LEAPS Position Paper on Horizon Europe Missions

20 March 2020

LEAPS
League of European
Accelerator-based
Photon Sources

Europe's Accelerator-Based Light Sources support Horizon Europe mission areas

1. Introduction

Finding an effective way to evolve from an exploitation model of the Earth resources to a sustainable one is an essential and imposing challenge humanity is facing today. A vital element of any long-term solution to this challenge will be new technology to meet our needs for energy and other resources and this, in turn, will require new materials and processes, predicted and realised through scientific research and innovation.

Research Infrastructures (RIs) are precious instruments in these endeavours, thanks to their capacity to serve broad scientific and industrial communities. Accelerator-based photon sources, i.e. Synchrotron and Free Electron Laser (FEL) facilities, have developed spectacularly over several decades and are today critical actors in the materials discovery and innovation chain.

In 2017 all European Synchrotrons and FELs joined forces within the new consortium LEAPS – the League of European Accelerator-based Photon Sources[1]*. Together they deliver X-rays a la carte to a multidisciplinary scientific community of more than 25.000 scientists encompassing physicists, chemists, biologists, and materials scientists, as well as experts from medicine, engineering, earth sciences and cultural heritage and provide a powerful platform to address Horizon Europe (HE) missions*[2]*.*

With their highly focused and coherent X-ray beams, they simultaneously allow the characterisation of materials from the bulk to sub-micron samples', penetrating and imaging them in 3-D with real-space resolution reaching down to the nanometre levels. The photon source brilliance and intensities available and planned across LEAPS Members enable high-throughput and time-resolved spectroscopic images at continuously varying time resolution, from the femtosecond to macroscopic time-scales, including the provision of entirely new possibilities for in-situ and operando experiments for tracking chemical and physical processes under realistic process or reaction conditions.

Europe is today at the forefront in many ongoing advancements in photon source technologies, which continue to boost the fascinating capability for understanding and to predict emerging properties and functionalities of materials.

The latest achievements are the two 4th generation synchrotrons now operating in Sweden (MAX IV) and France (ESRF-EBS). The latter is the first upgrade from a 3rd to 4th generation synchrotron through the adoption of new, cutting-edge technology. Through this upgrade, the users highly benefit from the unique capabilities of the renovated beamlines, and dozens of other facilities are also following such development route. The European FELs are at the vanguard of technological know-how as well.

Collaborative support, coming from EC, the Member States and Associated Countries, is essential for maintaining this global recognition, considering the intense competition due to massive investments for research and innovation in other regions of the world, particularly China, Japan and the USA.

This document aims to be part of the co-creation process of HE strategies and programs, in such a way that RIs, and LEAPS, in particular, may make the most effective contribution possible to the HE missions and grand challenges throughout the next decade and beyond. In the document, section 2 explains how RIs and LEAPS, in particular, are essential players for HE missions, with emphasis on how new developments will make this contribution most valuable. Section 3 changes perspective and brings forward suitable tools which HE programs may implement to best profit from RI contributions to HE missions; collaboration, diversity and integration are inherent to LEAPS' tradition and functioning, as made explicit when describing user development actions with an emphasis on industry. Section 4 looks into complementarity between LEAPS and other analytical RIs, again touching the different mission areas one by one. Finally, section 5 provides a summary of the most important take-home messages.

LEAPS facilities contributing to solving the Global Challenges

LEAPS engagement in COVID-19 research

In January 2020, the WHO declared the recent outbreak of coronavirus disease a public health emergency of international concern. LEAPS facilities with their dedicated and specialised biochemical characterisation techniques support the needs to improve our understanding of the newly identified virus and its possible future evolution as well as to contain the spread, and to develop precise diagnostics and treatment to improve the public health response and patient care.

Several LEAPS facilities have opened priority COVID-19 calls to give rapid access to beamtime for scientists studying the virus.

https://www.leaps-initiative.eu/

2. LEAPS as a key tool for HE mission areas

LEAPS facilities play a crucial role in ongoing efforts to address the vital problems our society is facing now and into the future. The research efforts for finding solutions towards climate change mitigation, curing cancer, clean water resources, smart cities, food security and other possible HE mission areas are already underway in a collaborative manner with other European research institutions, academia and industry, as depicted in Fig.1.

