPES, RIXS, and dichroism capabilities. These are especially relevant in understanding light-induced demagnetisation, transient superconductivity, and photo-induced switching in multiferroics.





Science Example

A heat engine extracts work as heat flows from the hot to the cold reservoir. In macroscopic systems this is achieved by avoiding direct contact between them; rather, the engine is cyclically connected to and disconnected from the reservoirs. This mode of operation, however, is rather impractical to be implemented at the nanoscale and nanoengines with no moving parts have been theorised. Linke and co-workers have now experimentally demonstrated a nanoscale heat engine in which only electrons at a specific energy flow between the reservoirs generating an electric current. The image is an artist's impression of the nanoengine with the hot and cold reservoirs coloured in red and blue respectively.

Josefsson, M., Svilans, A., Burke, A.M. et al. A quantum-dot heat engine operating close to the thermodynamic efficiency limits. Nature Nanotech 13, 920–924 (2018). https://doi.org/10.1038/s41565-018-0200-5

Area objectives

- **Develop a beamline for nano-ARPES** serving fundamental research on quantum materials and the quantum device communities.
- **Develop a tender/hard X-ray photoemission beamline** to study the electronic structure of the bulk, buried thin films, and interface states of quantum materials.
- **Continue extending beamlines capabilities for in-situ and operando studies,** as required for investigating the behaviour of quantum devices.
- **Attract seed funding to launch new research initiatives, conduct workshops, and prepare a science case** to fund activities dedicated to the study of the topology of light and matter, especially the use of X-rays with Orbital Angular Momentum.
- **Strengthen collaborations with Swedish universities and facilities involved in Quantum materials and device technology** development as well as with our user community through participation in joint development or research projects and student training.

Atomic, molecular and optical science

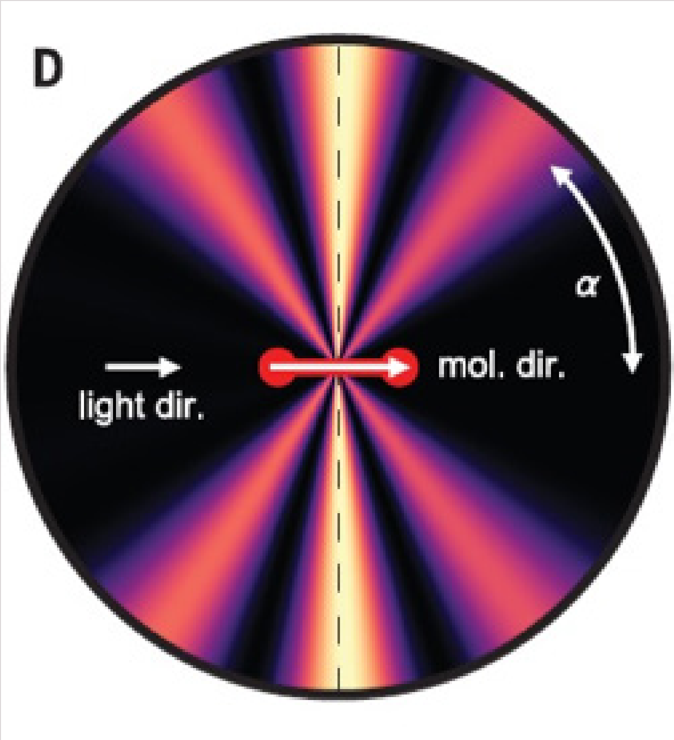
Atomic, Molecular, and Optical (AMO) science is a diverse and evolving international research discipline, to a large extent pioneered at MAX II, and thus with deep roots in Sweden. Molecular and cluster studies that focus on the role of electrons in atmospherically relevant systems help determine the character of chemical reactions. In contrast, liquid micro-jet studies on aqueous model systems have allowed us to infer important conclusions regarding the surface properties of aerosols and droplets in the atmosphere. Studying aerosols under realistic conditions using aerodynamic lenses opens the door to more accurate modelling of the influence of anthropogenic aerosols on health, climate, and weather. Most Swedish universities have strong research programs that specialise in different areas of AMO science, covering a wide range of systems and phenomena, ranging from small quantum systems (atoms, molecules, clusters) or reactive species (such as positive and negative ions) to surfaces and interfaces. This community's overarching aim is to execute controlled, precise experiments on well-defined systems supported by high-level quantum chemistry modelling.

The MAX IV beamlines are particularly relevant for AMO research. Research on particle beams and dilute targets benefits from the availability of a brilliant light source. The current AMO-relevant beamlines at MAX IV deliver high flux over a wide photon energy range (4.5-1500eV), enabling access to the valence and core orbitals of the lighter elements. Access to advanced timing modes on our storage rings supports coincidence and time-resolved experiments, and the brightness of the 3 GeV ring facilitates RIXS experiments on dilute gas-phase/liquid samples.

MAX IV is uniquely positioned to continue offering new capabilities to the AMO user community. This will include the development of specialised sample environments to enable measurements on samples that are as close to "real" systems as possible, as well as the refinement/development of cutting-edge measurement techniques. Access to higher photon energies, larger flux, and smaller spot sizes, such as can be delivered by our 3 GeV storage ring, will extend our experimental capabilities on offer to the AMO community and enable a new (and broad) range of experiments on neutral, heavy atom-containing polyatomic systems, molecular/ion beams, and liquid jet targets.

A Soft X-ray Laser (SXL) that delivers ultrafast soft X-ray pulses would further strengthen MAX IV Laboratory's contribution to cutting-edge AMO science. Key questions in the field concern the fundamentals of ultrafast charge transfer mechanisms, which are vital for understanding processes in large molecules, e.g., photosynthetic systems and DNA, or investigation of the role of electron and nuclear dynamics in molecular and cluster fragmentation. An SXL would also provide an opportunity for novel pump-probe schemes with a time resolution that enables investigation of such fundamental processes, i.e., a few femtoseconds (and potentially in the attosecond regime).


expert sensor box



Science Example

Photoionisation is an experimental technique that enables the investigation of a wide variety of phenomena and sample types, for example, atoms, molecules, clusters, liquid and solid samples. Typical experiments within AMO research involve research to investigate energy/charge transfer processes or reaction dynamics induced by photoexcitation. A large proportion of such AMO experiments are performed at synchrotron facilities as these powerful tools can provide a monochromatic beam of photons over a very broad photon energy range. Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) is a measurement technique that enables the detection of the electrons and ions emitted in a photoreaction and the subsequent determination of their kinetic energies and angle of emission from the parent molecule/cluster. Thus, allowing the researcher to piece together the dynamics of a reaction.

Grundmann and coworkers in Frankfurt have used a COLTRIMS reaction microscope, synchrotron radiation and an electron interferometric approach to determine the time delay between electron emission from the two center sites of the H_2 molecule. In other words, they have measured the time it takes for the synchrotron light to cross the hydrogen molecule – the shortest time ever measured –z 247 zeptoseconds.

Grundmann, S., Trabert, D., Fehre, K. et al. Zeptosecond birth time delay in molecular photoionization. Science 370, 339–341 (2020). https://www.science.org/doi/10.1126/science.abb931

Area objectives

- **Develop a tender/hard X-ray beamline** to enable tender X-ray Auger-ion coincidence measurements and depth-sensitive tender/hard X-ray XPS studies on neutral heavy atoms, ionic species, liquid micro-jet samples, and dilute gas-phase.
- **Develop experimental capabilities** to 'tailor' samples of small quantum systems.
- **Develop time-resolved and pump-probe methods** for relevant beamlines.
- **Achieve full control of incident polarisation** at all AMO-relevant soft X-ray beamlines.
- **Strengthen collaborations** with the user community through participation in joint development or research projects and student training.

Accelerator science

Accelerator science is the lifeblood of MAX IV, as it drives the performances and opportunities for our light sources to support a compelling user science program. It is also a vital research area on its own. Building upon the successful construction and operation of the first 4th generation storage ring worldwide, the accelerator science programme described below aims at meeting the short- and long-term needs of our user community, with the underlying goal of maintaining leadership in next-generation high-brightness X-ray sources. The programme includes shorter-term incremental improvements and longer-term, radical, game-changing proposals. The shorter-term initiatives target immediate needs and, at the same time, establish critical enabling technologies that set the stage for longer-term upgrades. Together they constitute a coherent set of activities in multiple time scales that make the most cost-effective use of synergies between the various efforts.

