Science and Technology Facilities Council

A Strategic Vision for the UK's Large-Scale Light Source User Facilities

November 2021

Foreword

The large national and international research facilities that we operate ourselves or through partnerships are vital elements of UKRI's support for UK science and innovation in both academia and industry. Among these facilities, large-scale light source user facilities exploiting synchrotron, solid state and free electron laser technologies are central to an incredibly broad range of leading edge, multidisciplinary, UK science and innovation advances. Here we outline a vision to provide UK researchers with the best access to light sources, nationally and internationally, matched to current and anticipated needs.

In 2019, UKRI initiated a future research infrastructures programme to identify and plan for the next generation of facilities that will be needed to meet the increasingly complex challenges across all areas of UKRI's remit. This strategic vision for future light source facilities provides a timely input to that planning process, not least by highlighting the important complementary capabilities of these different sources. It is increasingly rare for major advances to be achieved using a single investigatory technique in fields such as drug development and novel materials for energy systems.

It must be recognised that advances in new light sources on their own are not enough. We must also ensure that we are fostering the skills and expertise needed to exploit these new tools and their associated instrumentation. Equally important is the need to equip the facilities and their users with the data handling and analysis capabilities that will ensure that all of the hard-won performance gains can be captured and used.

As more attention is, rightly, placed on mitigating the effects of climate change and other unsustainable practices, we must ensure that these new research infrastructures have a strong focus on maximising the sustainability of their construction and operations. The next generation of tools that we develop must be part of the solution and not add to the problems by creating avoidable impacts on our environment.

As the Executive Chair of STFC, I am immensely proud of the contributions our existing light sources have and continue to make to supporting research into COVID-19. I strongly believe that elements of this strategic vision for future light sources can ensure that we continue to have the right tools to drive achievements across many similarly important areas of science and innovation, directly benefitting our own nation and helping to make the UK a science superpower. I hope you find this strategic vision report an informative and stimulating presentation of the opportunities that lie ahead.

Professor Mark Thomson

Executive Chair, Science and Technology Facilities Council

Executive Summary

User facilities employing cutting-edge light source technologies form a critical part of the research infrastructure that UKRI provides in support of the UK's research base across academia and industry.

Light sources are used to address science and technology challenges across a very wide range of research fields. In order to meet the capacity and capability requirements of this large user community, UKRI supports national facilities in the UK and access to multinational facilities overseas, which include synchrotrons, lasers and free electron lasers (FELs).

The UK's light source community is also well connected through formal and informal partnerships with a network of facilities around the world, which facilitate ad hoc access to supplement that supported by UKRI.

This strategic vision summarises the science and innovation challenges being addressed by light sources, and identifies where there are opportunities for sources with new performance characteristics to enable breakthroughs in research and exploitation in fields such as energy storage, drug development and the application of quantum technologies. It presents a compelling case for maintaining the current portfolio of UK facilities, and strong scientific and competitiveness arguments for significant upgrades. There is also an emerging case for increasing access to an additional new type of national facility, an X-ray free electron laser (XFEL) source, that would bring significant new capabilities not accessible through existing national sources.

Key elements of the Strategic Vision for Future Light Sources

- To maximise the range of applications and science gains, a balance of capabilities should be maintained, rather than focusing on any one source type. This can be achieved by a combination of upgrades to existing sources and increasing access to X-ray FELs.
- Future facility developments should seek to exploit the potential for synergies between the sources, for example in areas such as detector systems.
- Supporting the user communities is critical so that new capabilities can be fully exploited and researchers from fields with less experience of using the facilities and the techniques can achieve successful outcomes.
- Strengthening the UK's light source capabilities and research expertise will help the UK remain a partner of choice in international projects and help enable UK industry to achieve leadership in key technological areas such as photonics.
- There is a limited pool of expertise (in the UK and world-wide) with the skills needed to design, build, and operate large scale, complex light source user facilities. These skills are in demand across all research areas and industry. Being able to access these resources will be a critical constraint on any future source developments.

- Data volumes and rates from light source (and other) facilities is growing steeply. Data handling and analysis capability needs to be considered as an integral part of all future source development plans or there is a danger that the anticipated science gains will not be achieved.
- Light source facilities and the related technologies are areas of rapid progress, and upgrades and new facilities can take several years to bring online. There is a danger that existing facilities can fall behind international progress and the UK research community loose access to cutting edge capability if future developments are not planned in a timely manner.

Large scale light source user facilities require significant investments to build and operate. To help guide the optimal future developments of the UK's light source capabilities within the next twenty years, this strategic vision examines a broad range of options for each source type. Specific source types are not prioritised; rather the need to maintain and develop the full breadth of source types is considered such that the UK remains able to meet as wide a range of science and technology challenges as possible. The usual science and business case production process that UKRI follows on behalf of the UK government, our international partners and other interested stakeholders, will determine how development of each source type is implemented. For the largest sources, this planning and implementation cycle can last several years, while smaller sources and upgrades may proceed on a faster timescale.

To inform decisions that will maximise complementarity with future source specifications, this strategic vision seeks to provide a coherent framework in which the diversity of potential source developments can be set, considering the research benefits and the opportunities for synergies that each can achieve. Part One of the document sets out the role that light sources play as a key part of the UK's research infrastructure and presents an optimal plan for future capacity and capability. Part Two provides details of the science and innovation challenges that light sources are addressing, and also details the options that have been considered in developing the optimal future source plan.

Contents

Foreword

Executive Summary

1. Introduction 1

Part One 5

2. Why light sources have become so important 6

3. Light sources – characteristics and the status of current facilities 11

3.1 Light sources as part of the suite of probes 11

3.2 Characteristics and complementarity 12

3.3 The principal current sources 15

3.4 International context and trends 17

3.4.1 Introduction 17

3.4.2 Synchrotron radiation and Free electron laser facilities 17

3.4.3 High performance lasers 21

3.4.4 Electron microscopy facilities 22

3.4.5 Trends: Gaps, challenges and future needs 23

4. A plan for future light source provision 24

4.1 Summary of the principal source options 24

4.2 Future light source development planning 28

4.2.1 Factors influencing source development planning and timeline 28

4.2.2 Building the user community and skills 29

4.2.3 Data management and computation 29

4.2.4 A balanced development plan and timeline 30

4.2.5 New sources 33

5. Implementing the light sources development vision 34

5.1 Capacity and capability 34

5.2 International collaboration and partnerships 34

5.3 A holistic facility model 34

5.4 Building the user community 35

5.5 Innovation and industry 35

Part Two 36

6. The science and technology drivers for light sources 37

6.1 A diversity of applications 37

6.2 Life sciences challenges 38

6.2.1 Novel healthcare technologies 40

6.2.2 Complex biomolecular structures including plant science 42

6.2.3 Biotechnology and biological systems 44

6.2.4 Imaging across scales: Connecting the cellular and organism levels 44

6.2.5 Biological challenges at the atomic and molecular scale 49

6.3 Physical sciences challenges 52

6.3.1 Chemistry 53

6.3.2 Advanced materials and engineering 56

6.3.3 Energy materials 59

6.3.4 Properties of matter in extreme conditions 62

6.4 Underpinning functions 69

6.4.1 Detectors 69

6.4.2 Data handling and analysis 69

6.4.3 Sample preparation and environments 69

6.4.4 Specialist engineering 69

7. Future light source options 70

7.1 Option categories 70

7.2 Option details and analysis 70

Annexes 83

Annex 1: Profiles of principal sources 84

Annex 2: Glossary 92

Annex 3: References 95

1. Introduction

A central element of UK Research and Innovation's (UKRI) role is the provision of world-class science facilities for the UK's research and innovation communities. The Science and Technology Facilities Council (STFC) is responsible for providing the critical large-scale research infrastructures that support industrial and academic researchers across the whole spectrum of science, both in terms of operating the UK's own national facilities and of facilitating access to the network of overseas and multi-national facilities.

Light source facilities are perhaps the most diverse in nature, operation and scale of all the types of user facilities that UKRI supports. Our light sources range in scale from room-sized laser systems to synchrotron sources the size of a large sports stadium. They can generate photon energies covering 10 orders of magnitude – ranging from the infrared to gamma rays. As a result, these facilities are supporting cutting edge science and technology advances across many of UKRI's areas of interest, and are increasingly being used by industry. This strategic vision considers the future needs for multi-user central facilities, whilst recognising that several universities and research bodies will continue to other host light source systems.

The government's *Research and Development (R&D) Roadmap* [i] sets out its ambitions to further strengthen science, research and innovation across the UK, making them central to tackling the major challenges we face, and taking advantage of opportunities. Light sources will help deliver on many of these ambitions including:

- providing world-class, cutting edge infrastructure
- enabling innovation in areas such as energy storage technology and drug development
- supporting UK leadership in addressing science and technology challenges such as quantum technologies
- helping nurture talent, from apprenticeships to Future Leader Fellowships
- being a partner of choice in international collaborations and multi-national facilities
- supporting research and innovation across all regions of the UK through the widespread user communities.

Photon-based techniques are powerful ways to image, probe and reveal the nature of matter in all its forms – from atoms and molecules, to living cells and engineering structures. To answer the most challenging research questions will require photon beam generators that are pushing the boundaries of what is possible. These highly complex light sources are most effectively built and operated in well-founded research infrastructures that can be accessed by large, diverse and geographically spread user communities.

In 2019, UKRI published *The UK's research and innovation infrastructure: opportunities to grow our capability* [ii]. This analysis of the UK's science infrastructure identified that *"The ability to analyse complex structures in more detail and over time is increasingly important across a variety of disciplines. We need to invest in a variety of capabilities including both major upgrades and new infrastructures that may include synchrotrons, lasers, FELs, X-rays…."*

As well as enabling major science and technology advancements, light sources also play an important role in translational research and innovation by industry. A recent report by the Photonics Leadership Group [iii] identified the increasing value of photonics to UK society and the economy. Companies that manufacture or deliver services based on photonics technology produce goods and services worth around £13.5bn each year, representing a gross value added of £5.3bn to the UK economy. The continued growth of the UK photonics industry reflects the critical role that light plays in the development and manufacture of current and next-generation products. Whilst the photonics industry is much broader than the light source types covered in this strategy document, the fundamental physical, chemical and biological advances made in experiments at large-scale light sources offer a significant stimulus for many technological developments exploited by photonics companies and, more widely, by other technology industries.

Planning for UKRI's future infrastructure programme is underway, and each facility will need to develop its own robust rationale and business case for inclusion, and to secure the necessary investment. This strategic vision for large-scale light sources provides UKRI and other stakeholders with an overarching and holistic view of the opportunities and benefits of investing in new and upgraded facilities that use photons to probe, image and analyse the composition of matter in all its states. The document is structured in two parts:

RapID is a pioneering laser-based instrument that can pinpoint the chemical make-up of materials whilst they are still wrapped in packaging, enabling pharmaceutical firms to cut the time and cost involved in verifying the raw materials used in drug manufacture. The technique was first developed at the Central Laser Facility (CLF) and has since been commercialised by Cobalt Light Systems, now part of Agilent Technologies.

https://stfc.ukri.org/files/cobalt-light-systems-impact/

A research team, from HP Labs and the University of Bristol, is using Diamond Light Source to investigate pigment suspensions that change hue in reaction to an applied electric field. This is helping to develop more energy efficient display screen technologies than current liquid crystal technologies.

https://www.diamond.ac.uk/industry/Case-Studies/Case-Study-HP-Display-Technologies.htm

Part One provides:

- An introduction to light sources and why they have become important scientific tools (Section 2)
- A summary of the current source types and facilities in the UK, and those internationally that are accessed by UK users.
- An overview of how this suite of source types and facilities complement each other and provide a match to the capacity and capability requirements of the research base (Section 3)
- A vision for realising the optimal capacity and capability over the next 20 years (Section 4)
- Implementation factors that can help inform the decisions that will need to be taken for an investment programme in future light source provision (Section 5).

Part Two contains more detailed technical information, including:

- Details of the science drivers, challenges and innovation opportunities and the future capabilities and capacity needed to respond to the science challenges (Section 6)
- The future options for the principal source types and facilities (Section 7).

Short profiles of some of the principal light source facilities are included in an Annex. From an analysis of all the options for future light source provision, the strategic vision is for an ambitious, balanced development plan that will maximise the benefits across a wide range of science and technology areas. Therefore, the report does not prioritise between source types.

Several promising technology developments may provide new alternatives to the types of light sources detailed in this strategy, such as plasma wakefield accelerators as compact sources of X-rays, and room-sized synchrotrons using Compton scattering. Facilities based on these techniques are, however, unlikely to be able to fulfil the current and anticipated user demands within the twenty-year view taken in this strategy.

Supporting services, systems and technologies – such as detectors and instrumentation, accelerator and cryogenics technologies, and sample manipulation and environments – are essential components of all large science facilities. Although these are not covered in detail within this document, it is recognised that these will prove integral to the successful operation and exploitation of all the facilities discussed. Some of these elements are addressed in other strategy documents that STFC has prepared. [iv]

The next generation of research infrastructures, including light source developments, will result in a step change in the quantity and complexity of the data produced. **Enabling research community users to access and analyse this data effectively, including the use of artificial intelligence tools and remote access capabilities, will be as critical as the source technology developments in realising the anticipated science and technology gains.**

Building, operating and exploiting the light source facilities identified in this vision will require expertise and skills in a wide range of science and engineering specialisms. These skilled resources are already in high demand by research institutes and industry across the UK and internationally. **It is very likely that access to these skills will be a major constraint to how quickly the light source developments identified in this vision can be achieved.**

Part One

The first part of this strategy document provides an introduction to light sources and explains how they: are used as complementary probes of biological and material samples; enable imaging at extremely high spatial and temporal resolutions; and create matter in extreme and exotic states. The current status of light sources around the world is summarised, including those that are most important for UK users.

A strategic vision for the UK's future light source capability and capacity is then presented, drawing upon the analysis of options that is set out in more detail in Part Two.

Images courtesy of Diamond, EuXFEL and ESRF

2. Why light sources have become so important

Light sources and facilities, with their wide-ranging capabilities and diagnostic techniques, have become established as a critical component of the toolkit for researchers in the physical, biological and life sciences. Their use is helping to address complex science, technology and industrial challenges in all the goals set out in UKRI's Delivery Plan. [v]

The use of specialist light sources for imaging and probing applications in science, engineering and medicine, in universities, institutes and industry, has grown significantly over the past half-century.

Pushing the frontiers of human knowledge and understanding

- Synchrotrons help refine the structure of new high performance materials and the molecular structure of new drug compounds
- XFELs help to understand the properties of quantum materials
- Lasers can replicate the conditions at the centre of stars

Delivering economic impact

- Synchrotrons are solving metal fatigue problems in high value aircraft engine turbine blades, extending their safe operational lifetimes
- High power lasers can drive fusion reactions with the potential for a clean and safe nuclear energy source
- XFELs are helping optimise sustainable catalysts and light harvesting technologies

Creating social and cultural impact by supporting our society and others to become enriched, healthier, more resilient and sustainable

- Synchrotrons can investigate and help preserve rare cultural artefacts
- Lasers can reveal the presence of dangerous substances in cargo and luggage, making travel safer for everyone
- Lasers are helping to investigate resistance mechanisms to anticancer drugs

Meeting the Challenges

Figure 1: How light sources are helping to deliver UKRI's goals

A key aspect of this growth has been the development of source capabilities and the performance required by new applications increasingly going hand in hand, with each driving the other to break new ground.