Horizon Europe Mission areas

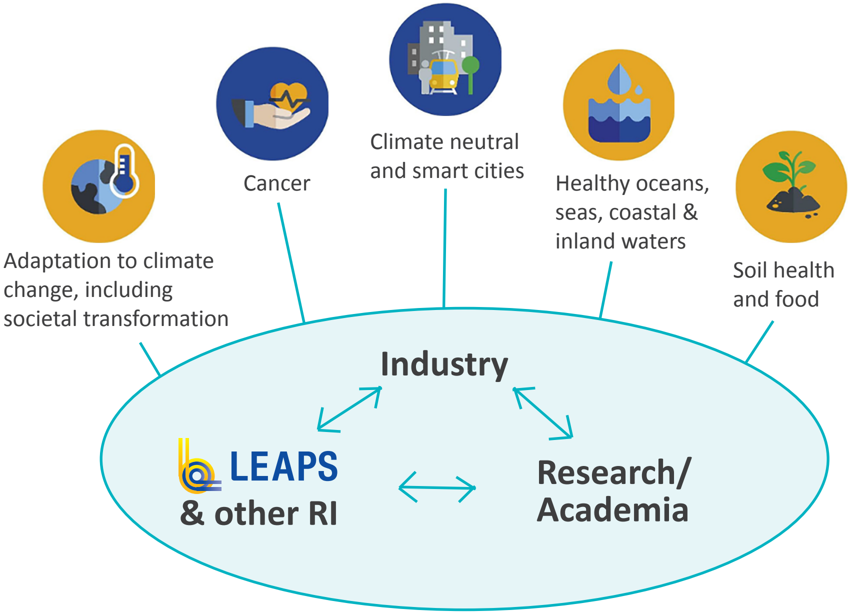


Fig. 1 – Interaction of LEAPS and other research infrastructures with industry and the scientific community in contibuting to Horizon Europe missions.

LEAPS facilities provide essential input on the mining and use of natural resources. The information from multimodal X-ray characterisation deepens our understanding of the formation of minerals, their interaction with the environment and specimen distribution within the soil, which lead to new ways to extract efficiently valuable resources and with reduced environmental impact. Such resources are further utilised by processing to new forms of materials, which very often provide unexpected properties enabling progress in electronics, construction, chemical industry, medicine, transportation, agriculture and others. LEAPS facilities have made significant contributions in guiding the discovery and optimisation of the desired properties of such advanced materials. Together with the advanced recycling, this leads to much more efficient use of the resources and contributes to the circular economy, one of the main sustainable goals of Horizon Europe. One good example is the exotic properties of 2D materials as graphene, which have been revealed and understood thanks to synchrotron-based techniques and has led to optimising the fabrication of products and fostered commercial applications.

Other significant challenges are the adaptation to climate change and the understanding of the anthropogenic impact on water and air quality. Some eight million tons of plastics enter the oceans each year. Among the most pernicious and pervasive of these is the nearly indestructible PET. At the same time, current recycling efforts still lack sustainability. Two recently discovered bacterial enzymes (PETase and MHETase) that specifically degrade PET represent a promising solution for sustainable recycling of PET. Synchrotron studies revealed the atomic structure of MHETase and PETase, thereby furnishing scientists with the necessary information to genetically mutate the enzymes to produce a variant that, even at the first attempt, accelerated the decomposition rate by a factor of three.

Scientific solutions in the field of anthropogenic impact on the environment arise by understanding molecular structures and reactions of relevance to biology and ecology, and also by sampling molecules and trace elements in the ecosystem. The advanced X-rays sources provide much larger photon fluxes than laboratory instruments, a decisive factor for photon-hungry techniques for analysis of trace elements and speciation in ‘real and dirty’ systems commonly present in the environment. This allows the identification of pollutants at the ppb level, for example tracing nanomaterials deposited in cells, living tissues or implants such as hip replacements.

Further in this topic, advanced photon sources also play an important role in providing multiscale insight into the next generation of materials needed to offset the greenhouse gas emissions in general. Materials able to capture, store or catalytically convert CO_2 to added value chemicals are routinely investigated at LEAPS facilities. Such materials operate at elevated temperatures and harsh environments. The invaluable information obtained thanks to the static and *operando* characterisations with ultra-bright X-ray probes, provides a fundamentally new understanding of basic operating principles that becomes practical guide towards large-scale use and commercialisation. Accelerator-based photon sources covering the entire wavelength range from x-rays to infrared are pivotal for the molecular understanding and design of novel catalysts.