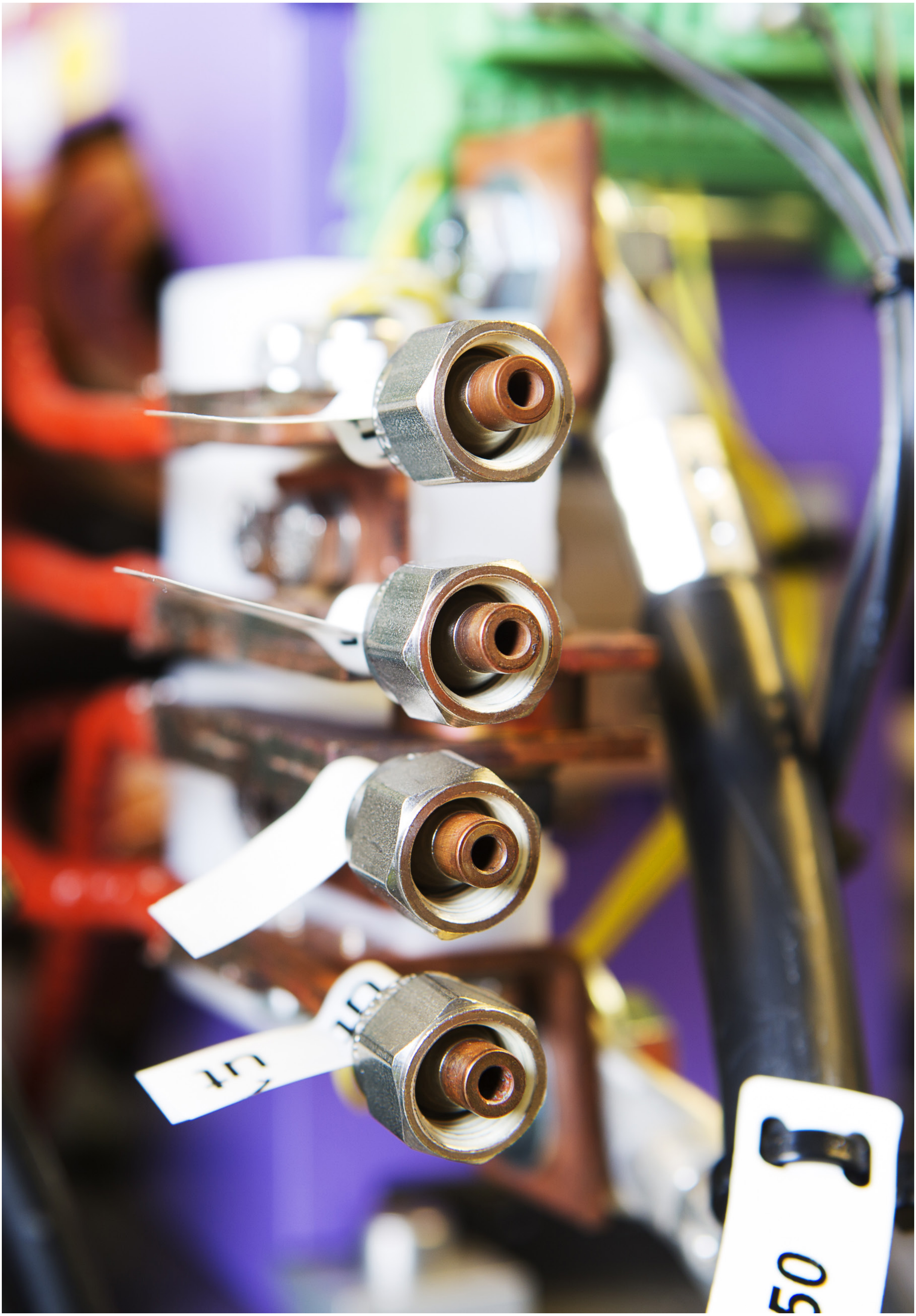
A crucial enabling factor for the success of this programme is the education and training of the next generation of accelerator scientists and engineers, which will be performed in collaboration with interested Swedish universities.

Building for the future

The international landscape of synchrotron radiation facilities has experienced major changes over the past seven years. In fact, since the successful commissioning of the MAX IV 3 GeV ring in 2015, several storage ring projects worldwide have gone from the proposal and design stages to construction, commissioning, and user service. Common to this impressive new wave of storage ring sources is the use of variants of the multibend achromat lattice pioneered at MAX IV. These developments confirm the leading role of MAX IV and emphasise the urgency of work towards further improvements that will keep the Laboratory competitive. During the same period, the landscape of high peak brightness sources based on free-electron lasers driven by linear accelerators has also seen significant advances, with new facilities commissioned in Europe, Asia, and the US.

Our existing accelerators constitute the backbone for further development over the next decades in both storage ring and linac-based high-brightness X-ray sources, as illustrated in figure 5. Our accelerator science programme foresees brightness improvements [1] in the 3 GeV ring aiming at the long-term goal of reaching the diffraction limit for 10 keV photons. In contrast, the efforts in the 1.5 GeV ring will include implementing transparent top-up injection [2] (replicating the successful implementation of a multipole injection kicker in the 3 GeV ring [3]) and advanced timing modes, initially using the TRIBs (Transverse Resonant Island) technique [4] and at a later stage using very fast kickers to get individual bunches into an offset closed orbit. Moreover, the potential of special accelerator operating modes in the 1.5 GeV ring for generating high flux IR/THz radiation through coherent synchrotron emission from short bunches will be further explored.

Despite their outstanding properties of high repetition rate high brightness and stability, storage rings cannot compete with free-electron lasers in terms of peak brightness and generation of ultrashort pulses. Anticipating a growing need for access to time-resolved tools in the femto- to attosecond regime, Sweden is also well prepared, through the early design choice of a full-energy linear accelerator injector at MAX IV, to join the few countries hosting free-electron laser facilities. A recently



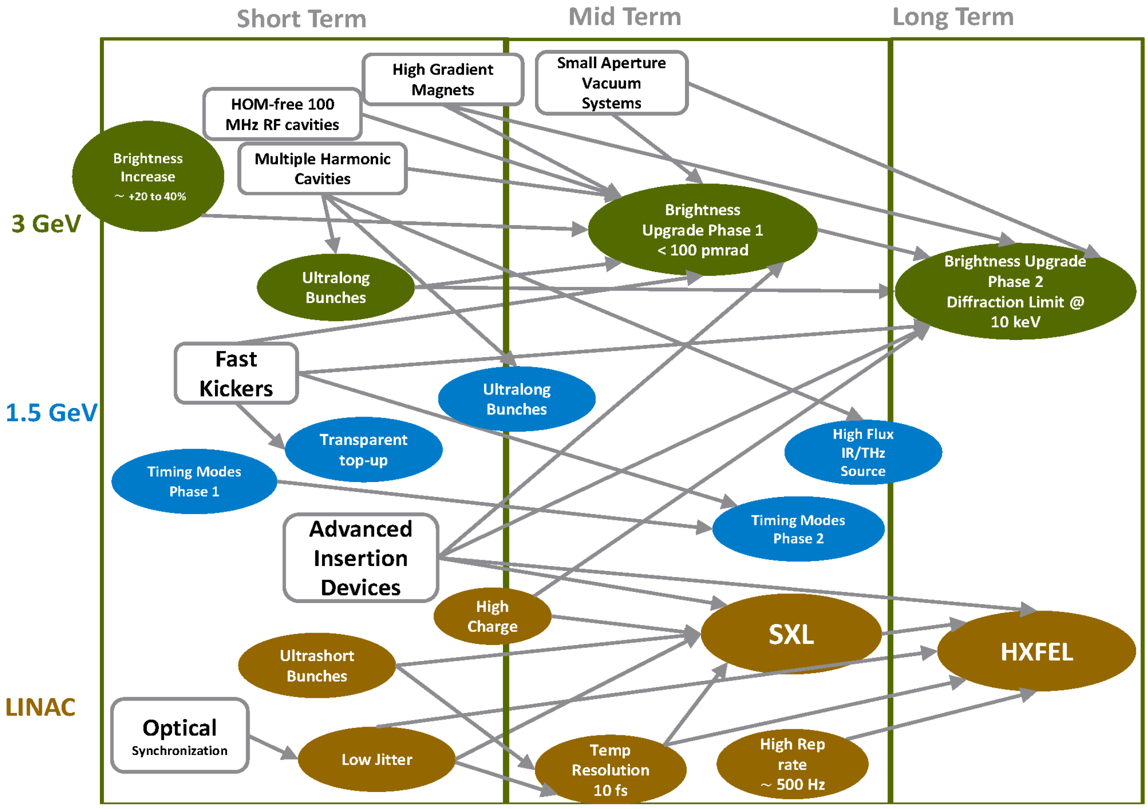


Figure 5: Accelerator Science Programme: developments over three timescales for each one of the MAX IV accelerators are indicated together with enabling technologies.

completed Conceptual Design Report [5] describes how a Soft-X Ray Free Electron Laser (SXL) can be implemented at a low-cost relative to the substantial leap of utility and competitiveness it would provide Sweden. Looking further ahead, adding a hard X-ray FEL at MAX IV would open possibilities for studies on ultrafastscience at higher photon energies.