Up to the late 1950s, light sources were all incoherent (i.e. with no inherent phase relationship) and effectively steady state in operation. Typical small-scale, stand-alone sources and applications included:

- Ultraviolet (UV) sources for lithographic processing
- Electron beam generated X-ray sources for low resolution medical imaging
- Incandescent lamp sources for simulating sunlight to test solar energy systems.

The first low power coherent photon sources – initially microwaves (masers), followed by infrared and visible light lasers – were invented in the 1950s and early 1960s. Initially described as "a solution looking for a problem", there has subsequently been a huge expansion in the performance characteristics of lasers such as frequency coverage, pulse energy and power, pulse length etc. This has enabled a multitude of applications benefitting science, medicine, technology and society, including industrial processing, high-speed fibre communications, consumer devices, fusion research, and photobiology.

Accelerator-driven light sources emerged through the 1960s and 70s. Synchrotron sources utilise the radiation emitted when electron beams travelling at speeds approaching the speed of light pass through strong dipole magnets or arrays of powerful magnets of alternating polarity – known as insertion devices – within closed rings.

Photon beams with a broad range of radiation energies and sustained stability can be generated, with intense X-ray beams the most frequently accessed, as these cannot be produced with comparable utility and versatility by other means. Free electron lasers (FELs) use periodically arranged magnets coupled with a linear accelerator and can generate ultrashort X-ray pulses of unprecedented brightness.

The UK built the first dedicated synchrotron light source facility – the Synchrotron Radiation Source (SRS) – at Daresbury in 1980, helping to pioneer the experimental techniques that are now used in synchrotron facilities around the world. The circular geometry of synchrotron machines makes them well suited to provide multiple beamlines, all running simultaneously, enabling a high throughput of scientific experiments. Coupled with the brilliance and tuneable nature of the radiation, particularly across X-ray photon energies, this has led to rapid advances in the life and physical sciences and engineering, as well as in more diverse fields such as cultural heritage, non-destructive imaging, and analysis in engineering and manufacturing.

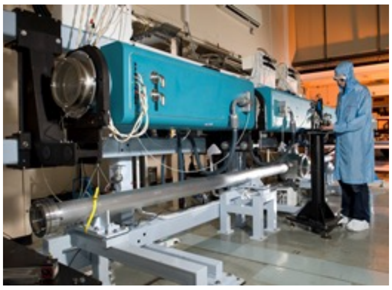
Different light source types – together with other probe and imaging techniques, including electron beams and neutrons – are complementary in what they can do. No single source type or technique can address all of the science challenges.

Light source development and application has resulted in major achievements across many scientific disciples, as illustrated by the numerous Nobel prizes that have been awarded within this field over the past fifty years.

Some of the Nobel Prizes that underpin the UK's light source facilities and some of the science achievements

The 1964 Nobel Prize in Physics was divided, one half to Charles Hard Townes, and the other half jointly to Nicolay Gennadiyevich Basov and Aleksandr Mikhailovich Prokhorov, "for fundamental work in the field of quantum electronics, which has led to the construction of oscillators and amplifiers based on the maser-laser principle."

This work led to the development of lasers including the high-power solid-state lasers such as the CLF's Vulcan laser.



The 1997 Nobel Prize in Chemistry was awarded (in part) to Sir John Walker for his work on the structure of Bovine F1 ATP synthase.

This work used research carried out at the UK's first dedicated synchrotron radiation source, the SRS at Daresbury Laboratory.

The 2018 Nobel Prize in Physics was awarded "for ground-breaking inventions in the field of laser physics" with one half to Arthur Ashkin "for the optical tweezers and their application to biological systems", and the other half jointly to Gérard Mourou and Donna Strickland "for their method of generating high-intensity, ultra-short optical pulses."

Many of the CLF's current facilities (and the new EPAC facility) are based on Strickland and Mourou's invention. The CLF also has several systems based on Ashkin's tweezers, that have been used for a wide variety of research in biological, life and environmental sciences.

Increasing automation, including remote access capabilities and the potential for high utilisation (especially at synchrotrons), has facilitated growing use of the sources by non-specialists and by industry – modern synchrotron facilities can be thought of as light source “factories”. The user communities for such facilities are now very large and well established, and are widely distributed across the UK, covering every region and major academic centre.

Over 14,000 scientists and 175 companies have used the UK national synchrotron, Diamond Light Source, to date, while the CLF’s suite of laser systems typically have over 500 total users each year.

UK researchers also make significant use of the international facilities open to them, with some 400 typically using the European Synchrotron Research Facility (ESRF) each year, and around 500 so far have used the newer European XFEL facility.

The mutual access arrangements between facilities around the world, and the many research partnerships that this promotes, mean that the UK’s light sources have extensive international connections. For example, Diamond Light Source has so far hosted over 5,000 users from more than 60 countries.

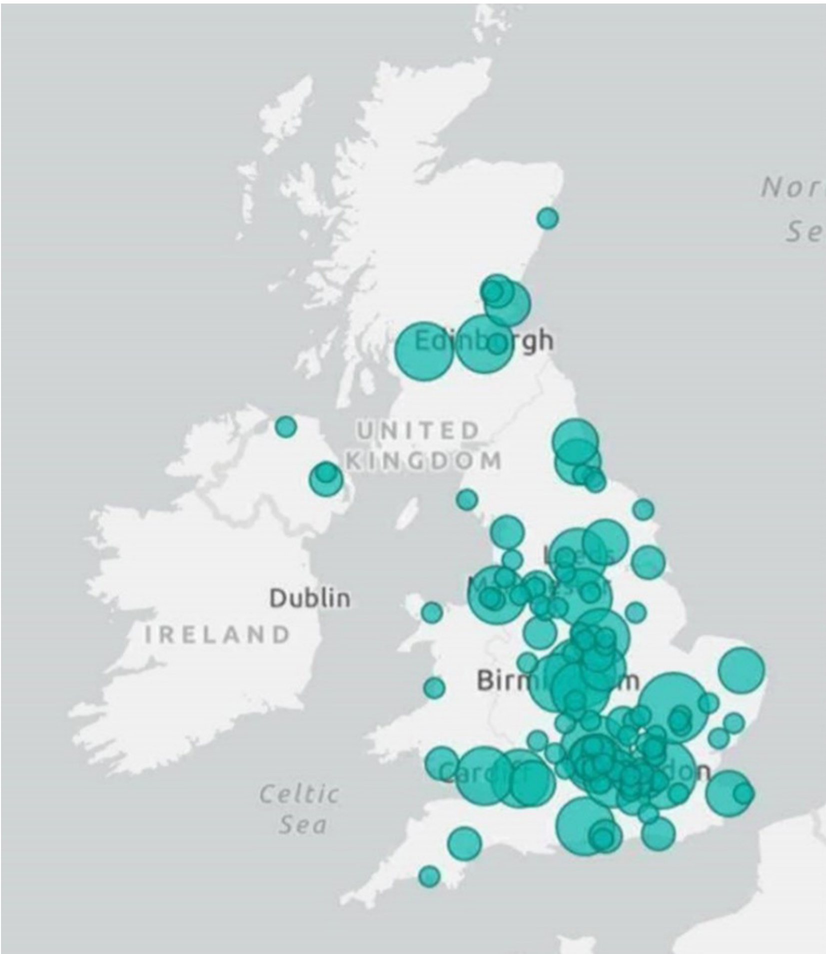
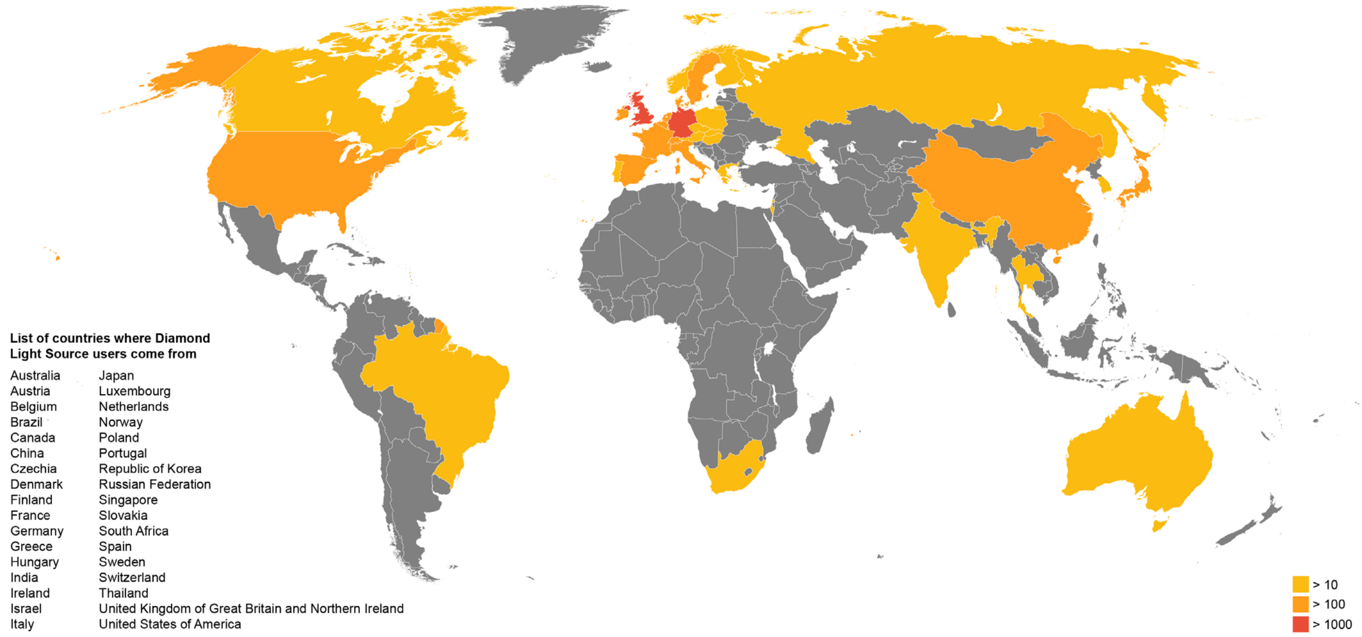


Figure 2: Geographic distribution of the UK light source user communities, with circle sizes proportional to the number of users in that location

There are strong links between the central facilities and the related research activities that are carried out at the home institutes and businesses of the users. This leads to the transference of cutting-edge techniques from the central facilities, so that they can be applied more widely across the UK science base, strengthening local capabilities.

Figure 3: Diamond Light Source users come from all over the world



3. Light sources – characteristics and the status of current facilities

3.1 Light sources as part of the suite of probes

Researchers today have access to many types of probe, some of which are illustrated in Figure 4. Some of these can be operated at small, laboratory scales, whilst others require large-scale infrastructures for effective operation.

The UK research community has access to all these types of probe at many national and international facilities. Whilst this report focuses on future large scale-research infrastructures for synchrotrons, X-ray FELs and high-power lasers, it recognises the important role that the other source types play.

Some notable examples of these sources include:

- Neutrons and muons: the UK's world-class ISIS spallation source and the Institut Laue-Langevin reactor source
- Electron and cryo-electron microscopy: high resolution EM and cryoEM facilities in the UK include ePSIC and eBIC, which are operated as user facilities by Diamond Light Source
- Terahertz and IR: the FELIX facility in the Netherlands is a specialist FEL that operates in the far infrared
- NMR: NMR spectroscopy and imaging systems are widely used in research, industry and medical applications.

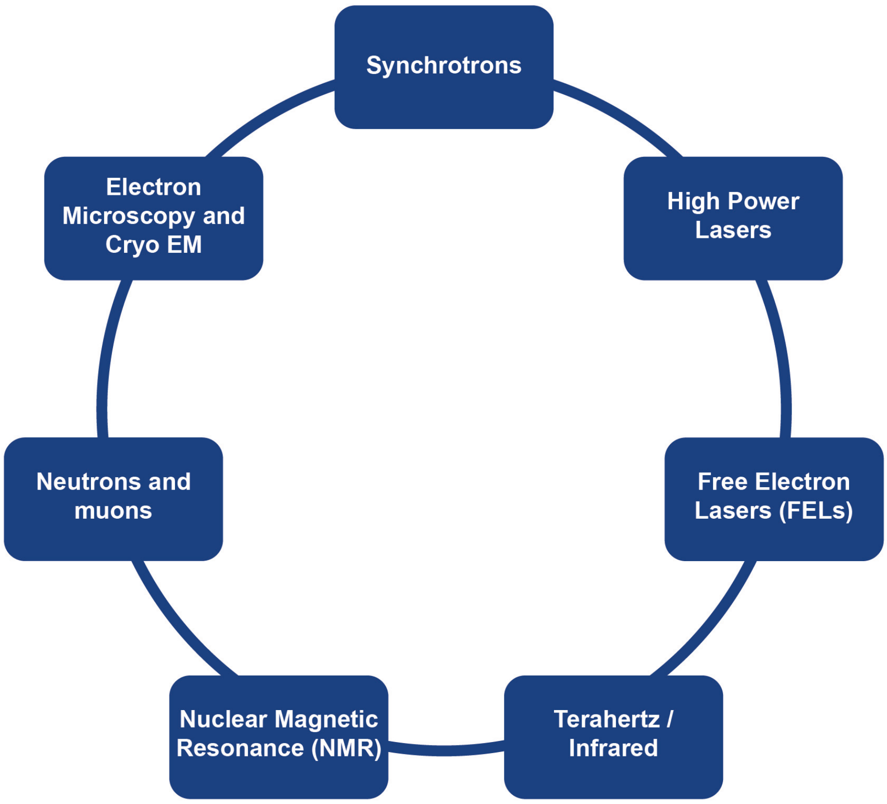


Figure 4: The suite of photon and particle sources

3.2 Characteristics and complementarity

Light is one of the most fundamental and powerful ways to probe and control the matter in the universe around us. A huge amount can be learned about the structure and dynamics of matter from scattering, spectroscopic and non-linear interaction channels; moreover, interaction with light can manipulate a material by, for example, electronic or vibrational excitation, exchange of angular momentum, heating, compression, melting, and acceleration. In these ways, light has been used as the basis of many technological applications, including microscopy, particle acceleration, laser processing, welding, probing nanoscopic geometric and electronic structures, using optical tweezers, and compressing matter to new states.

The specifics of the probing mechanism and any interactions depend critically upon the parameters of the light: for example, wavelength, brightness, intensity, coherence, polarisation and pulse duration. No single source can generate light across the full range of these parameters – this drives the need to have access to multiple types of source. In many cases, small-scale light sources (such as small conventional lasers, lamps, X-ray tubes), that can be operated locally at a laboratory or industrial site, are fully sufficient for the application. Accessing some crucial parameters that enable work at the frontiers of science and technology is, however, only possible at large-scale facilities: large-scale optical lasers are required for the highest intensities and high energy; synchrotrons are needed for stable high average spectral brightness X-rays; and X-ray FELs (XFELs) are needed for ultrafast measurements. Figure 5 illustrates where these large-scale light sources are positioned in the broader context of all possible light sources.