Increased urbanisation and growth in population present one of the biggest challenges of our time, where big cities are disproportionately large greenhouse gas emitters. Air and water pollution in such large urban areas drastically affect human health and well-being, with consequences for public health, safety and associated expenditure. To tackle these problems, the chief polluters (transportation, power production plants and industry) must significantly decrease their emissions. These sectors need to become virtually emission-free, using clean energy generation, conversion and storage schemes. For example, very significant improvements in battery and hydrogen fuel cells technologies are needed, what means developing complicated composite materials, integrated into devices, and improved so they deliver sufficient power densities and stability. Multiscale characterisation under typical operating conditions is essential for the understanding of the related processes, where several physic-chemical phenomena play a role. LEAPS facilities offer a unique combination of diverse complementary tools able to explore materials properties and evolution from Angstroms to several centimetres scale.They are already part of large collaborations with European industry and European research organisations to tackle these challenges. Also, the ability of FELs to probe high-speed processes, as charge dynamics that determine bond breaking and creation or charge reorganisation, is essential for rational design and fine-tuning of materials used in emission-free photovoltaics converting the solar energy to electricity. Therefore, LEAPS is well-positioned to significantly impact the development of the technologies necessary to reduce greenhouse gas emissions in urban areas.

To cope with the complexity of the system design, new development approaches like model-based system design technologies supported by artificial intelligence, self-learning and data-driven design methods will be implemented.

LEAPS facilities address public health from a fundamental perspective, such as infectious diseases or cancer research, which is still one of the significant scientific challenges of our time. X-ray microscopy reveals the mechanisms used by active substances to attack pathogens like the malaria virus. IR spectroscopy and microscopy can operate in vivo and provide orthogonal methods for biomarker discovery of metabolic diseases. More generally, membrane proteins (MPs) account for one-third of all proteins and two-thirds of therapeutic drug targets. Despite their obvious importance, their atomically resolved biochemical structures revealed by macromolecular crystallography (MX) are extremely under-represented in the worldwide Protein Data Bank (approximately 1 - 2%). This is mainly due to their hydrophobic nature, which makes crystallisation extremely difficult, limiting crystal sizes to the micron scale. In addition, their small molecular weight excludes them from high-resolution investigations using cryogenic electron microscopy (cryoEM). The upgraded 4th generation synchrotrons will be ideally suited to the investigation of MPs, owing to their small emittance, allowing both a tight focus tunable from the micron to the nanometre scale combined with the low divergence of the beam. A further advantage is the possibility to use serial techniques (serial synchrotron crystallography) in which the microcrystals are delivered either in a flowing medium such as lipidic cubic phase jets or on ultrathin support films.

X-ray crystallography techniques and multimodal imaging are also important in agricultural research, and an essential element in underpinning food security, improving public health and reducing environmental impact. The last century saw major advances in agricultural productivity, underpinned by scientific progress that yielded improved fertilisers (most notably the Haber-Bosch process) and herbicides as well as antibiotics and vaccines. These advances are now threatened by the rise of antibiotic and herbicide resistance. The impact on the environment due to intensive farming techniques, and risks from viruses and pollution, ranging from leaching to chemical processes enhances the need for new agrochemicals and methods to combat airborne and waterborne pollution. As outlined above, multiple advances in technology for x-ray crystallography beamlines will accelerate the structure-guided design of novel compounds and bioengineered reagents (e.g., designer enzymes with bespoke catalytic functionalities).

In the examples mentioned above, LEAPS facilities already provide advanced, multiscale characterisation, which has an essential impact on the fast progress in all science domains demonstrating that LEAPS transversal technologies are important in all mission areas. However, the current state-of-the-art of large light sources still has not reached the ultimate space-time-spectral resolution and high-throughput. The foreseen revolutionary upgrades in technology, as outlined later, will deliver significant improvements to overcome the present limits and will push further the advancements in material discovery, processing and recycling.

3. LEAPS in Horizon Europe programs

LEAPS is ready to contribute to the co-creation process of HE programs with the European Commission and other actors, in particular other RIs, for the best possible HE implementation strategies. Among the tools needed for such contribution, the key ones are joint development of advanced technologies (Fig. 2), a new approach to handling and analysing massive data and promotion and development of the user community, with emphasis on industry. Dedicated funding schemes for the development of these tools in HE would greatly boost LEAPS capacities in delivering solutions within the missions.