[1] M.Apollonio et al, Improved Emittance and Brightness For The MAX IV 3 GeV Ring, IPAC22.

[2] The injection process inevitably generates short-lived perturbations to the stored beam position and size. A transparent injection keeps these perturbations to a minimum, In the MAX IV 3 GeV ring these have been brought down to a world record sub-micrometer level.

[3] P.Alexandre et al, Transparent top-up injection into a fourth-generation storage ring, NIMA 986 (2021) 164739

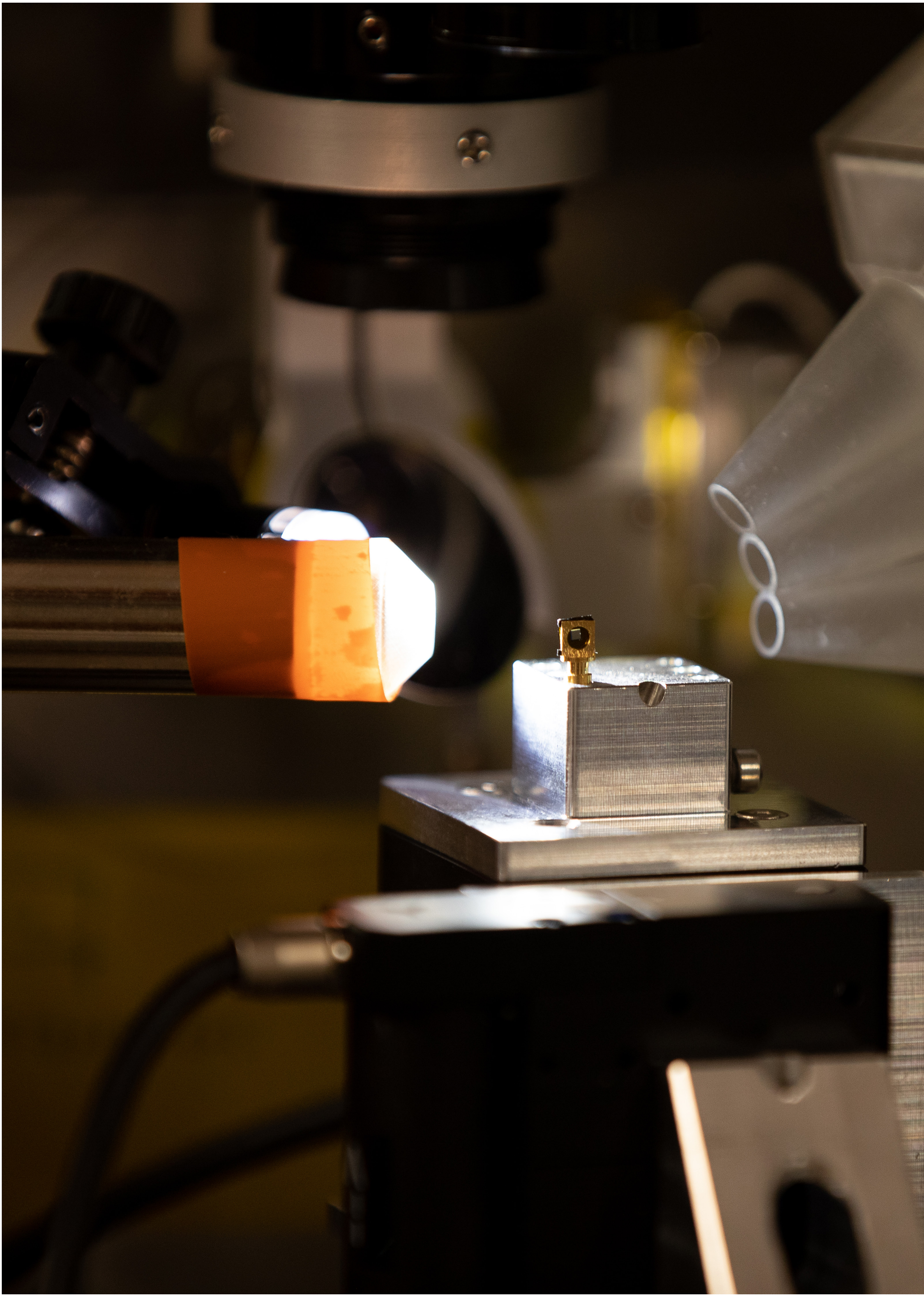
[4] D.K. Olsson and Å. Andersson, Studies on Transverse Resonance Island Buckets in third and fourthgeneration synchrotron light sources, NIM A 1017 (2021) 165802

[5] https://www.maxiv.lu.se/wp-content/plugins/sharepoint-plugin/ajax/downloadFile.php?site_id=MAXIV&version_series_id=59&repository_id=7902c653-bd51-4132-9352-2f9e2c0ddc77

Area objectives

To achieve our overarching goal of keeping the accelerators at the forefront, we will

- **Develop enabling technologies** that provide short and mid-term incremental performance improvements while setting the stage for future order-of-magnitude, game-changing jumps in accelerator capabilities.
- **Increase brightness by** for the 3 GeV ring and prepare a future quantum jump towards the diffraction limit at 10 keV.
- **Implement transparent top-up and continue to develop timing modes** for the 1.5 GeV ring.
- **Develop specialised run modes** for the production of high flux THz and IR radiation.
- **Continue to develop SXL** to deliver ultrabright and ultrashort soft X-ray pulses and prepare the MAX IV linac's future expansion to drive a hard X-ray Laser.
- **Ensure long-term competence in accelerator science** by educating the next generation of accelerator physicists and engineers
- **Further engage in international and national collaborative networks** in Accelerator Physics and Engineering.