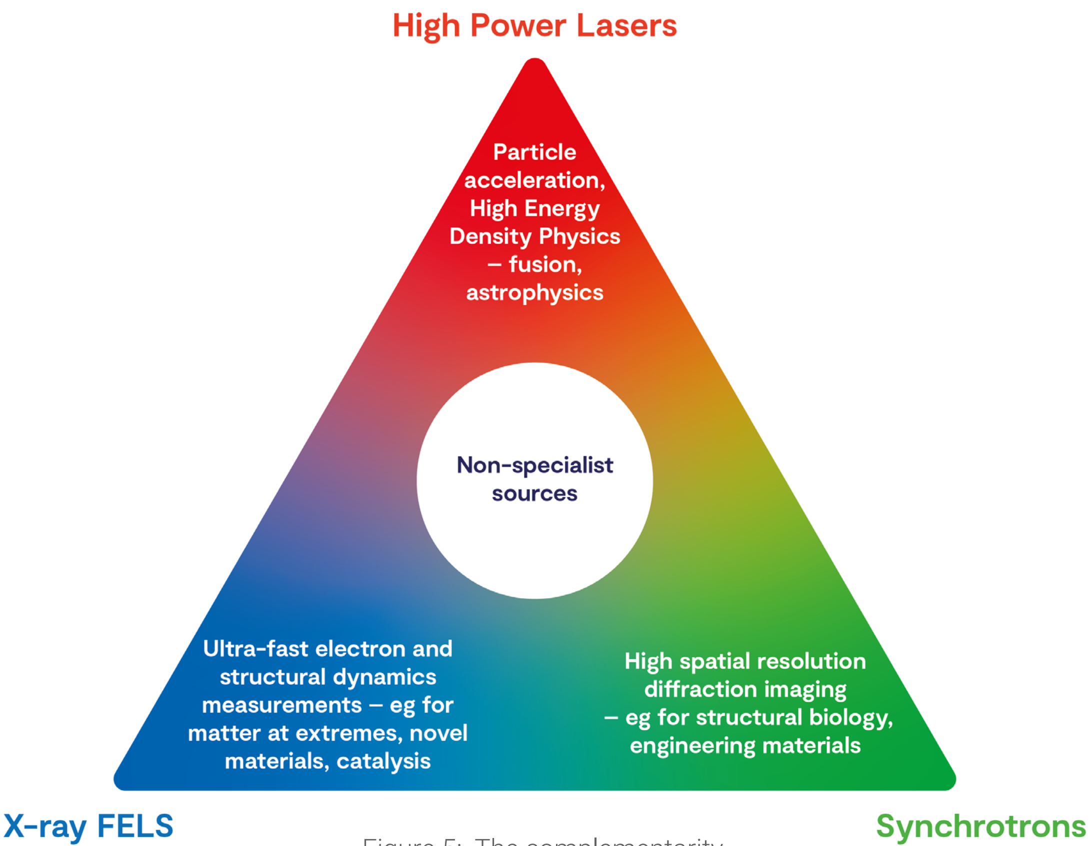


Figure 5: The complementarity of light sources

Examples of measurements that require dedicated large-scale facilities include:

- Probing (via scattering and spectroscopy) the structure of matter at atomic resolution (~ 0.1 nm) requires an X-ray wavelength, as the resolution limit of light is essentially linked to the wavelength. Thus, X-ray facilities such as synchrotrons and XFELs are required for resolving nanoscopic structure, and time-resolved X-ray facilities are required to resolve the corresponding structural dynamics.
- Accelerating free electrons into the relativistic regime (> 500 keV) requires ultrahigh intensity, high power lasers with typically sub-picosecond duration pulses.
- Driving matter into high density compressed states (e.g. for fusion energy, weapons research, and laboratory astrophysics and geophysics) requires high-energy nanosecond duration lasers.

The diversity of the science made accessible by large-scale infrastructures is illustrated in the following two charts. Figure 6 shows how the capabilities of differing sources cover the range required as defined by the parameters of pulse duration and wavelength.

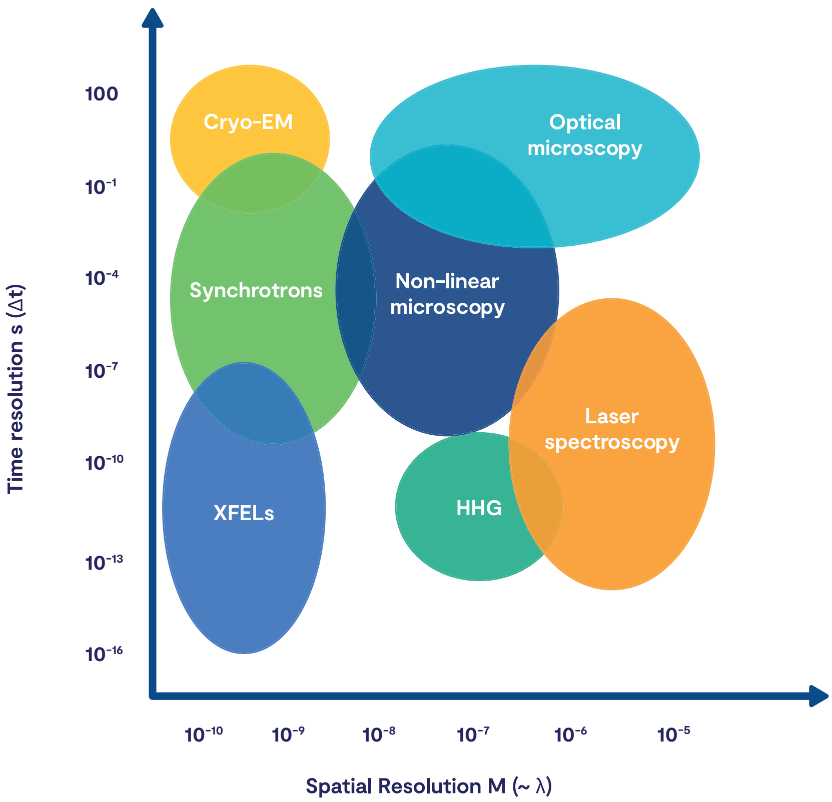


Figure 6: The temporal and spatial resolutions achievable with various lights sources and techniques

1 High Harmonic Generation (HHG) is a technique to extend the frequency of laser pulses by integer multiples of the original laser light

Each source type is mapped to the temporal and spatial resolutions of measurements; so, for instance, to resolve atom-scale structures with nanosecond resolution typically requires synchrotrons, whereas to resolve the same with femtosecond resolution requires an XFEL. Other ultrafast measurements (but without such high spatial resolution) can be achieved by a variety of laser methods, and high power optical lasers can also generate ultrafast X-ray pulses. Cryo-EM has become an increasingly important imaging technique over recent years. Although cryo-EM development is not specifically addressed in this light source vision, it is increasingly being deployed alongside synchrotrons to broaden the range of measurements that can be carried out. Figure 7 shows how the capabilities of differing sources cover the range required as defined by laser photon energy and electron ponderomotive energy (this latter parameter being an indicative measure of the strength of interaction between the light and matter).

Matter-light interaction is relevant to particle acceleration, strong field non-linear quantum electrodynamics (QED), laboratory astrophysics and fast ignition in inertial confinement fusion. Because the ponderomotive energy up-scales in proportion to the product of the intensity and the square of the wavelength, high power optical lasers can reach the highest fields (> 10^{13} Vm^{-1}) with ponderomotive energies exceeding multiple MeV. XFELs are also able to reach these high electric fields, but the ponderomotive energies are not comparable to those from optical lasers.

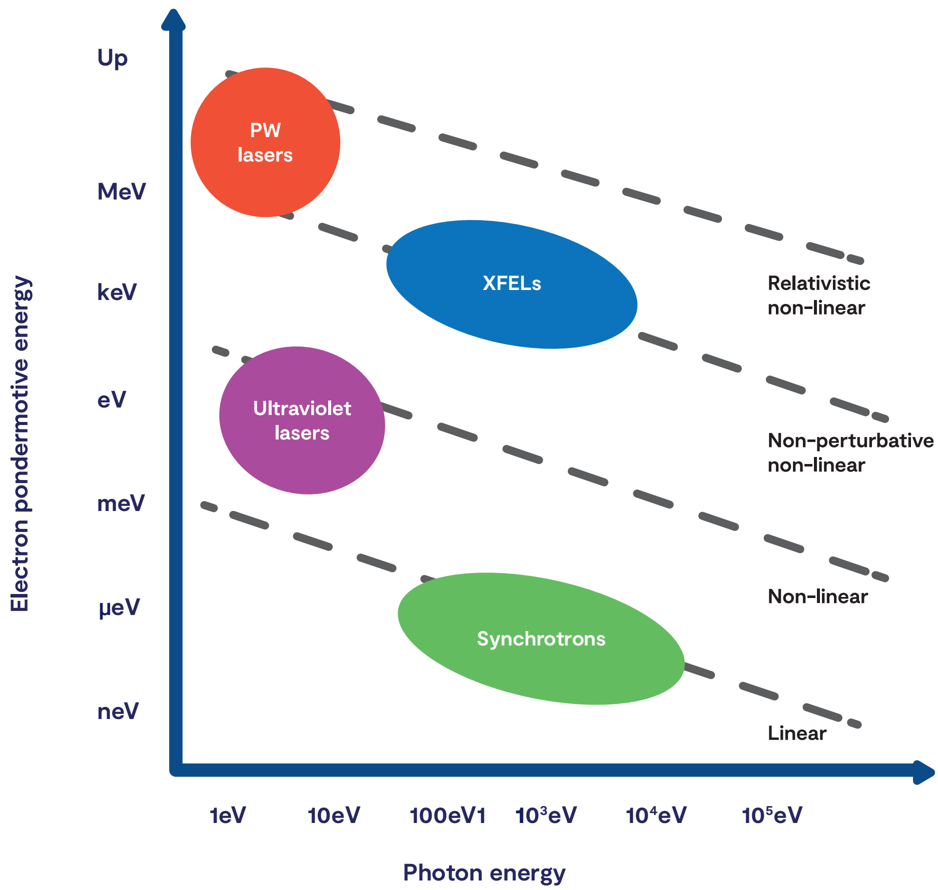


Figure 7: Regions of light-matter interactions in ponderomotive energy and photon energy parameter space for various types of light source

3.3 The principal currently operating sources

Table 1 lists the main light source facilities that are accessed by the UK's research and innovation communities at the present time. Further details of these principal sources are provided in Annex 1.

The most obvious benefit of international collaboration is that it offers the UK research community access to facilities that are beyond the scope or capability of national facilities. The UK membership of ESRF, for example, provides access to a synchrotron with a higher energy than the national facility, Diamond Light Source, together with an input into the way that ESRF is developed and operated. While the majority of beamlines at Diamond are very well matched to the needs of UK users, and with the required capacity, there are more specialised needs that can only be met by ESRF. The Engineering and Physical Sciences Research Council (EPSRC) operates the XMaS: X-ray Materials Science Facility at the ESRF beamline as a national research facility available to UK researchers.

There are other important benefits to international collaborations at centralised European facilities. The scale of operations and the input from a collection of international researchers provides excellent opportunities to develop cutting-edge technology that is shared among the partners, and ESRF sets the standards in key areas of synchrotron technology from which the UK benefits. The multinational nature of the workforce, with significant membership from partner countries, provides a critical route for the provision and development of staff in the national facilities of those countries, including the UK. This helps boost the available talent pool for the national facilities.

Table 1: Light Sources accessed by UK researchers (2021)

Source	Type	Location	Comments
Diamond Light Source	Synchrotron	Harwell	Includes eBIC and ePSIC and Life Sciences XFEL Hub
Central Laser Facility	Suite of lasers	Harwell	Vulcan, Gemini, Artemis, Octopus, Ultra, Physical Sciences XFEL Hub and EPAC (under construction)
Orion	High power laser	Aldermaston	Up to 15% access for academic use relevant to MOD
ESRF	Synchrotron	Grenoble, France	UK is a shareholder
European XFEL	FEL	Hamburg, Germany	UK is a shareholder
Extreme Light Infrastructure	Laser systems	ELI ERIC Czech Republic, Hungary	UK is not a member – potential for limited access via collaborations
		ELI NP Romania	
NIF	High power laser	Livermore, USA	Very limited access via annual call
Laserlab-Europe	Laser systems	Europe	A network of laser systems across Europe
Petra III, Swiss Light Source, SOLEIL	Synchrotrons	Europe*	Limited access determined by facility procedures
NSLS II, SSRL, Photon Factory	Synchrotrons	ROW**	
Flash, FELIX, Swiss FEL	FELs	Europe	
SLAC LCLS I and II, SACLA, PAL-XFEL	FELs	ROW	

* There are over 10 synchrotron sources in mainland Europe used on an ad hoc basis by UK researchers
** There are more than 20 synchrotrons sources outside Europe, some of which are accessible to UK researchers on an ad hoc basis.

3.4 International context and trends

3.4.1 Introduction

The UK science community in academia and industry accesses photon science facilities – synchrotrons, FELs and high-end lasers – primarily in the UK, but also globally, particularly across the rest of Europe. Some of these overseas facilities have UK membership and may be seen as part of the UK-funded portfolio of facilities, most notably the European synchrotron, ESRF, in Grenoble and the European XFEL in Hamburg. In 2018, the status of such facilities in Europe, together with future plans and an outline gap analysis, was presented in the *European Strategy Forum on Research Infrastructures (ESFRI) Roadmap*:[vi] this roadmap is being updated in 2021. The following sections of this document look at the light source facilities accessed by UK researchers, with Table 2 and Table 3 providing a summary of European SR facilities and FELs, respectively, and Table 4 detailing petawatt-class (PW) laser systems. Information on some of the other key international light source facilities accessed by UK users is also provided.

3.4.2 Synchrotron radiation and Free electron laser facilities

The synchrotron user community, in common with those for other large-scale analytic facilities (e.g. for FELs, high-performance lasers and for neutrons), uses a combination of its own national facilities, where available, international facilities, where they have membership, and other national facilities. This approach provides a very co-operative and dynamic provision of access to users across facilities worldwide. SR and FEL facilities banded together in 2017 to form the League of European Accelerator-based Photon Sources (LEAPS), which co-ordinates planning and joint activities across Europe. Diamond Light Source is a Member of LEAPS and is actively involved in collaborative projects.

Researchers from UK universities use approximately 75% of all peer-reviewed access time at Diamond and 10% of time at ESRF, but also enjoy substantial access to other facilities in Europe and further afield. By the same token, users from many overseas countries enjoy access to Diamond, accounting for approximately 25% of all peer-reviewed access time. This flexibility for users enables them to have access elsewhere when, for example, a national or international facility has a long shut-down for maintenance or an upgrade; it also offers users a greater range of capabilities as no individual synchrotron could or should aim to offer all types of measurement capability. ESRF, for example, excels for the very highest energy photons, and the ESRF-EBS (Extremely Brilliant Source) will enhance this further. For lower energy beamlines, Diamond, as well as the proposed Diamond-II upgrade, will maintain world-class performance in that region of the spectrum, so that both facilities continue to provide a wide range of opportunities for the large and diverse UK user community. This diversity of capability is particularly important for solving more complex problems that often need a combination of techniques or beamline parameters to be solved. Figure 8 illustrates the extent to which the publication of research enabled by synchrotrons uses individual or multiple facilities.