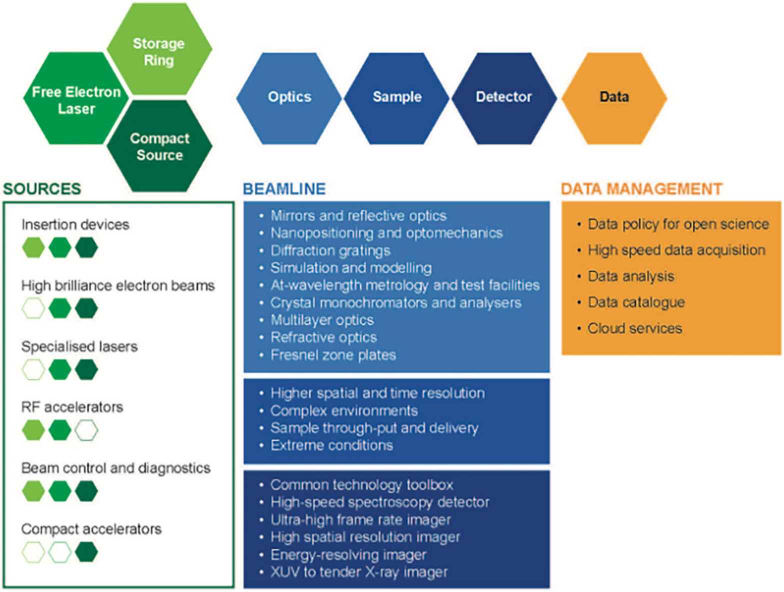


Fig. 2 – LEAPS key technological developments

Technology developments

The status of European synchrotrons and FELs is described in the LEAPS landscape document[3], which also outlines their plans for future upgrades. These transformative developments will enable the investigation of complex functional materials and biological systems at the relevant length and time scales, often under *operando* conditions. Together with complementary techniques, such as cryo-electron microscopy or neutron scattering, they are vital for solving scientific and societal challenges in the future, from enhanced care for an ageing population to cleaner, more efficient transport and manufacturing processes. The delivery of the requested science breakthroughs will require the development and effective exploitation of new technologies to enhance the capability and capacity of these facilities, through partnership and smart specialisation across LEAPS members. Thanks to the development of these new technologies, LEAPS will become a key tool to fulfil the goals of the HE mission areas, as described in the previous section.

Technological developments are proposed for every step on the path from the photon source to the analysis of the data collected, starting with the generation of yet more brilliant, coherent beams, passing through beamlines with better optics, sample environment and detectors. In a nutshell, a list of key technological developments for LEAPS will include:

- insertion devices for brighter, harder X-rays;
- next generation optical systems capable of optimising the X-ray beam characteristics for the experimental needs whilst preserving the source brilliance, thus enabling the full potential of finer, brighter, more coherent beams to be exploited;

- new detectors for X-ray spectroscopy, with the ultimate aim to detect a very single photon that carries relevant information from the sample;
- sample handling and environment allowing fast scanning, extremely precise (sub-nanometre), stable and reproducible, positioning systems or fast delivery systems

Data

All LEAPS RIs are already confronted with the exponential growth of data volumes resulting from year-on-year improvements in photon source properties, beam delivery and detector technology which will be boosted further by the planned upgrades to sources and beamlines. Far greater computational power will be required to enable researchers to visualise what they measure sufficiently quickly to make informed decisions about the next step in an experiment. Further processing on completion of measurements will involve quantities of data that cannot be transferred and analysed at most home institutions using current means. Future requirements for data handling are not scalable in terms of current technology, budgets or environmental impact and will need both improvements to hardware and development of new algorithms that will increasingly use artificial intelligence (AI). This challenge can only be met effectively through the creation of a pan-European collaboration in Information Technology (IT).

LEAPS RIs will collectively address the common technical challenges of data growth from experiment through analysis to scientific results through single solutions and deliver well beyond what they could deliver if they continued to act largely independently. Bidirectional collaboration with industry, open-source licensing, standardised open data access policy, federated access mechanism, data analysis services (involving high-performance computing where necessary) and data mining approaches are some of the key ingredients to make data, information and knowledge from LEAPS RIs more readily accessible to the scientific community and industry. A close collaboration between different RI communities is ongoing in this area for the photon and neutron facilities in the projects PaNOSC and ExPaNDs, in the strategic context of EOSC.

Both LEAPS RIs and industry suffer from an acute skills shortage of data scientists and scientific software engineers. Through an extensive programme of education, training and outreach, LEAPS RIs will complement university-based education and training programmes to develop specialists in these areas. LEAPS IT will open up innovation opportunities for RIs in several data, information and knowledge domains.