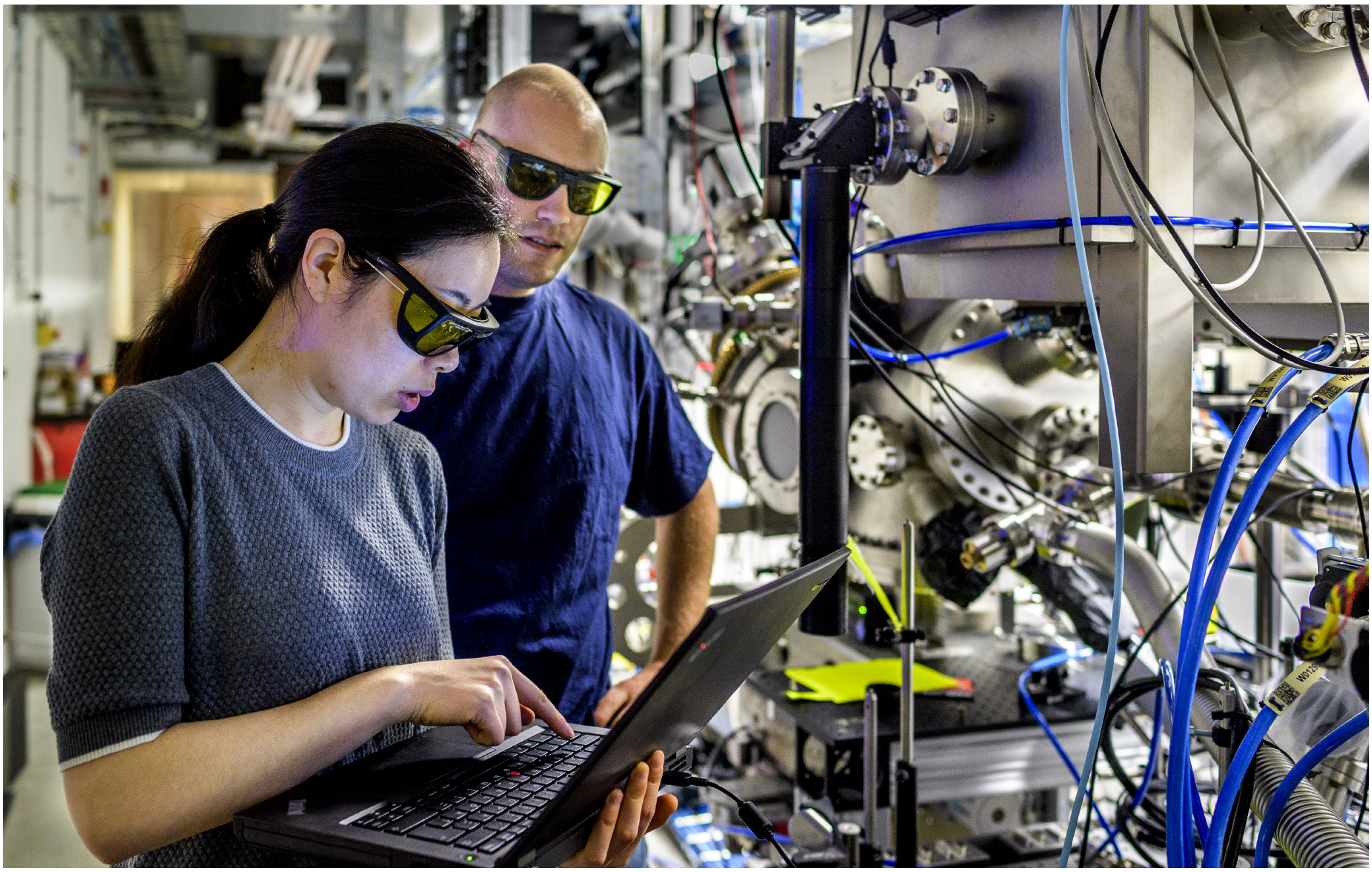
Enabling Technologies

Time-resolved methods

Storage ring-based X-ray light sources can uniquely probe the structure of matter over a broad range of length scales (from millimetres to Ångström) and also timescales (from hours down to tens of picoseconds). To fully understand a material property/function, it is critical to go beyond understanding the details of its time-average structure by probing its dynamic/kinetic information down to relevant time scales of interest. To support this goal, it is important to develop beamlines supporting in-situ and operando experiments that often require the development and integration of complex sample environments.

Beyond extending X-ray imaging techniques to time-resolved approaches, novel techniques exploiting X-ray coherence, such as X-ray Photon Correlation Spectroscopy (XPCS) or Speckle Visibility Spectroscopy (XSV), offer the unique opportunity to probe density fluctuations in equilibrium and out-of-equilibrium systems down to the atomic scale. Moreover, it offers the prospects to probe dynamical phenomena of disordered and amorphous matter that are not correlated to structural changes. Overall, X-ray imaging detectors with appropriate spatial resolution and fast data acquisition rates are essential. This also relies on the appropriate infrastructures to store, manage, process, visualise, and analyse the data generated by these detectors.

To extend further the range of accessible timescales down to the femto– to atto-second will require a source of coherent ultrafast X-ray pulses. A soft X-ray laser will ideally suit research directed to using pump-probe and/or diffract-and-destroy data collection strategies. There are significant synergies in the development of experimental stations and diagnostics between the storage rings and linac-based beamlines, which would boost time-resolved techniques.

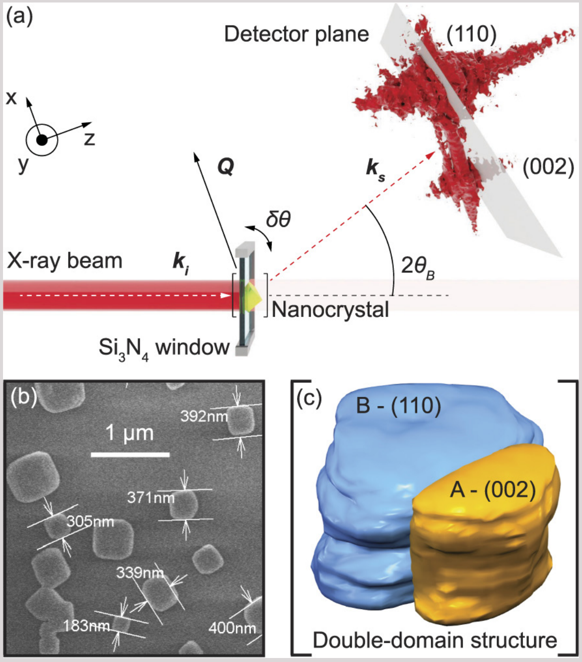


Imaging

A picture is worth a thousand words. Imaging with X-rays allows seeing inside objects and determining their structure at a resolution well beyond that obtainable with visible light. It also cuts across nearly all research areas due to the extended availability of diverse contrast mechanisms:

1. X-rays are sensitive to chemical contrast near absorption edges. This enabled X-ray techniques like fluorescence imaging to radically change our understanding of trace metals' prevalence and function in biological systems, for example, allowing us to map Zn in Alzheimer-diseased neurons. Other techniques, like Scanning Transmission X-ray Microscopy or infrared imaging, provide microscopic images where proteins, carbohydrates and lipids can be clearly identified.
2. Phase-contrast X-ray imaging is a unique tool to visualise small changes in sample density, such as at polymer interfaces and across cellular membranes. Furthermore, phase-contrast imaging deposits less radiation dose than absorption-based imaging, making it very attractive for investigating radiation-sensitive samples.
3. Polarised X-rays enable electron spin contrast for imaging magnetic states, e.g., the 3D magnetisation in a $GdCo_2$ film. X-ray OAM states are also an exciting new interaction mechanism for imaging spin-orbit systems.
4. Exploiting X-ray diffraction and scattering contrast in imaging modalities provides a unique handle on the order and disorder of matter, for example crystal defects and molecular packing in lignocellulose.
5. X-ray coherence imaging methods have rapidly advanced thanks to the development of ever brighter sources, fast and high-spatial-resolution imaging detectors, and phase-retrieval techniques. Due to the small emittance of our 3 GeV ring, we are uniquely positioned to capitalise on X-ray coherence imaging methods and will keep developing them.

While new X-ray imaging methods and technical capabilities are constantly evolving, it will be essential to manage our portfolio of imaging beamlines that can optimally address the current and future research needs of existing and emerging communities (e.g., cultural and natural heritage, geoarchaeology, etc.). This will also be accomplished by optimising user access to these techniques with user-friendly data collection strategies and efficient visualisation and analysis pipelines.



Three-dimensional coherent x-ray diffraction imaging of ferroelastic domains in single CsPbBr3 perovskite nanoparticles, by D. Dzhigaev, Z. Zhang, L. A. B. Marçal, S. Sala, A. Björling, A. Mikkelsen and J. Wallentin. New J. Phys. 23, 063035 (2021), DOI 10.1088/1367-2630/ac02e0

Science Example

CsPbBr3 is part of a useful class of materials – ABX3-type metal halide perovskites - showing tunable properties for optoelectronic applications. The interplay between chemical composition, crystal structure and phase transitions, provides the dial to tune these properties. For instance, highly efficient light emitters across the entire visible spectral range (410–700 nm) can be manufactured, by partially substituting Cl or I for Br giving cubic, tetragonal, or orthorhombic structure transitions, and the formation of twin domains can be induced. One important question is how such twin substructures modify transport and chemical properties in the vicinity of the domain boundaries relative to the bulk, as strain influences the bandgap and hence the emitted light.