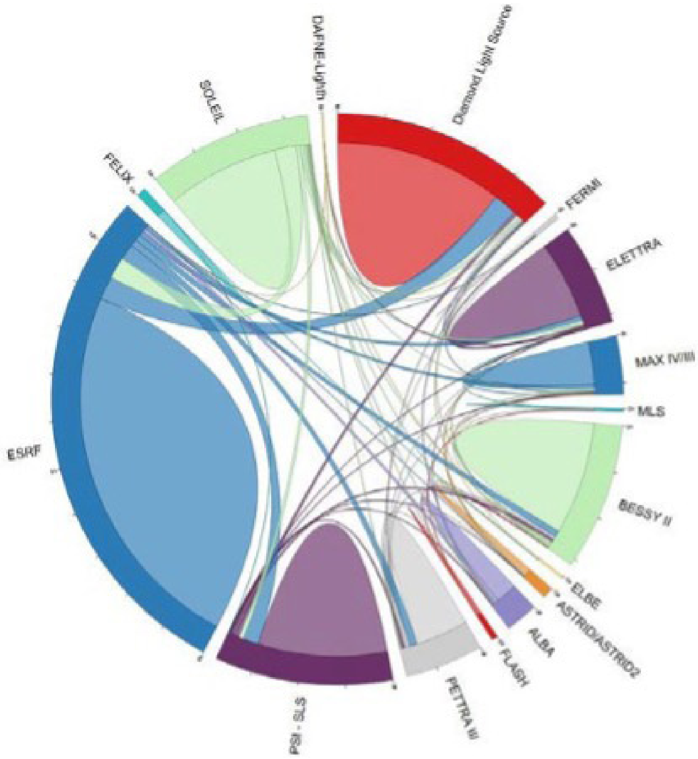


Figure 8: Mapping of European light sources cited in 2,300 publications, illustrating single and multiple use of synchrotron and FEL facilities

There are currently twelve synchrotron radiation (SR) facilities and six FELs open for transnational access across Europe (Table 2 and Table 3, respectively), serving a total user community of about 24,000; the current user community for FELs is in its infancy and is probably less than 1,000. FELs typically have fewer beamlines so the number of users that they can support is likely to remain lower than for SR sources.

Among SR facilities, most have storage ring energies of about 3 GeV, although ESRF is a 6 GeV machine, the best in its class in the world, and PETRA III has undergone extensive upgrades and is another 6 GeV facility. Most recently, Europe has seen first operations of the MAX IV facility, based on novel, disruptive Multi-Bend Achromat (MBA) technology for the storage ring that will offer unprecedented brightness and coherence, and the ESRF EBS came on stream in 2020 as a MBA upgrade that offers 100-fold increase in brilliance and coherence – significantly closer to the physical (diffraction) limit for hard X-rays. Several other national facilities in Europe also plan MBA upgrades in the next decade, with the Swiss Light Source upgrade SLS 2.0 planned for the end of 2026, the Petra III upgrade to PETRA IV expected in 2026, with this upgrade overlapping the timeframe for the proposed Diamond-II upgrade, creating a 'dark period' for researchers. Complementary improvements in detector technology have also been transformative. Accelerated throughput, increased remote access in techniques such as crystallography, and construction of more beamlines at some national facilities are all helping to meet the increasing demand for access.

Table 2: Summary of European SR Facilities

FACILITY	LOCATION	ELECTRON ENERGY (GeV)	EMITTANCE (nm rad)	FULLY SCHEDULED BEAMLINES (CONSTRUCTION/ COMMISSIONING)	START OF USER OPERATIONS
ESRF	GRENOBLE (FR)	6	0.13	30 +14 CRGS*	1994
PETRA III	HAMBURG (DE)	6	1.1	16 (24)	2010
ALBA	BARCELONA (ES)	3	3.6	8 (3)	2012
DIAMOND	HARWELL (UK)	3	2.7	33	2007
MAX IV	LUND (SE)	3	0.34	16 (29)	2016
		1.5	9	0 (5)	2016
SOLEIL	ST. AUBIN (FR)	2.75	3.74	29	2008
SWISS LIGHT SOURCE	PSI, VILLIGEN (CH)	2.4	4.4	16	2001
ELETTRA	TRIESTE (IT)	2.0/2.4	7.0/9.7	26 (2)	1994
BESSY II	BERLIN (DE)	1.7	6.4	47 (31)	1998
SOLARIS	CRACOW (PL)	1.5	6	4 (5)	2018
ASTRID2	AARHUS (DK)	0.58	12	10	2014
MLS	BERLIN (DE)	0.24-0.6	100	11	2008

*Collaborating Research Groups managing quota of access

The UK FEL user community mainly accesses US and Japanese facilities, plus usage of the Korean FEL is growing. There are exciting developments at the US facilities, where a capability for high repetition-rate operation – even to the hard X-ray limit – is being built. The UK does not, however, have much influence on these facilities and access is very restricted, although the scientific relationships are very good.

The ESFRI Landmark European XFEL and the SwissFEL are hard X-ray FEL facilities that saw their first experiments in 2017, adding to a suite of complementary Infrared (IR), UV or soft X-ray FEL user facilities already in operation. The TARLA facility is being built in Turkey and further projects are planned (MAX IV-FEL, POLFEL).

Table 3: Summary of European FELs in operation
or under construction

FACILITY	FELS LINES OPERATING IN PARALLEL	LOCATION	START OF USER OPERATIONS	ELECTRON ENERGY	PHOTON ENERGY	PULSE PROPERTIES	NUMBER OF END STATIONS
European XFEL	SASE-1 SASE-2 SASE-3	HAMBURG/ SCHENEFELD, GERMANY	2017 2018 2018	8.5 - 17.5 GeV	3.0 - >20 keV 3.0 - >20 keV 0.25 - 3.0 keV	1 - 100 fs 10 x 2,700 pulse/s	2 2 2
SwissFEL	ARAMIS ATHOS	VILLIGEN, SWITZERLAND	2018 2020	2.1 - 5.8 GeV	4.0 - 15 keV 0.25 - 2.0 keV	5 - 100 fs 100 Hz	2 2
FERMI	FERMI – I FERMI – 2	TRIESTE, ITALY	2012 2016	1.5 - 1.8 GeV	15 - 90 eV 80 - 400 eV	20 - 90 fs 10 - 50 Hz	5
FLASH	FLASH FLASH – 2	HAMBURG, GERMANY	2005 2016	1.25 GeV	30 - 300 eV 30 - 300 eV	20 - 150 fs 10 x 800 pulse/s	4 3
CLIO	CLIO	PARIS, FRANCE	1993	40 MeV	10 - 400 meV	0.5 - 5 ps 60 MHz pulsed: 25 Hz	
ELBE	FELBE TELBE	DRESDEN, GERMANY	2005 2016	40 MeV	0.5 - 250 meV	0.5 - 30 ps 13 MHz cw	7 1
FELIX	FELIX 1/2 FLARE FELICE	NIJMEGEN, NETHERLANDS	1993 2013 2007	15 - 50 MeV 10 - 15 MeV 15 - 50 MeV	8 - 400 meV 0.8 - 12 meV 12 - 250 meV	0.5 - 200 ps 1/3 GHz Pulsed: 20 Hz	12 4 2
TARLA		ANKARA, TURKEY	2019	40 MeV	5-400 meV	0.5 - 30 ps 13 MHz cw	

Further afield, the major non-European FEL projects are: LCLS, LCLS II and LCLS II HE in the USA; SACLA XFEL in Japan; and PAL XFEL in Korea. China has four FEL facilities, with the SHINE hard X-ray system due to start operations in a few years' time.

3.4.3 High performance lasers

Laser research infrastructures are distributed across Europe. Much of the user access and joint R&D is coordinated through the Integrated Initiative of European Laser Research Infrastructures, Laserlab-Europe (LLIV), which brings together 35 leading institutions in laser-based inter-disciplinary research from 18 countries; the European Cluster of Advanced Laser Light Sources (EUCALL) project also aims to bring together laser and X-ray research infrastructures. The Extreme Light Infrastructure (ELI), which aims to host the highest performance laser systems worldwide, is currently developing at three sites, with complementary capability to each other and the rest of LLIV: the ELI-ALPS pillar combines ultrashort pulse (USP) and ultrahigh intensity (UHI) at very high repetition rates; the ELI Beamlines pillar will provide ultrashort secondary radiation (X- and gamma-rays) and particle (electrons, ions) sources; ELI-Nuclear Physics offers a unique combination of the most powerful laser sources worldwide (2 x 10 PW) with a fully tuneable gamma-ray source (up to 19.5 MeV).

Outside of Europe, there are a range of large-scale laser facilities, which in general do support collaborative access to them. The largest, the National Ignition Facility (NIF) in the USA and the Laser MegaJoule (LMJ) in France support research into inertial confinement fusion and high energy density science.

There is a natural connectivity between XFEL sources and high-power lasers and both the European XFEL and the LCLS have significant high performance laser infrastructure on their High Energy Density beamlines. China, with its current construction of its new SHINE XFEL facility, is also constructing a 100 PW laser as part of it.

Table 4: Summary of world-wide PW-class lasers with a peak power of > 0.5 PW

SYSTEM NAME	HOST FACILITY	LOCATION	START OF USER OPERATIONS	ENERGY (J)	PULSE WIDTH (fs)	PEAK POWER (PW)	REP RATE
NOVA	LLNL	USA	1996	660	440	1.5	Single shot
VULCAN	CLF	UK	2002	500	500	1	Single shot
GEKKOXII	ILE	Japan	2003	420	470	0.89	Single shot
TITAN	LLNL	USA	2007	300	400	0.75	2/hr
Z-Petawatt	SNL	USA	2010	500	500	1	Single shot
Texas Petawatt	University of Texas	USA	2010	186	187	1.11	Single shot
PHELIX	GSI, LLNL, CEA	Germany	2016	400	350	1.14	Single shot
SG-II-U (PW)	SIOM	China	2010	1000	1000	1	Single shot
ORION	AWE	UK	2013	500	500	1	Single shot
OMEGA EP	LLE	USA	2008	1000	1000	1	Single shot
PETAL	CEA	France	2015	3500	500	7	Single shot
LFEX	ILE	Japan	2015	50000	10000	5	Single shot
ELI L4	ELI	Czech Republic	2021	1500	150	10	1/min
ELI-NP	ELI	Romania	2021	250	25	10	1/min
NIF	LLNL	USA	2009	1.80×10^6	3.60×10^6	0.5	Single shot
LMJ	CEA	France	2020	1.80×10^6	3.00×10^6	0.6	Single shot
UFL-2M-IR	IAP RAS	Russia	TBD	4.6×10^6	3.00×10^6	1.53	Single shot
SG-IV	SIOM	China	TBD	1.80×10^6	3.00×10^6	0.6	Single shot

3.4.4 Electron microscopy facilities

About 100 mid- to high-end EM instruments operate in Europe, most of which include aberration correction of the probe forming or imaging optics. ESTEEM 2 (Enabling Science and Technology through European Electron Microscopy) (funded under FP7) has brought together some 15 leading laboratories and associated SMEs to form a networked infrastructure that provides transnational access to advanced EM instruments: ESTEEM3 (funded under H2020) will continue this work. An EU Design Study (DREAM) is being planned that will explore the creation of a pan-European Research Infrastructure for advanced EM at a scale similar to SR and Neutron, and will include two of the highest spatial resolution microscopes in the world (at Juelich and Harwell) and several instruments capable of providing sub 10 meV energy resolution (at Daresbury and Orsay). The recent development of direct electron detectors has helped to revolutionise the use of cryo-EM in structural biology, with an exponential growth in installations that increasingly complement X-ray protein crystallography, and in the physical sciences through faster frame-rates and significantly improved detector resolution.

3.4.5 Trends: Gaps, challenges and future needs

Brighter sources and faster detectors produce larger, often more complex, data sets that are becoming more challenging to process and analyse, both during an experiment (to make informed decisions about how best to proceed) and afterwards. The increasing use of multiple probes is adding even more complexity to the data sets generated. This area of work not only requires significant investment in hardware to transfer, store and process data, but also coherent development of software including greater exploitation of AI techniques, and many more people – data scientists – who are expert in such methods.

Many of these research infrastructures (RIs) require more powerful, compact accelerator sources and better detectors, both of which could involve highly synergic collaborations across types of RIs. There are technical challenges specific to individual types of RI; for example:

- diffraction limited storage rings for SR for harder X-rays, offering coherent imaging down to tens of nanometres, and study of fluctuations to 100 picoseconds;

- coherent pulsed sources for EM that operate in both stroboscopic and single shot modes, also requiring detector development.

Improvements to high performance lasers will require: new or larger materials for robust optical components; a new generation of online, in situ diagnostics of the laser fields to control the experimental environment fully; and increased laser peak power (at least 100 times) by shortening pulses, increasing energy and/or developing techniques for the coherent combination of multiple beams – for example to create and study electron-positron pairs from the vacuum. In general, there is a movement from “single shot” facilities to higher repetition rate as diode pumping becomes more accessible and cost effective.

Increasing demand for SR facilities could be met over the next decade through the upgrade of existing facilities, with the current programme of MBA upgrades and the construction of additional national or regional facilities. Exploitation of complementary FEL facilities is still at a relatively early stage, but likely to grow strongly in this period. The very strong growth in demand for Cryo-EM will require an increase in the number of instruments and the development of higher throughput methods. For high-performance lasers a key challenge is to transform existing networks into more robust and reliable user-oriented operations at, or approaching, 24/7 availability.

4. A plan for future light source provision

The options for developing the UK's future light source provision need to be considered against the opportunities and risks to the diverse science, technology and innovation challenges. Although this is a complex picture, the principal elements that underpin the source plan can be summarised and an outline plan can be developed that:

- creates a timeline of developments that seeks to manage the resource inputs (engineers and scientists) needed
- identifies any links between options and how these can be optimised
- outlines the potential impacts on the needs and research priorities of various science communities
- Includes mitigation measures where necessary (for example were sources will be off-line for extended periods)
- identifies key decision timings.