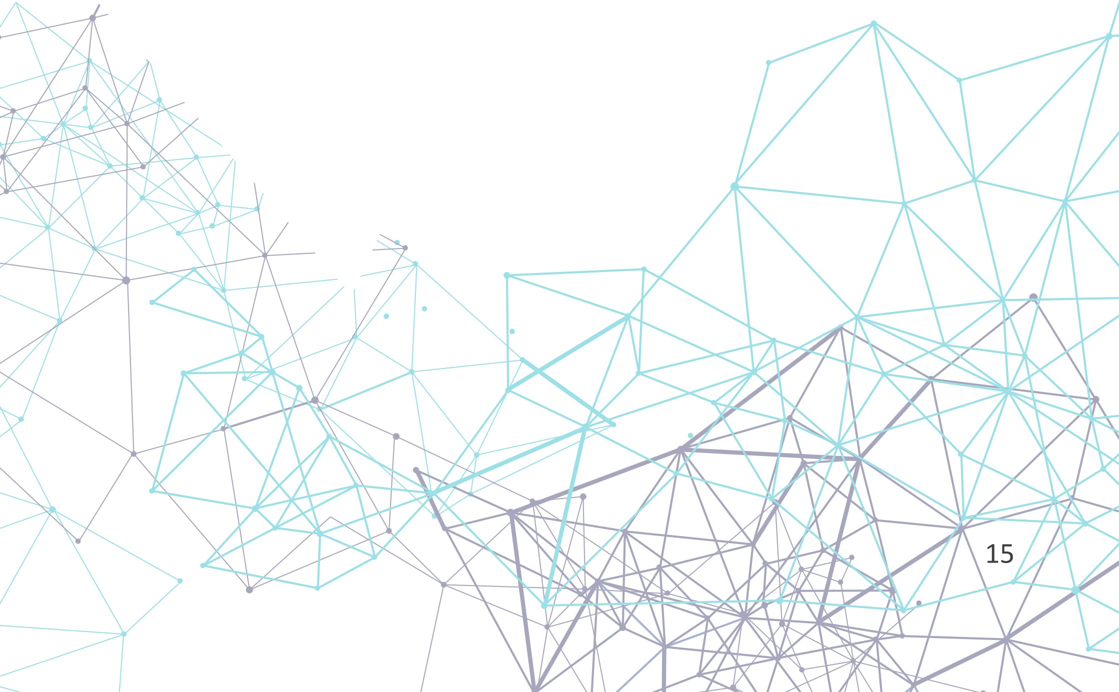
User Community

LEAPS engagement with the scientific user communities will help them to build a wider bridge to meet the global challenges and missions of HE. It will enable the existing users of its facilities – from both academia and industry – to exploit their full potential. It will lower barriers to access the advanced capacities of its facilities for new users from all European countries, new research communities, and industry – in particular, SMEs. It will also support and engage with science communities worldwide.

LEAPS will provide the next grade of optimum conditions for users, stimulating their widest participation in response to the needs formulated by their communities. Countries that do not host LEAPS facilities will be better integrated, and this will widen and strengthen the European User Community.

To this aim, LEAPS could implement priority access schemes to its facilities and development of dedicated services to certain user communities of the HE missions. Such support will likely be defined in the next Work Programme for 2020, to be updated in spring 2020, and the subsequent Work Programmes.

Another very interesting option is the joint development of scientific instruments by key user groups and beamline experts of LEAPS facilities towards future needs in addressing the global challenges defined in HE and in particular to contribute to HE Missions. Thereby, bridges from Pillar 1 (Science Excellence) to Pillar 2 (Global Challenges and Industrial competitiveness) of HE could be efficiently built.



4. Complementarity between European Facilities for Analysis (EFA) in the context of Horizon Europe

This section briefly addresses the complementarity of different types of analytical facilities concerning HE mission areas. It contains a summary of the outcomes from a collaborative meeting held at Brussels on 21st February 2020, in which representatives of relevant RI networks in Europe had the opportunity to exchange impressions and discuss joint approaches for the benefit of science and society. In particular, the meeting, organised by LEAPS, was attended by DREAM (electron microscopes), EMFL (High Magnetic Fields), LaserLab (lasers), LENS (neutron sources), and RADIATE (ion sources), plus representatives of networks which include different kinds of instrumental techniques, like CERIC-ERIC.