Bragg coherent X-ray diffraction (BCDI) provides a perfect tool to probe the internal 3D nanoscale structures of single crystallites of typically sub-micron size, provided care is taken to tune photon flux, spatial coherence and exposure time (SEM picture of particles in (b)). The measurements map the 3D Bragg diffraction profile (seen in (a)) and can then be used to reconstruct the particle in real space (c). Surprisingly, all investigated particles show the same two domain structure, with similar atomic structure, size, and adjacent domain orientations. (Coherent) imaging techniques, boosted by 4th generation light sources, pave the way towards rapid, high resolution imaging experiments and aid the development of novel perovskite-based devices towards the limits of their capabilities.

Data, artificial intelligence and machine learning

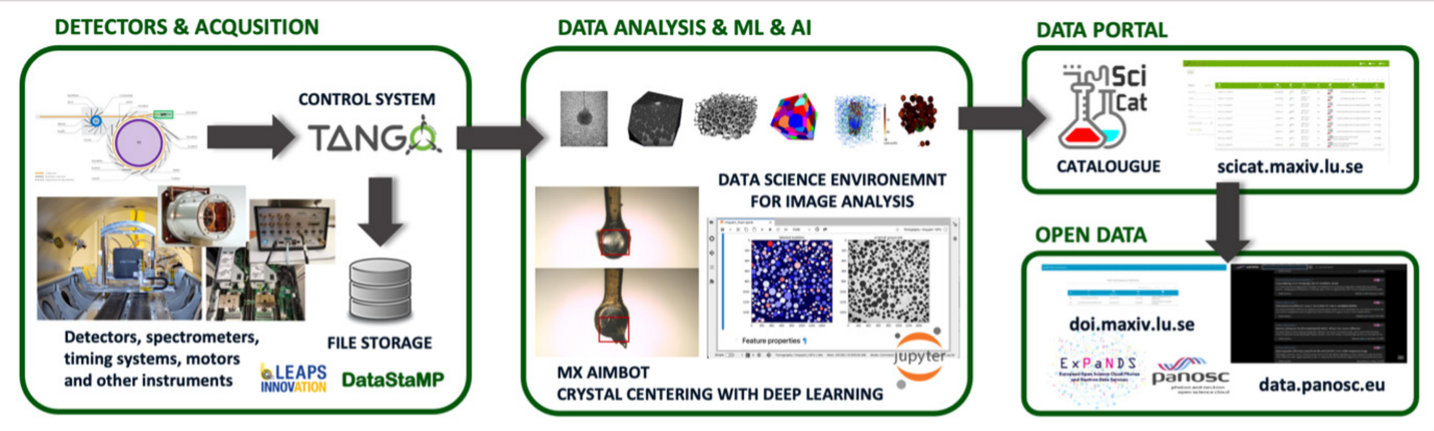
Data-Driven science is a mission-critical part of the operation of all our beamlines and capabilities. Over the next decade, the Open Science, Artificial Intelligence (AI), and Machine Learning (ML) revolution will bring new requirements and opportunities for MAX IV and our user community. This will affect all parts of our IT infrastructure; hardware and software control systems are key tools for driving our accelerators, as well as unique and challenging experiments at our beamlines. Network and high-performance data storage infrastructures are vital for recording data from advanced detectors. MAX IV, with LUNARC and the Swedish national computing infrastructure, provide services supporting experiments at our beamlines before the experiment starts and long after it ends when data analysis occurs.

The transition toward an open science system in Europe sets high requirements for data management at research infrastructures. The modern data management practices at MAX IV build on extensions to data acquisition and metadata harvesting, as well as centralised data storage. This allows a variety of modern and complex services to be efficiently provided for all science disciplines and our scientific data to be shared with other e-infrastructures across Sweden, Europe, and the world. We are participating in the development of an EOSC and a LEAPS initiative in data acquisition and compression. Remote operation and virtual participation in experiments bring new requirements to the control system and the overall support environment.

To optimise MAX IV operation and performance using ML and AI, it is imperative to steer synchrotron technologies towards global industrial standards where possible. ML and AI are becoming important in all levels of system diagnostics, facility and accelerator operation and smart feedback to users during beamline experiments. In the next decade, AI/ML will be used for electron beam and beamline parameters optimisation and, where applicable, for getting the best performance from MAX IV beamlines. To fully exploit these targeted collaborations, resourcing and projects will be needed.

We must continue and deepen collaborations with gateway environments providing access to data processing, analysis, and visualisation tools. We will strengthen connections with scientific communities on the development of synchrotron instrumentation, including synchronisation and motion controllers, sensors, detectors, and data handling protocols. It is also vital to ensure their good integration into the scientific experiments and on-demand access to computing resources. This is all necessary to create a vital data analysis environment where also ML and AI methods can be fully utilised to reveal the potential of the MAX IV light sources.