4.1 Summary of the principal source options

A comprehensive list of the development options for all the source types is presented in Part Two of this report (see Section 7). A summary of the principal source options that can enhance the current capabilities is presented in Table 5. It identifies the main risks and opportunities and any links between the options. The likely implementation timescales and capital costs are indicated in broad terms:

- Implementation time bands:
  - Short: can be implemented within 3 years
  - Medium: can be implemented within 3 – 10 years
  - Long: can be implemented within 10 – 20 years
- Capital cost bands:
  - Low: capital cost < £100M
  - Medium: capital cost between £100M and £750M
  - High: capital cost > £750M

Table 5: Summary of Principal Options – page 1
synchrotrons

Source	Options	Links	Science, innovation and industry opportunities	Risks and mitigations	Timescale	Capital costs
Diamond	Major upgrades	Reinforces existing links to laser/cryo EM imaging/RFI capabilities	Higher flux, lower divergence, higher energy beams critical to achieving step change advances across a wide range of physical, life sciences and engineering. In particular in high resolution imaging and operando studies of processes in real time as well as higher-throughput crystallography and lower damage for softer or biological samples. Very large user base including significant UK industrial use.	Building on existing infrastructure means low technical risk. Dark period can be minimised and access to ESRF and other sources provides some mitigation. Additional to the routine upgrades needed to maintain machine performance.	Medium	Medium
	Build new facility	Reinforces existing links to laser/cryo EM imaging/RFI capabilities	Photon energy range can be extended to even higher values with even greater impact on operando and engineering applications.	Will not be available for a considerable time (of the order of 15 years) so UK community will see much delayed benefits and will lose access (with serious damage to UK research and innovation) to a national synchrotron unless Diamond continues to run in parallel for much of this period with associated costs.	Long	High
ESRF	All options	Complementary to national capabilities	Recent upgrade means UK users can exploit new capabilities, but access level is capped. Enhances international partnership opportunities.	Significant addition to UK's capacity, but restricted access means ESRF cannot service all the needs of the UK's user community.	n/a	Low

Table 5: Summary of Principal Options – page 2
XFELS

Source	Options	Links	Science, innovation and industry opportunities	Risks and mitigations	Timescale	Capital costs
UK FEL	Build test facility	Can make use of existing infrastructures such as CLARA	Reduces technical risk to building a future full user facility but limited opportunities for new science.	Loss of momentum in the UK user community. Will need to enhance links with overseas groups to maintain science gains.	Short	Low
	Build full scale facility	Specification linked to other developments: EPAC, Vulcan, Diamond, Cryo EM and ultrafast electron diffraction.	Opportunity to design world-leading and unique capabilities that could enable dramatic science gains and make the UK a leader in FEL science and techniques.	Correct choice of beam and detector instrumentation is required to ensure the anticipated outcomes. Ambitious technical design carries an element of risk, but all underpinning technologies are proven.	Long	High
European XFEL	All options	Long term use may be influenced by decisions on UK FEL.	Enhances international partnership opportunities and facilitates science gains at low cost, but access level is capped.	An important capability but capped capacity means the European XFEL cannot service all the UK's needs, with consequent risks to science outcomes and the user community. Other overseas FELs may also be options but would be subject to making suitable agreements and the availability of suitable capacity.	n/a	Low

Table 5: Summary of Principal Options – page 3
lasers

Source	Options	Links	Science, innovation and industry opportunities	Risks and mitigations	Timescale	Capital costs
Laser imaging dynamics systems (RCaH)	Upgrade	Strengthens links to RFI and national / international networks, e.g. Bioimaging UK; Euro Bioimaging and European access and research networks, such as Laserlab-Europe.	Laser imaging, dynamics and manipulation techniques are particularly important for bio, life and physical science. There is significant cross fertilisation.	Current capabilities can quickly fall behind requirements if not kept up to date. Available space limits to RCaH may be a restriction, especially for the desire to increase capacity for industrial use.	Short	Low
EPAC	Upgrade	Links to industry and EU programmes e.g. EuPRAXIA	Phase 2 expansion will deliver the capacity to develop long term strategic partnerships with diverse industries and drive translational research. Creating new capabilities through links with projects such as EuPRAXIA creates the opportunity to internationalise EPAC, attracting inward investment.	Underutilisation or inefficient use of EPAC capabilities.	Medium	Low
Vulcan	All options	Numerous national and international links, and links to the UK defence community.	Opportunity to create a world-leading high-power capability, maintains UK leadership	Loss of Vulcan would mean UK HED science being primarily dependent on non-UK facilities, e.g. in Europe, Asia and the USA	Short	Low

4.2 Future light source development planning

4.2.1 Factors influencing source development planning and timeline

The overarching consideration is the UK's strategy for future research and innovation priorities. The government's industrial strategy[vii] identifies research challenges in: AI & Data Economy; Clean Growth; Future of Mobility; and an Ageing Society. *The UK Research and Development Roadmap* sets out the government's approach to meeting these challenges. Research infrastructures, including light sources, are a key element in enabling these long-term aims to be met. Inevitably the focus of research needs will change over time in response to new policy requirements, funding constraints, science breakthroughs and external factors (such as the COVID-19 pandemic, where light sources such as Diamond played a vital role in supporting research on the virus structure).

Light sources, with their extremely diverse fields of application, are well suited to supporting and responding to the nation's evolving research and innovation needs and priorities. Given the increasing number of research areas with needs for access to lasers and synchrotrons (see Part Two), there is no case for a reduction in capacity or capability. In a constrained budget, user consultations invariably prioritise existing national capabilities over international facilities. However, within the principal options collated in Table 5 above, the future development programme across the source types could either create a balanced and highly-flexible capability, or particular capabilities could be enhanced. There are strong scientific arguments for upgrades to existing facilities to maintain international competitiveness and open up new research opportunities; further, specific new capabilities (in particular for dynamic studies) would be created by investment in a UK-based Free Electron Laser. Access to XFEL enabled science will be important whether or not a UK facility is constructed.

The approach adopted in this strategic vision is to set out a "balanced" development plan that will result in the broadest range of capabilities, in order to support science and technology advances in many fields. This approach will also maximise opportunities for UK facilities and researchers to forge new and stronger partnerships with the international research communities, bringing the potential to leverage access to leading facilities around the world.

All research infrastructures need to develop in order to keep pace with the science and innovation challenges they are addressing, and to take advantage of advances in technologies that can Increase their efficiency and reliability. For light source facilities, it is important to recognise that there are different upgrade/renewal cycles for each source type. Synchrotrons typically operate for 10 years or more between major beamline upgrades, and over 20 years for major machine upgrades, whereas lasers of the kind operated in the Laser Support Facility can be reconfigured and upgraded every few years.

There is a continuing need for diversity in source types and capabilities, to cover the science challenges across diverse and cross-disciplinary domains. By taking a holistic view across all the options for the future development of light sources and the capabilities needed, there is an opportunity to maximise the overall gains that can be achieved. Decisions on each source development opportunity must take into account the wider context of all the UK's light source activities, so that the performance specifications can be fine-tuned where possible to maximise the synergies and the complementarity.

4.2.2 Building the user community and skills

Over recent years there has been a steady broadening of the UK's light source user community, within both academia and industry. As a result, there are now expert users and researchers that make only occasional use of the facilities and techniques. To support the continued expansion of the user base, all the facilities need to continue to target new groups and help the growing number of non-expert users to achieve their research aims. Such an approach may be particularly needed in the industrial communities, where the specific expertise required can be thinly spread, and in the research domains where the application of light sources is less well established.

Support for the user base will be especially important for the new facilities and research techniques, such as those being developed at the new generation of FELs, to ensure that their exploitation is not constrained to a small group of expert users. The future development of facility capabilities and the growth in expertise in the user community will help to keep the UK as a partner of choice in collaborative international research that is undertaken by, and in many cases led by, UK researchers.

It will also be important to review and evolve the access modes to the facilities on a regular basis, to include a greater emphasis on timely and dynamic access, and to facilitate effective remote access, with the necessary support to remote users by local facility teams. Remote access will also support the future sustainability of facilities, by minimising the need for individual visits and reducing the impact of travel.

Retaining and enhancing technical expertise at the facilities – both instrument scientists and support staff – is a key requirement to delivering reliable operations, and maintaining the UK community and its international reputation. Sustaining technical expertise at all levels will be key to realising the UK's strategic light source vision. Although this is a challenge for all research infrastructures, light source facilities provide excellent training opportunities for young engineers and scientists, and can play an important role in securing the skills pipeline.

4.2.3 Data management and computation

The current generation of light source facilities has already experienced massive growth in the quantities of data generated by their suites of instrumentation. As a result, increasing attention is being directed towards ensuring that this data can be effectively and efficiently extracted, stored and analysed. All the source development plans set out in the following sections will inevitably create further step changes in the needs for greater data management and computational power. Any future source specifications must include the information technology and artificial intelligence capabilities needed to realise the predicted research gain.

4.2.4 A balanced development plan and timeline

The development of the UK's future light source provision will build upon a world-class track record. We have a strong knowledge base in the design, construction and operation of new sources and photonics instrumentation, and in the techniques needed to apply the capabilities to leading edge research and innovation. It is, however, a fact that the available pool of the required specialist skills in engineering, design, optics, instrumentation etc – nationally and internationally – is a critical limitation on how quickly progress can be made. An important consideration is to minimise disruption to the user communities and, where possible, put in place mitigations for any extended down-times of each source type, to minimise the constraints on research progress.

Figure 9 illustrates the high-level decision planning and actions for future light sources.

Tables 6 to 8 set out the details of the components of the balanced development plan. Links between sources are indicated together with potential timings for key decisions and implementation actions.

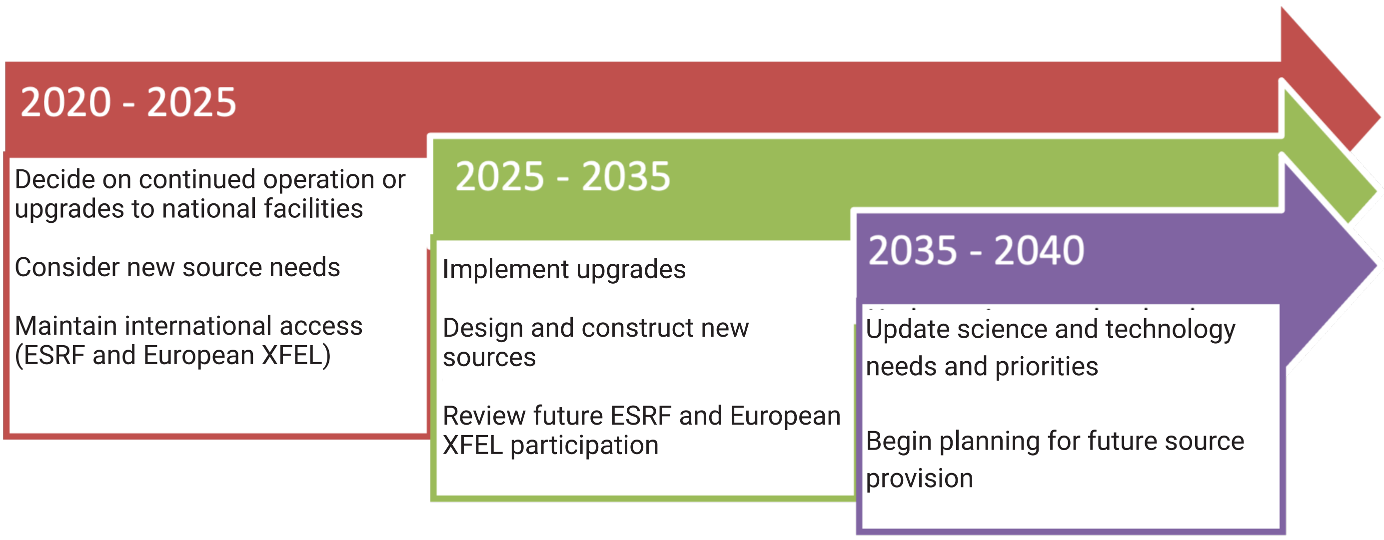


Figure 9: Decision planning and actions for future light sources

Table 6: Synchrotron Sources

Source	Strategic Plan	Anticipated Timing
Diamond	Implement a major upgrade to the machine, the instrument suite and computation facilities. This will: • Provide the UK with a world-class 4th generation synchrotron source, with a significant increase in capability in both source characteristics and detection efficiency. • Allow recycling of much of the hardware • Minimise the downtime for users To further mitigate the dark period impacts, UK access to suitable overseas sources will need to be secured.	Finalise design Year 0 Secure financing Year 1 Begin construction Year 2 Begin commissioning Year 7 Begin full operation Year 8
ESRF	Maintain ESRF membership reviewing regularly. Investment in any future ESRF upgrades should be considered against DII specification and performance and user needs.	Review continued participation every three years (notice period is 3 years).
Other	Maintain active links with the world-wide network of synchrotrons so that: • Ad hoc arrangements for mutual access are maintained • Opportunities for collaborative partnership research programmes can be identified • UK is engaged in, and can benefit from, international advances in synchrotron science and technology.	Ongoing

Table 7: FEL Sources

Source	Strategic Plan	Anticipated Timing
UK XFEL	Whilst building a small-scale facilitiy would add some increase to capacity, building an internationally competitive UK facility will provide the greatest gain in capabilities and opportunities for research benefits. The UK FEL specification should: • Build on world-wide experience so that research gains can be maximised • Take account of Diamond upgrade and EPAC capabilities to maximise complementarity The existing FEL test facilities should be used to support development of the optimal design and minimise the technical risks.	Finalise design Year 0 Initiate detailed design planning and test programme Years 1 - 4 Finalise design and secure funding Years 4 - 5 Begin construction Year 5 - 8 Begin commissioning Year 9 - 10 Begin operation Year 10
European XFEL	Maintain European XFEL membership but review regularly. Investment in any future upgrades needs to be considered against UK FEL specification.	Review every five years
Other	Maintain active links with the world-wide network of FELs so that: • Ad hoc arrangements for mutual access are maintained • Opportunities for collaborative partnership research programmes can be identified • UK is engaged in, and can benefit from, international advances in FEL science and technology.	Ongoing

Table 8: Laser Sources

Source	Strategic Plan	Timing
Vulcan	Maintain Vulcan operations in the short term and complete current beamline upgrade. Make the investment decision for the Vulcan 2020 project.	Secure interim continuation of Vulcan Year 0 Initiate upgrade Year 1
EPAC	Complete Phase 1 build, commission and operate Transfer Gemini to EPAC building Develop plans for Phase 2 expansion	Phase 1 build Year 0 Commissioning and operation and Gemini relocation Year 1 Initiate planning for expansion Year 2
Imaging and dynamics systems	Upgrade and develop system capabilities as techniques evolve, linking to RFI and other national/international capabilities, especially in data/scientific computing	Ongoing
Other	Maintain active links with the world-wide network of laser facilities so that: • Ad hoc arrangements for mutual access are maintained • Opportunities for collaborative partnership research programmes can be identified • UK is engaged in, and can benefit from, international advances in laser science and technology.	Ongoing

4.2.5 New sources

The development of the potential new source types identified in Part Two: Section 7 – Table 12 have not been considered in detail as, in the main, they are not yet close enough to becoming user facilities. Some of the conventional source developments, however, in particular for high power lasers and FELs, will provide the means to carry out further research that will advance understanding of how these new source types could be constructed and the potential performance capabilities they could bring.

5. Implementing the light sources development vision

Implementing the development plan for future light sources will necessarily depend on overarching factors, including the availability of funding for new capital projects, UKRI's research infrastructures programme, and the plans of the international facilities. As a result, determining the detailed implementation programme for any or all of the light source options that have been set out is beyond the scope of this strategic vision. This section does, however, set out the factors that should be key considerations of any decision process.

5.1 Capacity and capability

Maintaining capability, and identifying the opportunities for enhancing capability, is the main theme of the strategic vision across all the light sources that have been considered. Of equal importance to the "beam factors" such as brightness, coherence, pulse length, repetition rate and so on, are the instrumentation and techniques that need to be deployed to detect the photons through imaging, spectroscopy and scattering, and to collect and analyse the data generated. These are critical to realising the ambition of cutting-edge infrastructure in the government's R&D Roadmap.

The typical build/upgrade timescales for large and complex user facilities means that capacity must be well matched to user demand, as significant changes to capacity cannot be achieved quickly. This plan builds on the established model of having a national capacity that is complemented and supplemented by formal arrangements to access international facilities, and less formal partnerships with other national facilities.

5.2 International collaborationand partnerships

International collaboration both strengthens the activities at national facilities and, through shareholdings in international facilities, provides the UK community with additional capabilities, capacity and development opportunities in technology and skills.

The UK light source community, including the facilities and the research groups that use them, is well connected with its international peers. The source developments identified in this strategic vision can provide a stimulus to strengthening these established links and opening opportunities for new collaborations. This will help keep the UK as the partner of choice in the increasingly important areas of photonics technologies and photon-enabled science in key research areas.

5.3 A holistic facility model

Future light source facility developments should build upon all the experience to date and adopt a holistic approach that:

- Facilitates options for future upgrades
- Encompasses a complete instrumentation approach and is not purely source-centric
- Embeds all the necessary data and associated computational needs, so that the science outputs can be fully exploited
- Maximises the user experience, including facilitating remote operation and supporting non-expert users

- Takes maximum advantage of opportunities to minimise the environmental impact of source construction, operation and decommissioning.