Cancer

Analytical methods combined with multi-modal and multi-scale scale and beyond are needed for understanding the complex processes, which happen on a time range up to weeks, involving dynamics from tissue down to the molecular level. Structural determination is an essential step in drug discovery where electron microscopy and NMR efficiently complement X-ray macromolecular crystallography. In addition to early detection, preventing cancer requires understanding, in particular, the effect of food additives or nanoparticles. Here again, neutron scattering, laser spectroscopy, electron microscopy make important contributions complementing those of synchrotron facilities. Finally, regarding cancer treatment, lasers can be used for diagnostics. Ion accelerator and laser communities are joining forces to develop cheaper hadron treatment facilities. Ions, laser and neutron facilities are also involved in the production of nuclei for cancer treatment.

Climate neutral and smart cities / Adaptation to climate change

The main contribution analytical facilities make to the climate-neutral, and smart cities and adaptation to climate change missions is in materials development, including developing less energy-hungry processes for building and structural materials manufacturing (lean steel, green concrete/cement), catalysts for lower emissions, energy (batteries, supercapacitors, fuel cells), information technology (quantum materials) or resource valorisation and recycling. Here again, the complementarity between analytical facilities is essential: synchrotron and neutron facilities provide *in situ* and *operando* characterisation techniques, bridging scales from macroscopic to atomic. They are complemented in particular by electron microscopy, which provides the ultimate spatial and chemical mapping resolutions.

Soil health and Food

Soil health requires understanding composition, co-localisation and speciation of elements present in soils, as well as transport mechanisms and remediation processes. Synchrotrons provide the sub-ppm elemental analysis (x-ray fluorescence), speciation, chemical state of elements (XANES, EXAFS, photoemission...) and correlative imaging (IR, UV, soft x-rays, hard x-rays) combined to electron microscopy which provides the highest resolution. Neutron scattering is essential for hydrogenated samples. Ion facilities provide the highest sensitivity to traces, accelerator-based mass spectroscopy having a sensitivity down to atoms. Lasers have the unique capability to be transportable to the field. Food research requires, in addition, structural and textural information where neutrons efficiently complement x-rays for organic matter. Lasers have the remarkable ability to provide non-intrusive spectroscopy sensing inside a package for food quality control.

Healthy oceans, seas, coastal and inland water

Like for soils, the analytical capabilities of synchrotron facilities are essential for speciation of elements, including their chemical state and binding, determining bioavailability. They are complemented in particular by ion facilities for trace element analysis including the use of radioactive tracers for investigating ocean streams, monitor the rate of carbon sink, coastal water flows, groundwaters (accelerator-based mass spectroscopy). Electron microscopy is essential in the investigation of nanoparticles, e.g. microplastics. Lasers add the possibility of remote sensing.

5. Summary and conclusion

RIs are a compendium of technical developments, scientific imagination and revolutionary ideas devoted to answering basic knowledge questions and now increasingly addressing specific societal problems. Boosting RIs' capacities is a high return investment. Joint commitment in this sense from the funding agencies of Member States and Associated Countries and EC programs is an opportunity to make Europe and its industries strong players in the sustainable future of our planet.

LEAPS members are actively participating in moving forward in HE Missions areas, and ready to contribute in designing reachable objectives. The LEAPS technological roadmap depicts the areas where upgrades will have the leading role for the step-change in understanding basic properties of matter and for helping industries in developing materials and drugs, tackling Mission goals.

Collaboration within the European Research Area (ERA) with other RIs communities takes advantage of the complementarity among experimental techniques, as made clearly explicit in the first EFA joint meeting held at Brussels on 21st February 2020. The strength of EFA lies in its scientific and technological capacities and in its users, hailing from all European countries, beyond those that host the facilities. The Member States, Associated Countries, and their facilities should optimise the funding instruments under HE available to researchers and innovators across all Europe for the benefit of the society.

References

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2 https://leaps-initiative.eu/wp-content/uploads/2019/11/LEAPS_Strategy2030_June2018.pdf
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Mission

LEAPS will use the power of its combined voice to ensure that member light source facilities continue to be world-leading, to act as a powerful tool for the development and integration of skills with a view to address 21st century global challenges, and to consolidate Europe's leadership in the field.

Vision

A world where European science is a catalyst for solving global challenges, a key driver for competitveness and a compelling force for closer integration and peace through scientific collaboration.

Working together in LEAPS