[13] Set out in the DataStaMP project

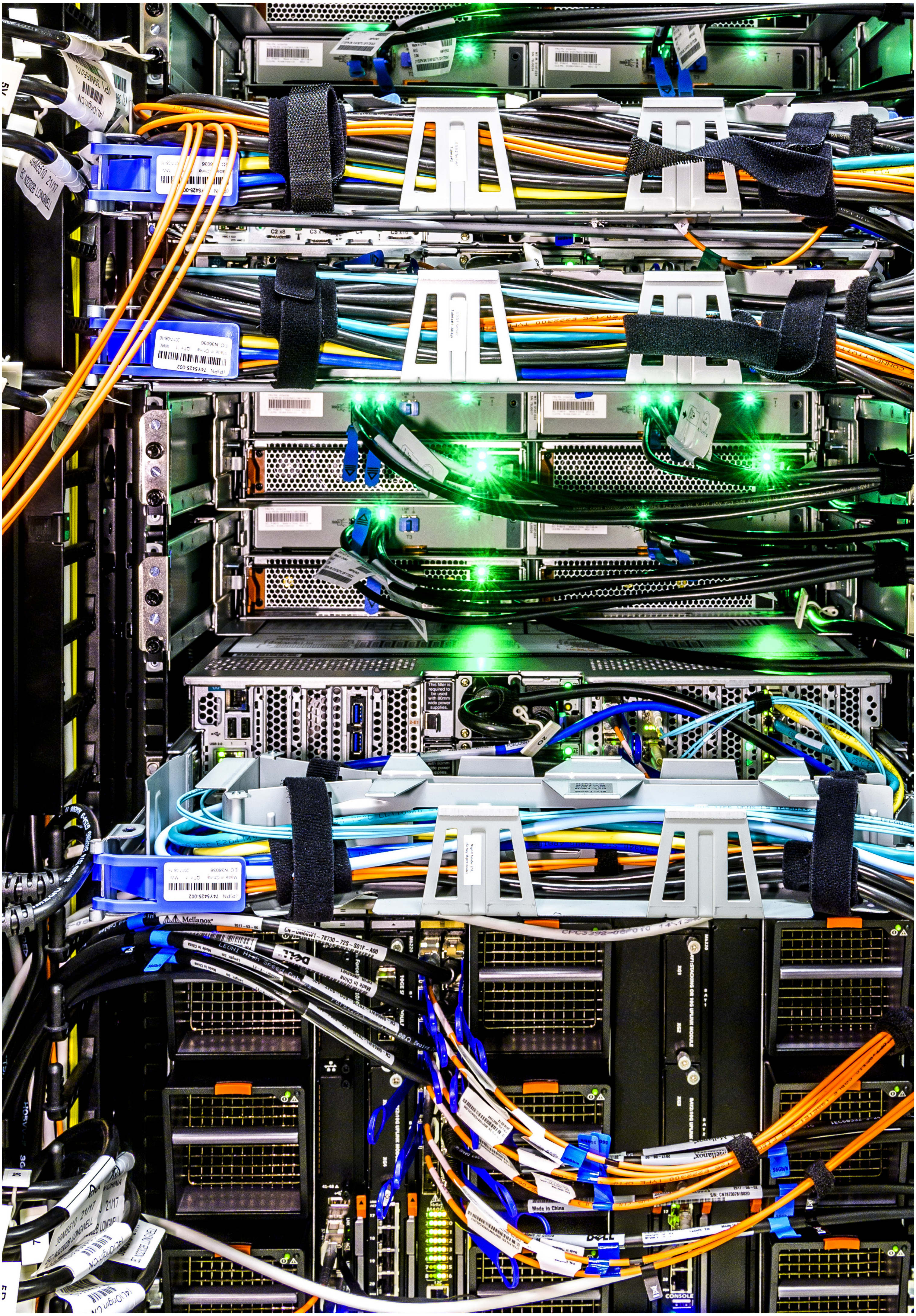


Science Example

Experimental control, X-ray photon detection, timing, data acquisition and data storage belong to the key ingredients of novel and challenging experiments at MAX IV. Data flows from x-ray detectors are growing, robust and effective tools for data analysis are demanded. MAX IV must provide data analysis environment fitting needs of multiple scientific domains. Machine learning and artificial intelligence are finding applications in optimisation of MAX IV accelerators, x-ray optics, beamline parameters, as well as user experiments. Experimental metadata needs to be archived, and MAX IV data should be accessible in Open Data catalogues and EOSC. MAX IV will work together with national (LUNARC, LBIC, LINXS, PReSTO, CiPA and NAISS), Nordic region (QIM) and other photon and neutron facilities (LEAPS Innovation) on developing all elements of the complex data workflow to maximise the value of MAX IV data.

[1] Z. Matěj, R. Mokso, K. Larsson, V. Hardion, D. Spruce, The MAX IV imaging concept, Adv Struct Chem Imaging, 2, 16 (2016); 10.1186/s40679-016-0029-7;

[2] S. Diego et al., ExPaNDS General Architecture description in relation to the EOSC services, Zenodo, (2020); 10.5281/zenodo.3697704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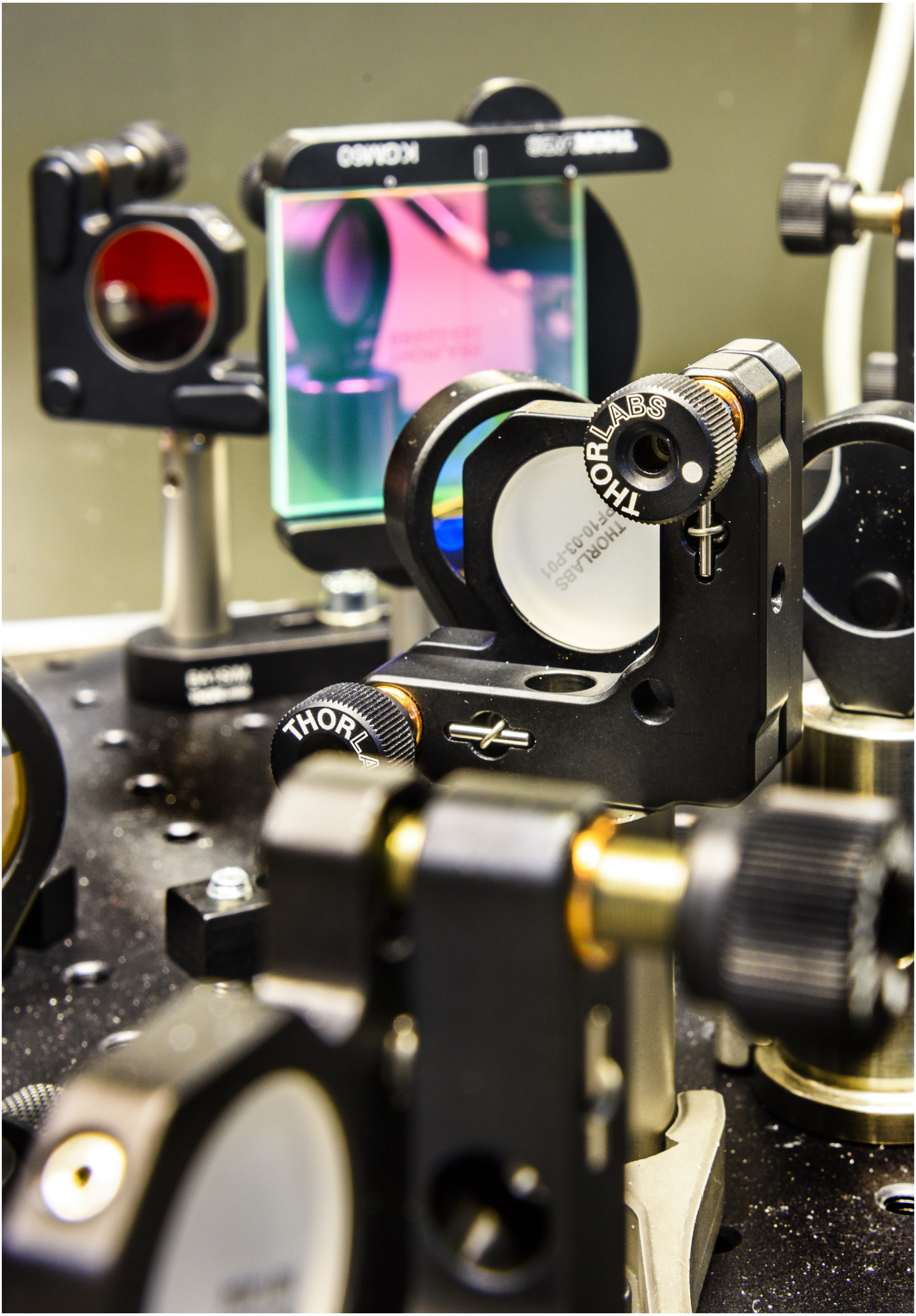
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Objectives for enabling technologies

Continue investing in state-of-the-art detectors, essential for time-resolved and imaging methods. Strengthen coherent X-ray scattering and time-resolved studies, by

- Investment in coherence preserving and manipulation beamline optics.
- Supporting the development of methods and data processing algorithms that utilise coherence.
- Continuing to develop experimental stations' diagnostics for coherent ultrafast X-ray sources.
- Benefitting from collaborations not only in Sweden but also from other synchrotron facilities.

Develop platforms and infrastructures to support imaging

- Strengthen collaborations among complementary (imaging) beamlines and with gateway environments (e.g., LBIC, QIM, CiPA, LINXS, PReSTO, etc.).
- Offer users tailored approaches by providing training alongside guided access to experiment planning, sample preparation, data processing, and analysis and visualisation tools, which is especially beneficial to new and upcoming communities.

Provide a robust open science framework for MAX IV research data.

- Access portal to metadata associated with experiments.
- Sustain a long-term home for MAX IV research data.
- Engagement of Swedish e-infrastructures including LUNARC.
- Integration to EOSC Photon and Neutron Data Services.

Maximise the potential of AI/ML methods for data collection and analysis

- Identify optimisation opportunities in diagnostics/monitoring, beamline alignment, facility and accelerator operation.
- Investigate AI/ML autonomous experiments for some applications.
- Investigate AI/ML-guided expersiments.


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Financial Strategy

MAX IV Laboratory is Sweden's largest national research infrastructure. The total investment in us to date is about 4.5 billion SEK. Maximising the return of science and innovation from MAX IV is, and remains, a national priority. The potential for return on investment is directly proportional to performance and the number of operational beamlines, of which we now have 16 out of 30 possible. To stay at the forefront, the facility must continue to develop its accelerators and existing beamlines and their capabilities further, as well as filling the remaining beamline ports. To stay internationally competitive, a healthy level of reinvestment annually for beamlines is 5-8% of the initial investment.

The cost to build a new individual beamline, 150–200 million SEK, is small compared to the initial and total investments in the Laboratory. A beamline takes about four years to build and about one year of commissioning to bring into user operation. MAX IV Laboratory has the capacity to continue building about one new beamline per year. Every new beamline requires an additional 20–30 million SEK/year to the operations budget.