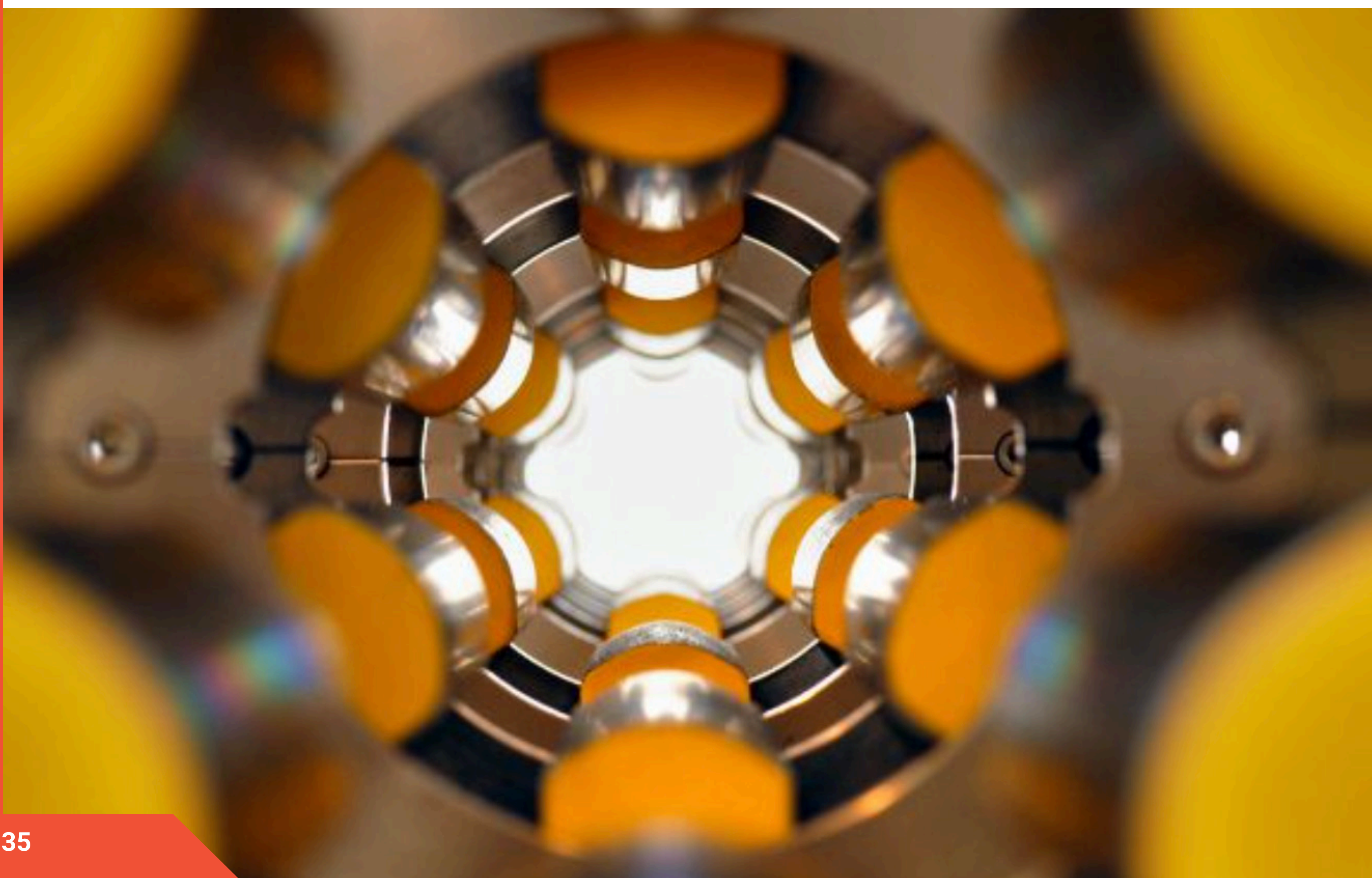
5.4 Building the user community

The success of all research infrastructures depends upon an effective combination of machine performance and user expertise. The light source facilities discussed in this vision must work, individually and in collaboration, to maximise the potential for their users to achieve their science and innovation goals. The facilities must be proactive in helping their user community to be able to exploit the new capabilities made available to them. Facilities should also seek to broaden the user base into new research disciplines and industrial sectors that are likely to need more directed support than the established areas.

5.5 Innovation and industry

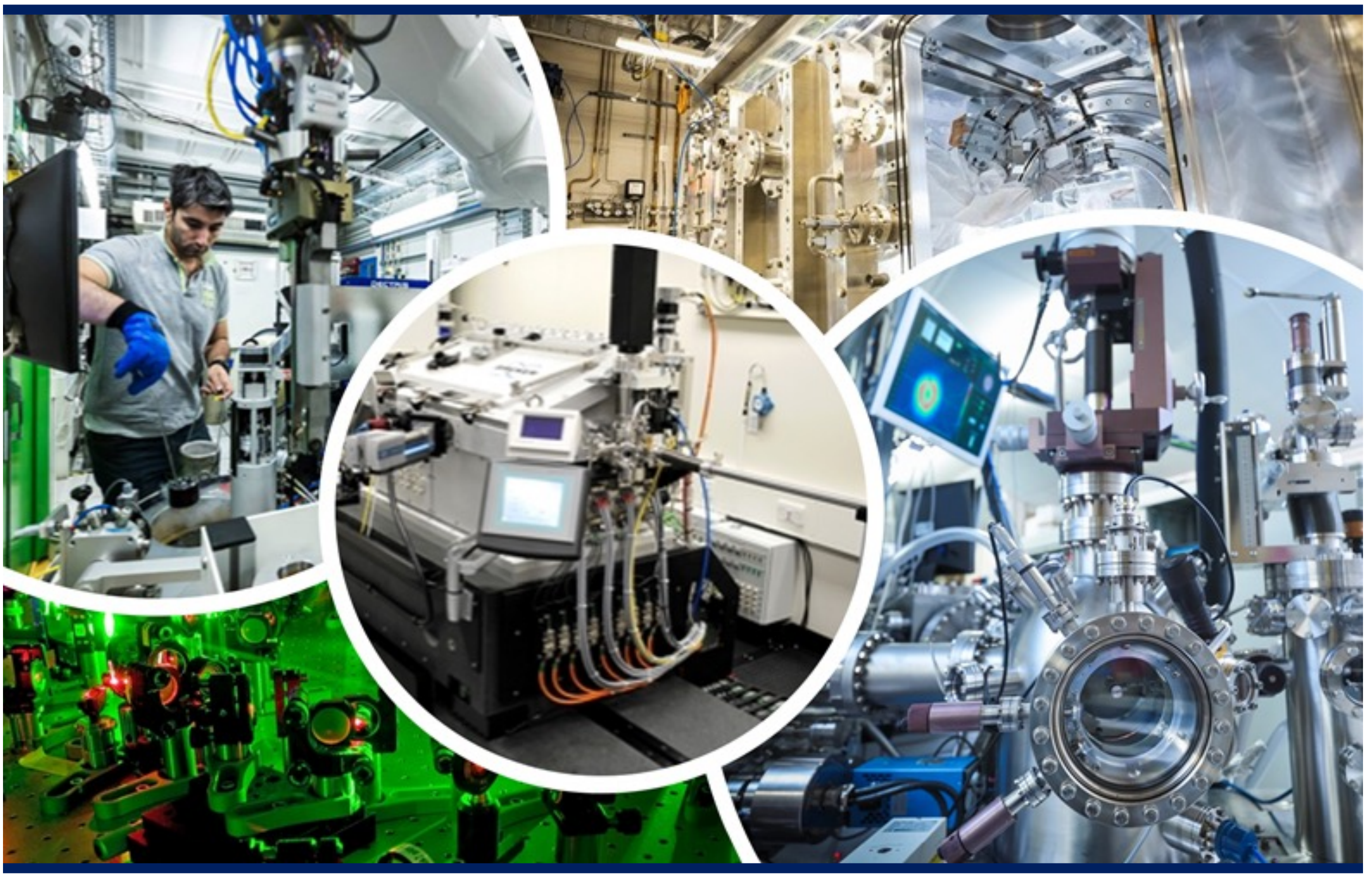
Developing and implementing the new generation of source technologies will require leading-edge optical, mechanical, electronic and cryogenic engineering equipment and skills. Supporting these developments will provide UK supply industries with opportunities to grow their capabilities and, in turn, provide a showcase for their capabilities to the worldwide marketplace for advanced instrumentation.

The UK's light source facilities already have a strong track record of collaboration with industry, which has led to many successful, innovative products as well as spin out companies. The new source capabilities proposed in this strategy will support further innovation in important technologies and business sectors, such as pharmaceuticals, energy storage and advanced materials.



Part Two

The second part of this strategic vision report sets out the evidence base for how light sources are being used to enable research and innovation in key challenge areas for science and technology. It also details a comprehensive set of options for future developments across all the principal sources for the UK's research base, which underpin the optimal development plan presented in Section 4.2 in Part One.



Images courtesy of Diamond, EuXFEL and ESRF

6. The science and technology drivers for light sources

6.1 A diversity of applications

The immense breadth of light source applications is highlighted in several recent reports, including:

- Diamond-II – Advancing Science [viii]
- ESRF Orange Book [ix]
- National Academy of Sciences Opportunities in Intense Ultrafast Lasers – Reaching for the Brightest Light [x]
- UK XFEL Science Case. [xi]

The following sections aim to highlight where new capabilities can provide solutions to challenging problems in science and technology, illustrated by examples of recent breakthroughs. Although the emphasis is on highlighting how light sources are addressing key research needs in the Life Sciences and Physical Sciences, their application is much broader than this, as illustrated in Figure 10.

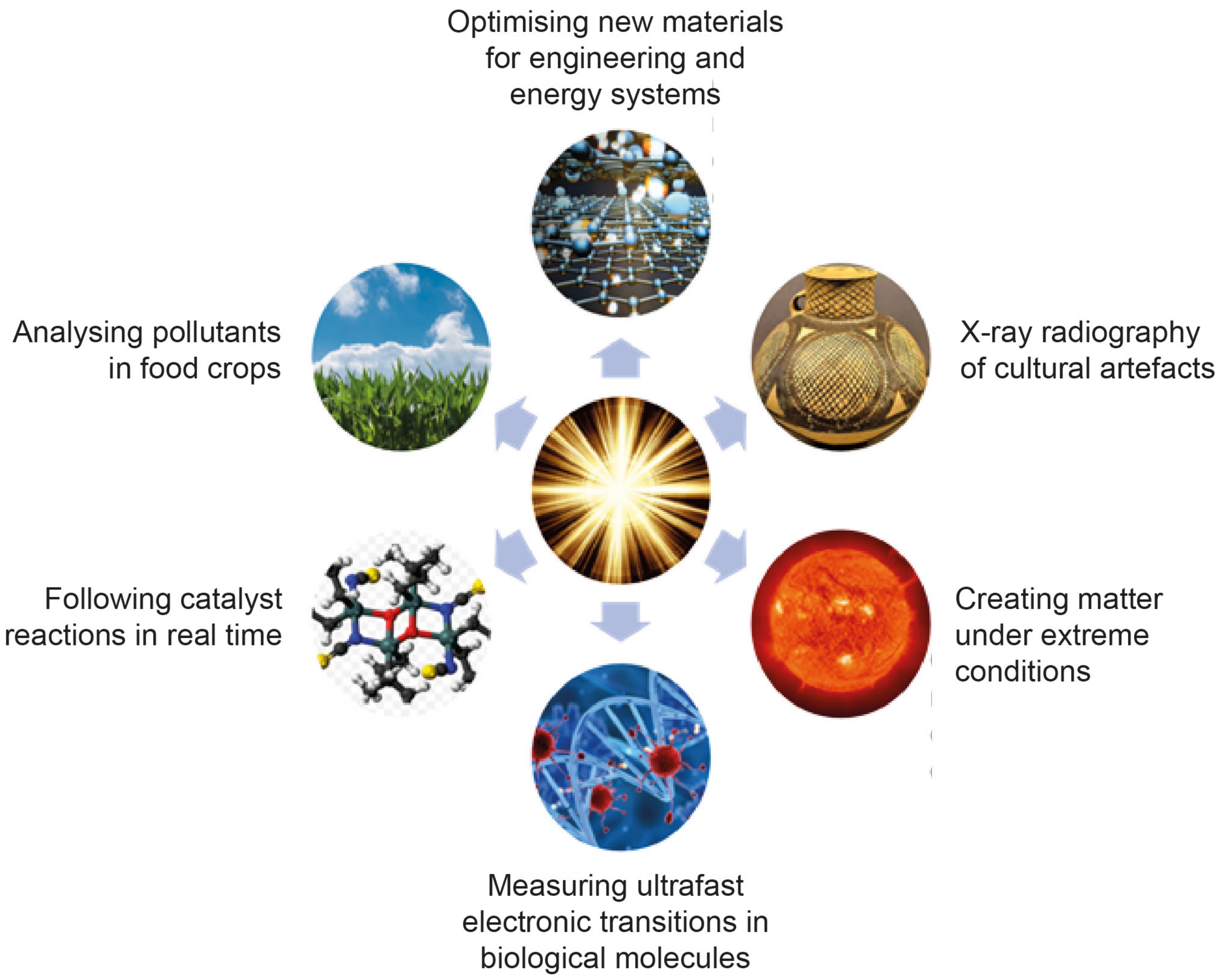


Figure 10: How light sources are used in different disciplines

6.2 Life sciences challenges

To enrich our understanding of biological structure and dynamics involves gaining knowledge across a broad range of scales:

- spatial, where atomic-level details describe life in terms of fundamental chemistry, through to imaging organisms and macroscopic structures such as bone

- dynamic, where structural and electronic changes need to be measured at timescales important to fundamental processes, ranging from femtoseconds to minutes.

Biological science remains immensely complicated. To understand the workings of cells through all forms of life requires in-depth, molecular level knowledge of many elaborate hierarchical structures. Deciphering the often weak and transient interactions between these structures, and the diverse roles they play in the make-up and biological functions of cells, requires both single and correlative measurements that are pushing the boundaries of current photon and electron-based probes. Future progress in structural biology depends on the availability of an increasing range of techniques that can provide structural information in in-situ cellular contexts. To meet this need, there is a requirement for advanced spectroscopy and imaging facilities that can extract structural information from biological systems that operate on timescales ranging from femtoseconds to milliseconds.

Life is a non-equilibrium thermodynamic process that changes through time, but we have little idea of the operando interconnectivity between the different scales involved – from the multi-cellular to the cellular (microscale), from subcellular organelles to the molecular level. Understanding the structure and dynamics of macromolecules, combined with a mapping of the distribution of interacting molecular species within the cell (including metabolites, ions, etc.), will significantly improve our quantitative understanding of the mechanisms underpinning life processes.

Observing the dynamics of molecules requires data collection at ambient temperature from femtosecond X-ray pulses. Understanding macromolecular dynamics will enable a better understanding of the effects of drugs in the behaviour of macromolecules and provide experimental data to test the predictions from molecular dynamics simulations, something that is not possible using averaged rate data. Ultrashort pulses open the femtosecond regime for studies, and time-resolved serial crystallography can investigate the microsecond regime – some of the most interesting molecular dynamic behaviour in the solution phase occurs between these two regimes. Together, XFELs, synchrotrons and lasers allow measurements spanning the femtosecond to millisecond time domain, and will provide a complete assessment of protein-drug kinetics, and enable optimisation of drugs targeted to transition states.