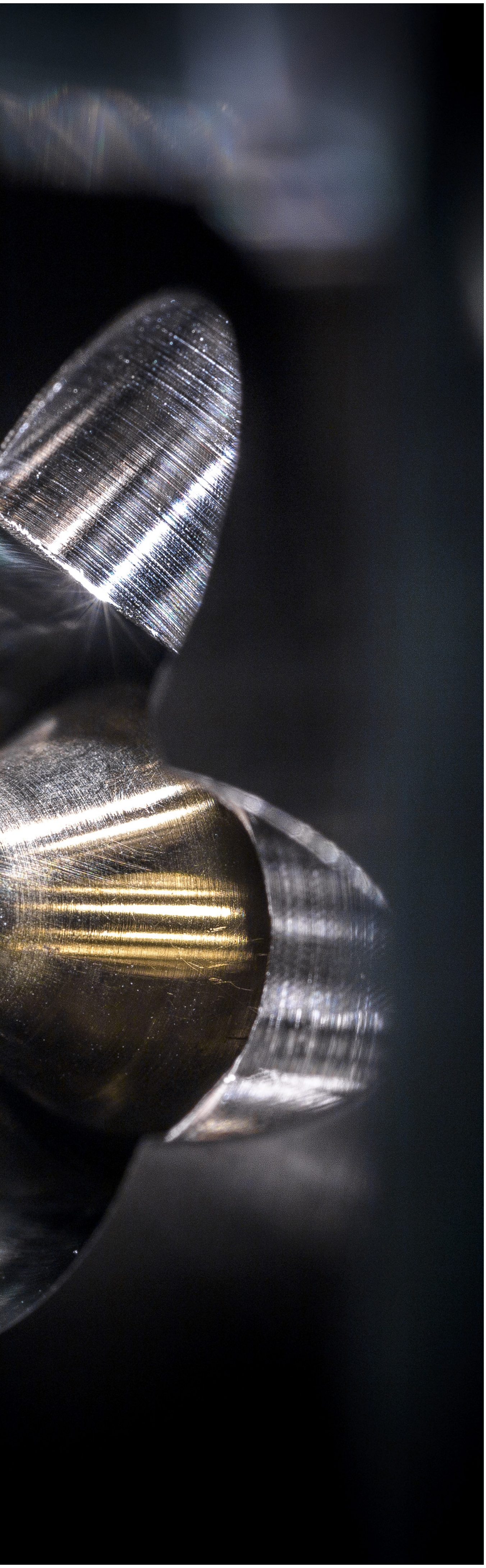
Given the scale of these future investments, the only realistic scenario is for the Swedish government to be the majority funder for the bulk of the future development of MAX IV. Inspired by the funding model for SciLifeLab, we will work toward an independent funding stream directly from the government. MAX IV will work with its user community, especially the Swedish universities, to ensure that the bulk of the funding is planned in the coming Swedish Research Bills ("Forskningspropositioner").

In addition to funding from the Swedish government, MAX IV Laboratory and its user community have benefitted from generous provisions from private foundations, especially the Knut and Alice Wallenberg foundation and the Novo Nordisk foundation. We are most grateful for these crucial contributions, without which the initial investment could not have been raised. We hope that private foundations can provide a crucial boost to get initiatives off the ground early for strategically important beamlines. The Laboratory has also benefitted from generous contributions from sources outside Sweden for beamline investments, beamline operations, and various projects (see Appendix 2). MAX IV will build on existing and new strategic partnerships with its Nordic and Baltic neighbours to further develop its technical capabilities and science programs.

Overall, MAX IV will actively develop its research capabilities in close collaboration with key stakeholders, seek collaboration with partners to identify scientific areas of interest for joint development and increase strategic communication with funders to enable the user community to take full advantage of new funding calls.

The process for doing this is closely tied to our Roadmap. We expect to maintain a prioritised list of up to seven beamlines that MAX IV will aim to realise. MAX IV will actively pursue funding for the top two beamlines on the Roadmap list. In addition, MAX IV will support all beamline proposals included in the Roadmap in maintaining updated documentation (such as Conceptual Design Reports, etc.). The complete list is updated via calls for Expressions of Interest and the evaluation of these. This procedure is described in further detail in the Roadmap document. The proposed SXL will be a significant undertaking and will be managed in a separate track in the Roadmap.

Additions and modifications to existing beamlines will be included in a cost-book-like process driven by the beamlines and their users. MAX IV will seek to partner with user groups, e.g. at universities, to get these funded and realised.



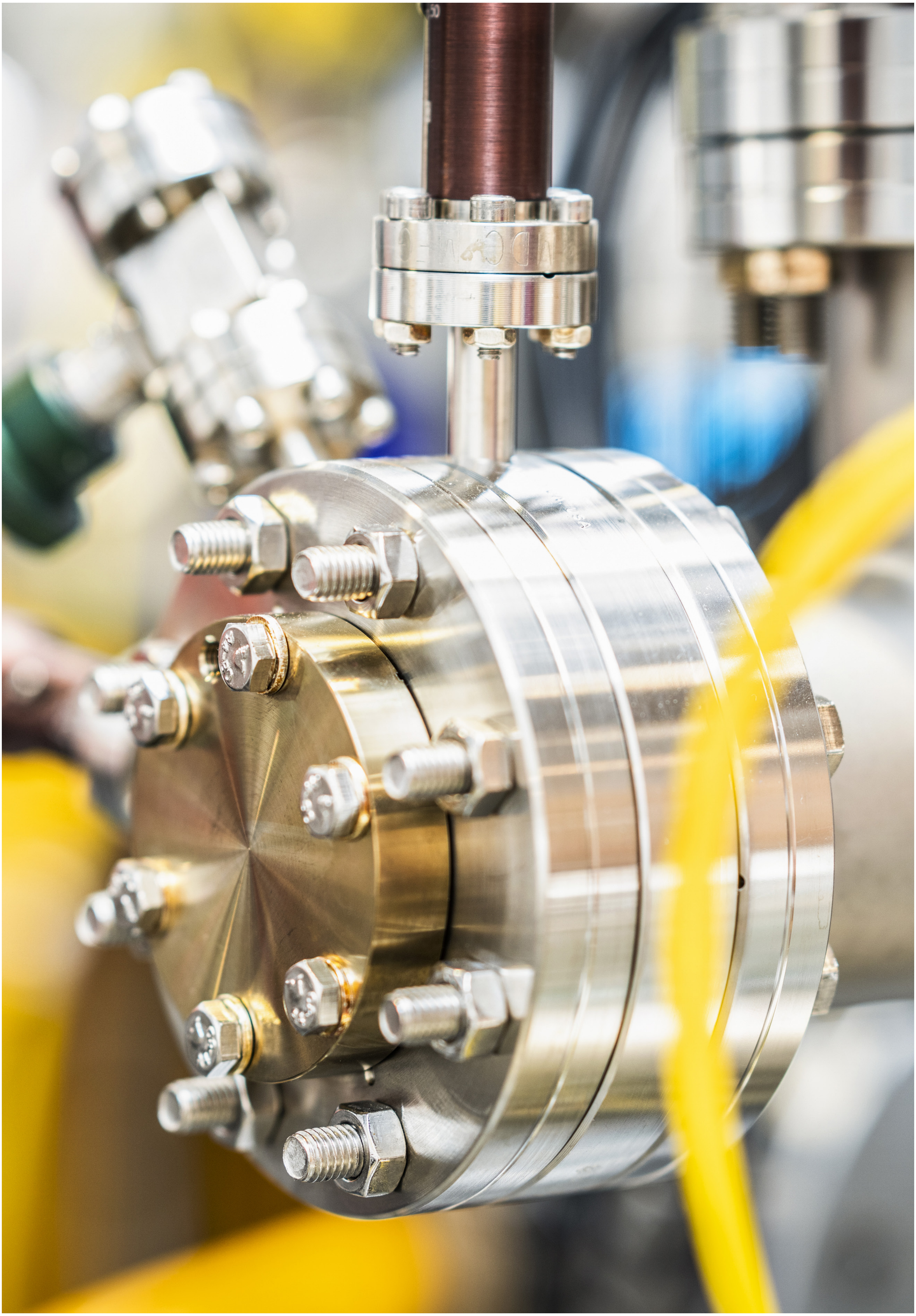
Appendices

Appendix 1 – List of Abbreviations

AI	artificial Intelligence
ALS-U	Advanced Light Source Upgrade
ARIE	Analytical Research Infrastructures of Europe
APS-U	Advanced Photon Source Upgrade
APXPS	ambient pressure X-ray photoemission spectroscopy
ARPES	angle-resolved photoelectron spectroscopy
CDR	conceptual design report
CPO	Central Project Office
CTH	Chalmers University of Technology
DataSTaMP	data storage and management project
DDR	detailed design report
DESY	Deutsches Elektronen-Synchrotron
EOSC	European Open Science Cloud
ESRF-EBS	European Synchrotron Radiation Facility Extremely Brilliant Source
ESS	European Spallation Source
EuXFEL	European XFEL
E-mynd	Swedish Energy Agency
EXAFS	extended X-ray absorption fine structure
FEL	free electron laser
Formas	Swedish Research Council for Sustainable Development
GU	Gothenburg University
HEPS	High Energy Photon Source
ILL	Institut Laue Langevin
IR	infrared
IRO	Industrial Relations Office
KAW	Knut and Alice Wallenberg Foundation
KI	Karolinska Institutet