The UK's biological science community that uses light sources as a core part of its research is strong and growing as new techniques are developed. Over 2,500 researchers from the biological sciences fields and the health technology industries used Diamond and ESRF in 2019.

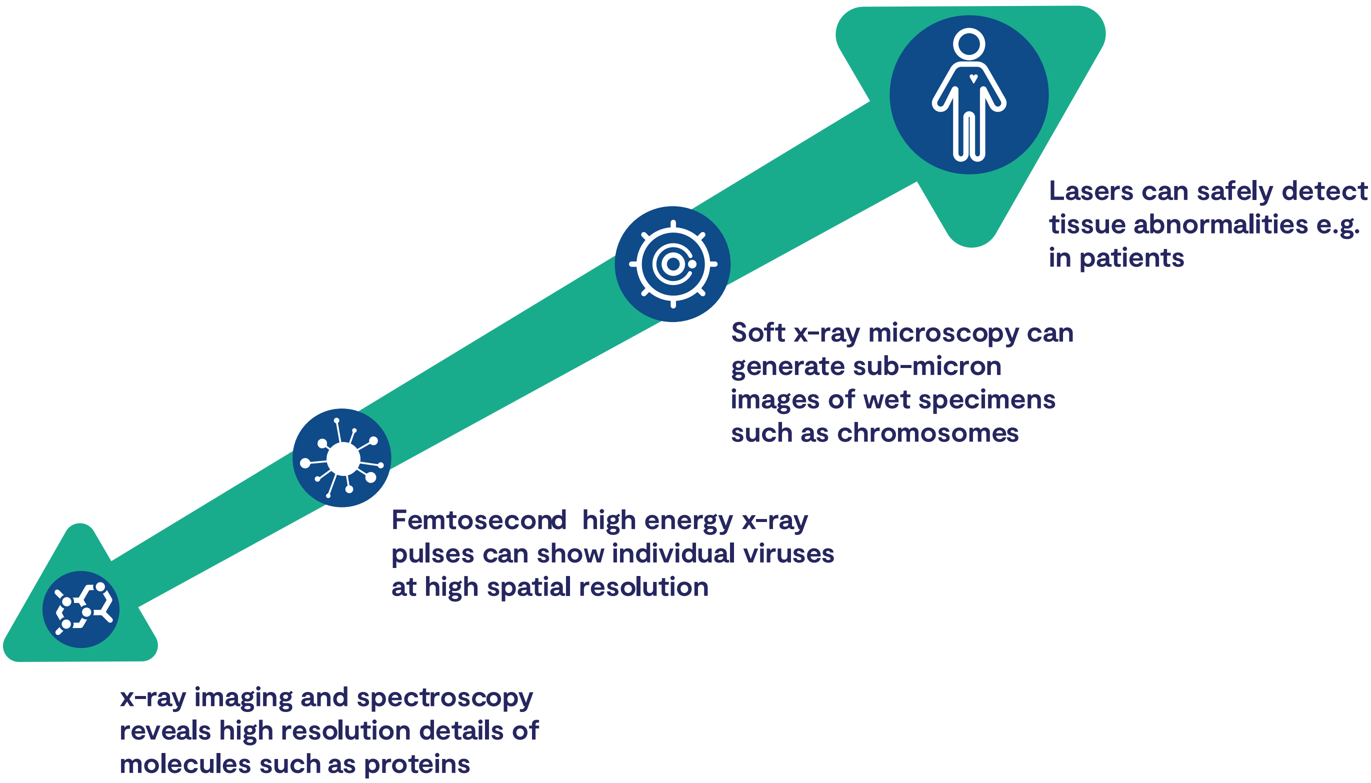


Figure 11: Improving understanding of biological structures on widely different scales

6.2.1 Novel healthcare technologies

Improving public health is a critical driver for advancement in many fields including biology, medicine, chemistry and engineering. Recent developments in X-ray imaging tools can now directly reveal the intricate structural changes during tumorigenesis in a single cancer cell, while advancements in nano-imaging and nano-spectroscopy can identify and map the distribution of metal ions throughout brain tissue, for example in relation to neurodegenerative disease. This high level of detail is uncovering relationships which suggest new leads for the next generation of medicines and treatments. Advancing the science of metallomics (the role of metals in biology) is a high priority. Increased flux and better spatial resolution, coupled with greater control over sample environments, will enable new insights into the way that cells, proteins and polymers take up and release biometals and disease-relevant metal ions and minerals.

In response to the COVID-19 outbreak, light sources are being used to research the virus. Microscopy techniques have been used to investigate how the virus infects cells, and how potential treatments might work.

Currently many serious diseases are diagnosed through inconvenient, painful, and sometimes dangerous, invasive procedures. There is a need to develop methods by which the molecular signatures of disease can be detected non-invasively through the skin. The use of laser-powered Spatially Offset Raman Spectroscopy (SORS) and its related technique of Surface Enhanced SORS (SESORS) has the potential for medical diagnosis of, for example, bone diseases such as osteoporosis, and for the biopsy-free characterisation of lesions detected by mammography.

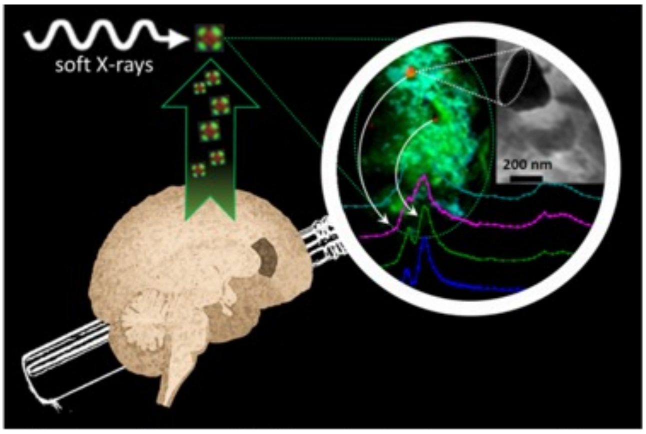
Cancer is a global public health problem of epidemic proportions. Personalised anti-cancer therapies target specific molecules that cause uncontrolled cell proliferation. A big hurdle in personalised medicine is finding why some patients benefit, yet others do not respond. Improving patient selection will save money in the National Health Service (NHS), cut down the costs of drugs, and reduce the size and cost of clinical trials. The use of machine learning approaches in laser-powered super-resolution nanoscopy is being trialled at the laboratory and the clinic as a tool to search for specific tumour fingerprints in lung cancer, that will predict which patients will benefit from a particular treatment.

Clinicians, together with scientists from Diamond Light Source, have demonstrated that synchrotron-based IR micro-spectroscopy and imaging can be used to study chemical speciation of human tissue and cells for cancer diagnosis in a non- destructive manner. A successful pilot study looked right inside cells – both lung cancer cells and normal cells – in tissue samples taken from lung cancer patients.

Fast in-line phase contrast tomography and advanced image analysis tools are being used to unravel, for the first-time, key failure mechanisms of electro-spun polymer fibre mats which are being used for tissue replacement and repair and in prosthetics.

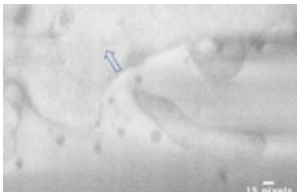
Case Study 1 – Alzheimer's disease

Alzheimer's disease is a neurodegenerative disease that is associated with dementia and shortened life expectancy. The disease is characterised by the formation of protein plaques and tangles in the brain that impair function. As well as protein plaques, perturbed metal ion homeostasis is also linked with pathogenesis, and iron levels in particular are elevated in certain regions of the brain. Synchrotron X-ray spectromicroscopy has been used on samples from the brains of two deceased patients who had Alzheimer's disease to differentiate the iron oxide phases in the samples. This work revealed that the chemical reduction of iron, and indeed the formation of a magnetic iron oxide called magnetite that is not commonly found in the human brain, had occurred during amyloid plaque formation, a finding that could help inform the outcomes of future Alzheimer's therapies.



Synchrotron soft X-ray nano-imaging and spectromicroscopy reveals iron and calcium biomineralization in Alzheimer's disease amyloid plaques (Image: Diamond Light Source)

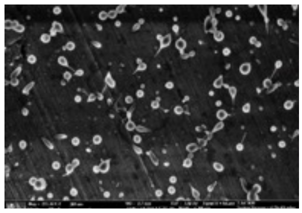
Case Study 2 – Imaging techniques to understand the biology of the SARS-CoV-2 virus, and to investigate potential treatments

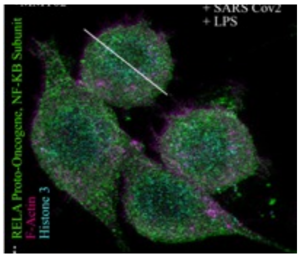


High resolution Serial cryoFIB/SEM volume imaging, showing the location of the virus in the cell at high resolution and near-native state tissue samples.

Image: Peijun Zhang (eBIC/DLS, Oxford University); Luiza Mendonça (Oxford University); Marisa Martin-Fernandez/Octopus group (CLF).

High resolution SEM of BioCyto's proprietary polymer nanoparticles that have been developed to carry anti-COVID drugs into neural tissue. Find out more at www.biocyto.org



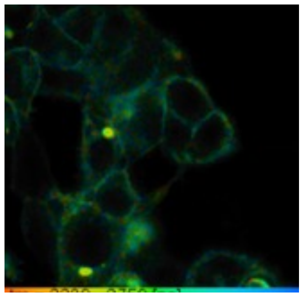


Super-resolution optical microscopy to investigate the cellular location and mode of action of drugs designed to prevent excessive immune response to the virus, a common cause of serious illness and death.

Image: Gokhan Yilmaz (Metamorph Therapeutics Ltd.).

Fluorescence lifetime imaging (FLIM) to study the interaction of SARS-CoV-2 spike protein with its target receptor at the cell surface.

Image: Siva Ramadurai, Ray Owens (Rosalind Franklin Institute); Stan Botchway, Kathryn Welsby (CLF); StreamBio; The Antigen Company.



6.2.2 Complex biomolecular structures including plant science

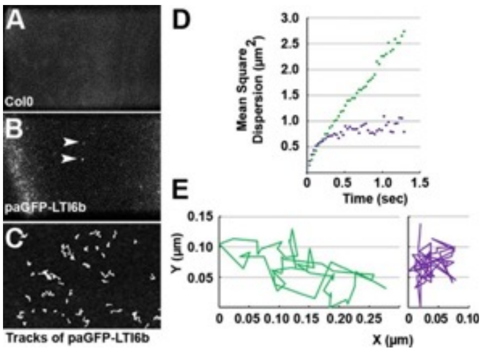
Laser imaging stations can be used to investigate processes in plant cells, addressing fundamental questions in plant biology.

This topic covers a huge area of science, and there are many challenges. For example, researchers wish to gain a better understanding of how plants can survive (and can be modified to survive) under extreme conditions such as drought. Optical microscopy has always been important for understanding the fundamentals of plant biology, and the more recent developments of super-resolution and single molecule microscopy techniques have provided insights into the molecular interactions important for plant growth, survival, and pathogen resistance.

Spectroscopic and molecular crystallography studies at synchrotrons are mapping toxic metal uptake in plants. This can reveal the amount, distribution and chemical environment of elements such as iron and zinc in grains, with different treatments that can be used to enhance uptake to increase nutritional value; it can also be used to study plant defence systems and resistance to attack by pathogens.

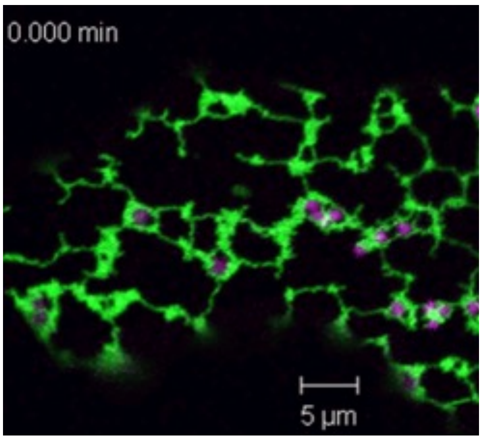
Case Study 3 – Laser-based optical microscopy in plant biology

Understanding the fundamentals of plant biology is important to address problems that affect agriculture, such as drought and pest infestation, problems that are likely to become more common as a result of climate change. The Octopus microscopy facility at the CLF has been used by the plant biology community to investigate many aspects of plant biology, using a number of laser-based imaging techniques.



For example, single particle tracking has shown how plant proteins move around the plasma membrane of the cells, and how this is affected by the plant cell wall.

Martinière A, Lavagi I, Nageswaran G, et al. Cell wall constrains lateral diffusion of plant plasma-membrane proteins, Proc Natl Acad Sci U S A 109, 12805 (2012) DOI: 10.1073/pnas.1202040109



Combined optical trapping and confocal microscopy has been used to investigate the interactions in plant cells between Golgi bodies and the endoplasmic reticulum, cell components involved in the synthesis and transport of proteins.

Photograph courtesy of Hawes Group, Oxford Brookes

6.2.3 Biotechnology and biological systems

Biotechnology across the agricultural, medical, energy, and environmental sectors is of tremendous benefit to society. The development of bio-inspired materials for widespread commercial and medical applications is creating a new era of renewable and bio-compatible products. These developments need to be facilitated by an understanding of the nanoscale structure of materials and how bulk properties emerge from the hierarchical assembly.

This level of physical characterisation and precision measurement demands:

- brighter/harder X-ray sources to improve depth of penetration
- improved spatial resolution to image submicron features
- new technologies in chemical mapping including circular dichroism (CD) spectroscopy, infrared (IR) spectroscopy and X-ray fluorescence imaging
- improved beam characteristics (coherence, emittance and divergence).

Bio-inspired systems are leading to new forms of paint, hydrophobic and anti- bacterial structures. Coherent X-ray imaging techniques can play a critical role in understanding these structures, but the application of these techniques is limited by the available photon flux.

To understand the effects and efficiency of cellulosic biomass processing requires biophysical characterisation. High resolution CD imaging could provide answers to questions that are difficult to answer using X-ray methods, such as homogeneity of the crystalline state or functionalisation.

6.2.4 Imaging across scales: Connecting the cellular and organism levels

The challenge of imaging biological systems, including human biology, is multi-scale and requires chemical imaging of compartmentalised environments of different tissue types (bone, muscle, etc). This requires multi-modal imaging and in situ measurements with enough resolution to visualise the structures, and brightness to distinguish from typically high levels of background.