KTH	KTH Royal Institute of Technology, Stockholm
KU	Karlstad University
LBIC	Lund Bio Imaging Centre
LEAPS	League of European Accelerator-based Photon Sources
Linac	linear accelerator
LINXS	LINXS Institute of Advanced Neutron and X-ray Science
LiU	Linköping University
LnU	Linnæus University
LTP	long term financial plan
LTU	Luleå University of Technology
LU	Lund University
LUNARC	Center for Scientific and Technical Computing at Lund University
MBA	multibend acromat
MIK	multipole injection kicker
ML	machine learning
MSCA	Marie Skłodowska-Curie Actions
MU	Malmö University
MyFab	Swedish research infrastructure for micro- and nanofabrication
NLF	Northern Lights on Food
NNF	Novo Nordisk Foundation
NUFI	Danish Ministry of Higher Education and Science (Nationalt Udvalg for Forsk ningsinfrastruktur)
OAM	orbital angular momentum
PAC	Programme Allocation Committee
Petra III	Petra III storage ring, DESY
PReSTO	software stack for integrated structural biology
PV	photovoltaic
RF	radio frequency
QiM	Center for Quantification of Imaging Data from MAX IV

RISE	Research Institutes of Sweden
RIXS	resonant inelastic X-ray scattering
SAXS	small angle X-ray scattering
SciLifeLab	Science for Life Laboratory
SDGs	UN global sustainable development goals
SIP	Strategic Innovation Programmes
SLS	Swiss Light Source
SLU	Swedish University of Agricultural Sciences
SNIC	Swedish National Infrastructure for Computing
SPELEEM	spectroscopic photoemission and low energy electron microscopy
SPF	Short Pulse Facility
STM	scanning transmission X-ray microscopy
STXM	scanning tunneling microscopy
SU	Stockholm University
SVS	Science Village Scandinavia
SXL	soft X-ray laser
UmU	Umeå University
UU	Uppsala University
Vinnova	Swedish Governmental Agency for Innovation Systems
VR	Swedish Research Council
WAXS	wide angle X-ray scattering
XANES	X-ray absorption near edge structure
XAS	X-ray absorption spectroscopy
XES	X-ray emission spectroscopy
XFEL	X-ray free electron laser
XMCD	X-ray magnetic circular dichroism
XPCS	X-ray photon correlation spectroscopy
XPS	X-ray photoemission spectroscopy
XRF	X-ray fluorescence microscopy



Appendix 2 – Foreign funding

Several projects with various purposes and funding spans were developed at MAX IV in collaboration with foreign partners. Table A1 summarises the past and ongoing collaborations since MAX IV's inauguration in 2016. The outputs of these projects range from joint research activity products (for example sample environment developments) to training of future generations of scientists performing excellent science as users or staff of synchrotron facilities and to transnational access routes for new user communities. The most tangible results of these collaborations have been the construction of, currently, three beamlines relying largely on foreign contributions.

To date, three beamlines currently being part of the MAX IV portfolio were constructed or are currently being built thanks to the contribution of funders from the neighbouring Nordic countries. These initiatives have strengthened the links with user communities from these areas and allowed our facility to develop, addressing the needs of many users. The FinEstBeAMS, DanMAX and MicroMAX beamlines were built based on such international collaborations.

Finnish and Estonian contributions

The financing and construction of the FinEstBeAMS beamline (Finnish-Estonian Beamline for Atmospheric and Materials Sciences) at MAX IV is the result of support for synchrotron-based research in Finland and Estonia at a national level. The Estonian side of the FinEstBeAMS collaboration, headed by Ergo Nõmmiste from the University of Tartu, obtained funding from the European Union (through the European Regional Development Fund) for the project "Estonian beamline to MAX-IV synchrotron". Marko Huttula from the University of Oulu coordinated the preparation of three Finnish Research Infrastructure funding applications that long-term homed funding from the Academy of Finland. University of Oulu, University of Turku, and Tampere University of Technology have been the main Finnish partners in this project.

Marco Kirm from the University of Tartu became the principal Estonian spokesperson of FinEstBeAMS in 2019. Marko Huttula has been the general coordinator of research activities at FinEstBeAMS. The Estonian and Finnish partners continue to invest in FinEstBeAMS after its completion. The researchers at the Institute of Physics of the University of Tartu have recently obtained a grant that will be partly used for instrumentation of FinEstBeAMS, including the acquisition of a third grating for its monochromator.

Danish contributions

Danish involvement at MAX-lab has a long and successful history, with Danish researchers

Table 1: Summary of past and ongoing projects relying on foreign funding.

Country	Funder	Years	Purpose/Project title
EU	EC – Horizon 2020	2015–2018	Cremlin
EU	EC – FP7	2011–2016	Bio-Struct
EU	EC – Horizon 2020	2015–2018	Eucall
EU	Interreg - Tillväxtverket	2015–2018	ÖKS Interreg
EU	EC – Horizon 2020	2015–2020	iNEXT
EU	EC – Horizon 2020	2019–2021	Calipso+
EU	EC – Horizon 2020	2018–2021	Mummering
EU	Interreg - Tillväxtverket	2019–2022	HALOS
EU	EC – Horizon 2020	2019–2022	ExPaNDS
EU	EC – Horizon 2020	2020–2023	iNEXT Discovery
EU	EC – Horizon 2020	2021–2026	NEP
EU	EC – Horizon 2020	2021–2025	LEAPS-INNOV
Finland	Academy of Finland	2017–2021	Operation Collaboration Agreement
Lithuania	Vilnius University	2019–2026	Research Collaboration Agreement
Finland and Estonia	Universities of Tartu, Oulu, Turku and Tampere	2013–2025	FinEstBeams beamline construction
Denmark	Novo Nordisk Fonden	2018–2031	MicroMAX beamline construction and operations
Denmark	NUFI, DTU, AU, UCph	2016–2022	DanMAX beamline construction and development

being frequent guests at many beamlines and covering a wide range of scientific disciplines. The close proximity to Denmark and effective collaboration with MAX IV provided a setting for outstanding science. The DanMAX consortium was formed in 2009 involving Aarhus University (AU), Technical University of Denmark (DTU), and Copenhagen University (KU). The first step towards realising a beamline dedicated to studying "real materials under real conditions in real time" was an infrastructure grant of 35 million DKK from the Danish Ministry of Research. This led to subsequent investments from the three universities, the Capital and Central Denmark Regions and MAX IV Laboratory, and in 2015 an agreement was reached to initialise the DanMAX project. The DanMAX user consortium combines approximately 50 staff members from five major Danish universities and 17 industrial companies. The academic partners of the DanMAX consortium are AU, DTU, KU, University of Southern Denmark, Roskilde University, and Aalborg University. The persons leading the initiative on the Danish side are Bo Brummersted Iversen (AU), Kirsten Marie Ørnsbjerg Jensen (KU), and, previously, Henning Friis Poulsen (DTU).

The Novo Nordisk Foundation has funded the protein crystallography beamline MicroMAX with 255 million DKK. This grant does not only include beamline construction but also operating the beamline until 2031. The beamline is now commissioning, and it will create new possibilities in structural biology in time-resolved experiments. MicroMAX also allows studying the molecules that are most interesting but most difficult to study because they only provide microcrystals and thus this beamline is highly complementary to BioMAX. MicroMAX is part of the Copenhagen Bioscience Cluster – a cluster of world-class research centres and infrastructure within biomedicine and biotechnology in Greater Copenhagen.

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