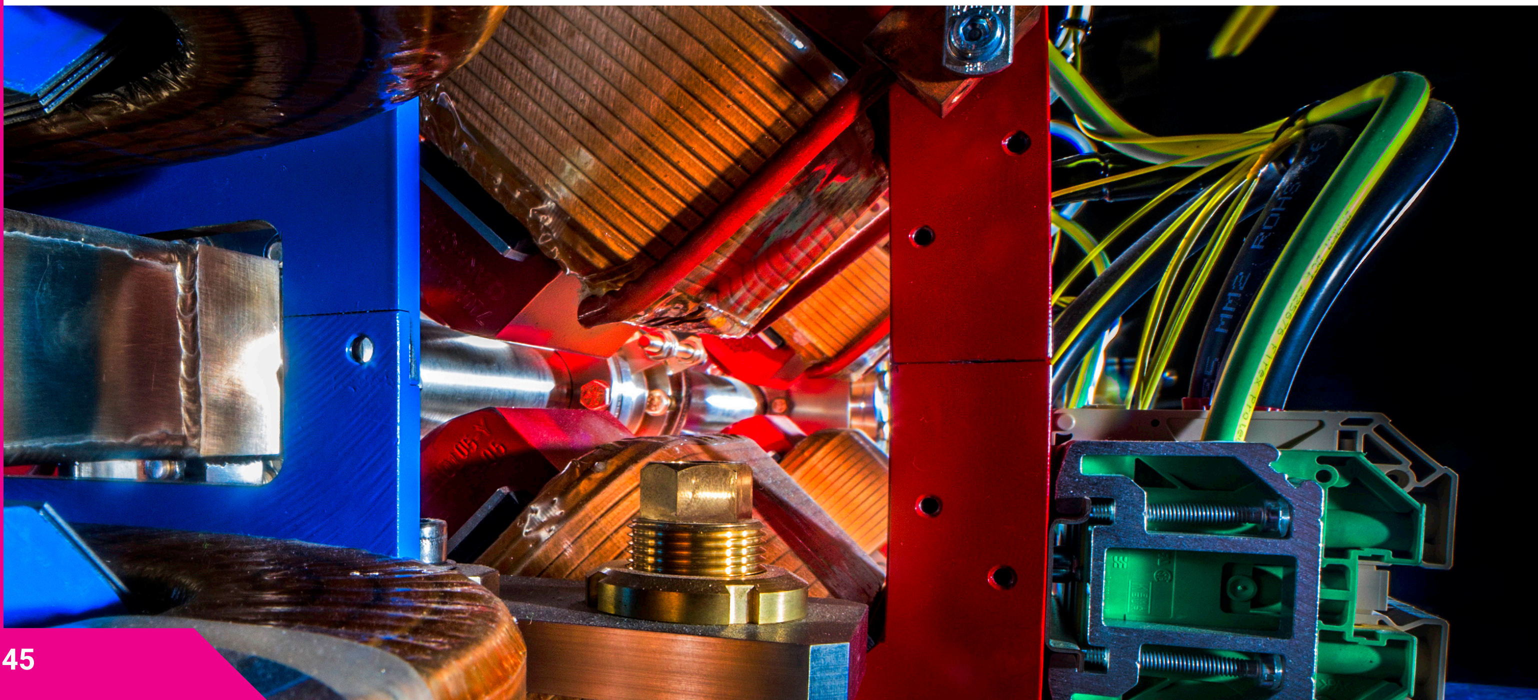
Imaging of cells and biological materials at atomic and molecular resolution

Imaging of cells and biological materials has been dominated by light and electron microscopy. These techniques will continue to flourish, as super-resolution microscopy and cryo-electron microscopy (CryoEM) provide 0.1 – 10 nm resolution imaging within cells, and their correlation provides a platform to study the structural biology of interacting macromolecules in the cell, whilst also connecting this structural information with macromolecular interactions.

However, a limitation of CryoEM arises from the poor penetration depth of electrons, so that only thin slices (~100 – 200 nm) of a biological specimen can be imaged with <1 nm resolution. In contrast, X-rays have a high penetration depth but poorer resolution (~10 nm). New techniques, such as full-field soft X-ray cryo-transmission microscopy, coherent diffraction imaging and cryo-ptychography, have achieved proof of principle status, but require the higher fluxes of emerging next-generation synchrotron sources to enable a reduction in scan times, and higher energy X-rays to reduce the impact of radiation damage to biological materials. Imaging at tens of nanometre resolutions for large tissue samples will be possible.

Correlative light and electron microscopy (CLEM) combines the ultra-high resolution of electron microscopy with the molecular specificity available from targeted labelling in optical microscopy. To date, there has been a resolution gap between optical and electron microscopy, but the development of sub-diffraction limit optical imaging brings the resolution of the two techniques much closer together, potentially increasing the power of the correlative approach. The development of EM-like sample fixation methods, in particular the use of cryo-fixation, for super-resolution optical techniques is key to unlocking the potential of ultra-high-resolution CLEM.

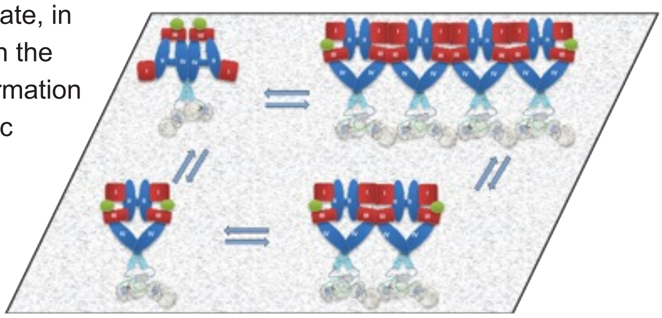
Ultimately, the use of very high-resolution optical methods has the potential for annotation of electron tomograms, identifying specific molecular types which can be averaged for structure determination. This brings us closer to the goal of in situ structure determination.



Case Study 4 – Combining sub-diffraction limit optical microscopy with long timescale MD simulation to understand the architecture of molecular complexes in cells, in health and disease

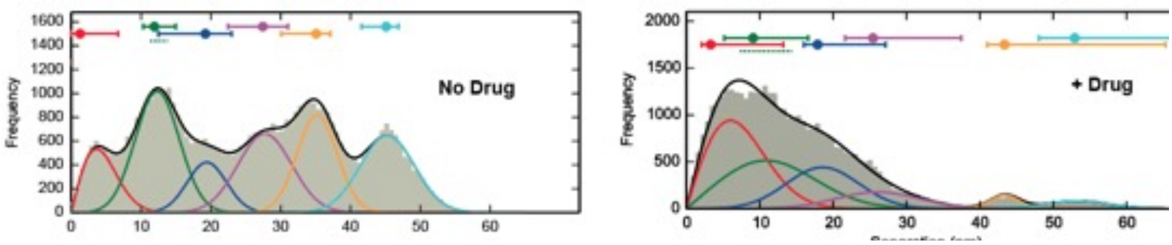
Atomic resolution structure determination methods have shed a huge amount of light on the structure-function link; however, there is also a requirement for in cellulo methods to determine how the larger scale organisation of biological macromolecules affects biological function. For example, the Epidermal Growth Factor Receptor (EGFR) family of molecules controls important cell functions, is involved in the development of many cancers, and is the target of anti-cancer therapies.

The method of Fluorescence Localisation Imaging with Photobleaching (FLImP) was developed at the CLF's Octopus facility and uses single molecule localisation to characterise complexes of macromolecules with < 5 nm resolution. FLImP has been used to investigate the oligomerisation of EGFR in the native state, in mutations associated with cancer, and in the presence of anti-cancer drugs. The information obtained has been combined with atomic resolution structures of EGFR domains, and with long timescale MD simulations to produce a model of EGFR oligomerisation in the cell.



Model for EGFR oligomerisation based on FLImP data

The FLImP measurements have demonstrated "fingerprints" of molecular architecture associated with different mutations. A collaborative project between the CLF and clinicians is investigating the potential to use FLImP as a tool to stratify patients for optimal cancer therapy, and for early warning of the development of drug resistance.



FLImP "fingerprints" of EGFR structure, with and without the addition of an anti cancer drug

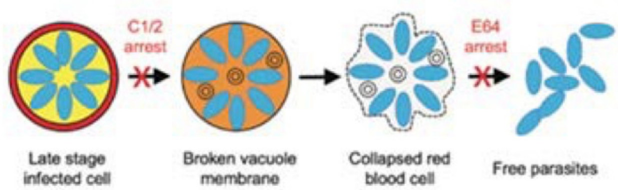
Laser-based optical tweezer systems are important new tools, for example for the capture of bio-active particles and the probing of their chemistry using spectroscopy techniques. Imaging stations are used to monitor biochemical processes and interactions on length scales from 1 nm upwards. They have played an important role in capturing subcellular organelles whilst imaging under the confocal or super- resolution microscope, allowing the investigation of the molecular mechanisms of inter-organelle interactions, critical to maintain cell homoeostasis.

Optical tweezers are also being used for the manufacture of micron-sized polymer particles, and the characterisation of polymer particles. Confocal stations are used to monitor the assembly and interaction of polymers with biological systems. Confocal and super-resolution imaging stations can provide information on the interaction of drug and probe molecules with cells and tissues, with applications in therapies and diagnostics. Raman technologies can probe deep within tissues and can be used for imaging and diagnosis of bone disease and cancer.

Often the most powerful approach is by a combination of techniques. For example, in-cell studies of the mechanism of malarial infection, using full-field soft X-ray microscopy to get tomographic (3D) images of whole red blood cells as infection propagates, have been combined with electron tomography.

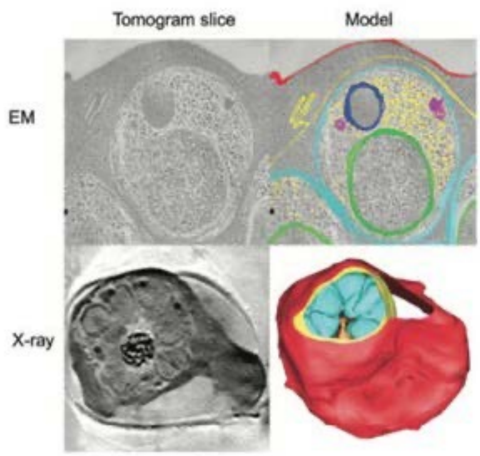
Case Study 5 – Combining X-ray and electron tomography to visualise key steps in the malaria infection process

Malaria parasites develop within red blood cells inside a membrane-enclosed parasitophorous vacuole. An essential step in their life cycle is the exit of mature parasites from the blood cell, a multistage process termed egress. To do this, the parasites orchestrate a highly regulated sequence of membrane permeabilisation and breakage steps culminating in the explosive release of parasites for a new round of infection.



Schematic of the main steps in egress with points of arrest by compound 1/2 and E64 indicated

Using a combination of cryo X-ray and electron tomography, Hale *et al*[1] discovered a previously unidentified permeabilisation of the vacuolar membrane at the start of egress that preceded membrane rupture. To collect these data, parasites inside red blood cells were synchronised so that they were at a similar stage of the infection cycle. Two pharmacological blockers (Compounds C1/2 and the cysteine protease inhibitor E64, see schematic) were used that could stall egress at different stages. The strategy enabled visualisation of the final minutes of egress, revealing that the blood cell membrane abruptly loses its structural rigidity and collapses around the parasites. The image is rich in detail and provides significant context, however, it is just one of a small, limited dataset. The increase in flux and sample throughput in Diamond-II would provide suitable datasets for machine learning. Already, we are seeing that machine learning algorithms can improve protein folding predictions, cancer screening and guide self-driving cars. Diamond-II will enable larger numbers of samples to be measured that will not only increase their statistical relevance but also provide deeper insights through the application of artificial intelligence.



Electron and X-ray tomograms of cells arrested early in egress by Compound 1 or 2. Red cell membrane, red; vacuole membrane, yellow; parasite cell membranes, cyan. Other colours, parasite organelles and ribosomes.

1. Hale VL et al. Parasitophorous vacuole poration precedes its rupture and rapid host erythrocyte cytoskeleton collapse in Plasmodium falciparum egress. Proc Natl Acad Sci U S A 114, 3439-3444 (2017) DOI:10.1073/pnas.1619441114

Chromosome structure
We still have very little understanding of the organisation of genomic information in space in a non-dividing cell. The mechanism of action remains elusive due to a lack of tools for in vivo investigations, with the available tools only probe a set of specific loci at a time. For example, nucleoid associated proteins (NAPs) facilitate chromosome organisation and there is a need to investigate the many NAPS, their effects on nucleoid organisation and the role they play in multiple control mechanisms in reaction to stimuli. The dynamical response to effectors is ripe for investigation by multiple integrated methods of imaging, microscopy, scattering and diffraction.

A three to five order of magnitude increase in brilliance will enable sampling over larger areas and will bring the in-plane resolution into the subcellular regime, supporting single cell analysis at a level that has not been possible to date. This would bridge a critical gap in provision for life sciences experiments, overcoming current constraints at nanoprobe beamlines worldwide. Such a performance increase is achievable with the next generation of synchrotrons and detectors.

Membrane proteins
A key area where fundamental science is closely meshed with biomedical applications is in the understanding of membrane proteins. These are implicated in a wide range of pathological behaviours, but are very difficult to prepare and study. Drug advances will need a step change in throughput allowing the investigation of thousands of such structures, which requires high fluxes and novel sampling environments so that smaller crystals can be used – overcoming the current bottleneck of needing to grow large samples. XFEL-enabled serial femtosecond crystallography (SFX) techniques can now use nano crystals, and can yield structures under physiological conditions and free from radiation damage.

6.2.5 Biological challenges at the atomic and molecular scale

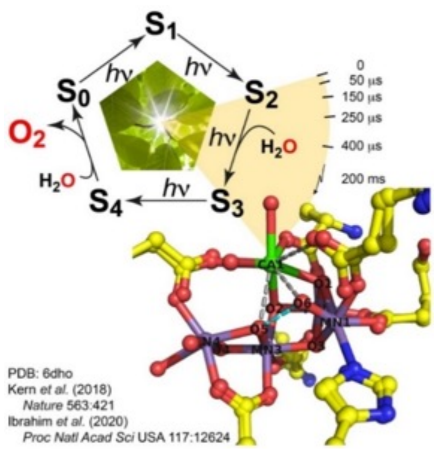
Achieving a molecular description of cellular organisation will transform fundamental science and our understanding of disease processes, allowing more effective definition of drug targets.

Advanced imaging techniques can provide structural information, including the use of both single molecule and ensemble techniques to determine intra- and inter- molecular distances on length scales from 1nm upwards. For example, Förster resonance energy transfer (FRET) and fluorescence lifetime imaging microscopy (FLIM) techniques can be used to measure nanometre distances and, together with atomic resolution structure and molecular dynamics simulation, determine macromolecular conformation. These measurements can be made either in living cells or on isolated proteins and protein complexes. Super-resolution imaging techniques based around single molecule localisation are being used to characterise molecular complexes at the sub-5 nm level (see Case Study 6 on the following page).

Case Study 6 – Time-resolved serial femtosecond crystallography correlated with X-ray emission spectroscopy provides unprecedented and detailed mechanistic insights into the photosystem II reaction cycle

A remaining frontier challenge in structural biology is to determine time-resolved structures at atomic resolution directly from systems engaged in function, at physiological temperatures and pressures. Serial femtosecond crystallography (SFX) methods developed at XFELs present revolutionary opportunities to solve structures from slurries of nano- to micron-size crystals. Sample delivery is often coupled with reaction initiation strategies that include optical pump – X-ray probe and/or mixing methods, all of which are making important advances towards this goal.[1, 2] These methods yield structural and functional information with high temporal and spatial resolution from the same sample. The resulting molecular movies enable scientists to watch the most complex systems in biology as they work.

Photosystem II (PS-II) is a high-value, benchmark system for time-resolved SFX studies. The enzyme is responsible for the “great oxidation event” approximately 2.4 billion years ago, that transformed the earth from an anaerobic reducing atmosphere to the O_2 rich and oxidising atmosphere today. PS-II is a large integral membrane protein expressed in all plants and most photosynthetic microorganisms. The protein uses four visible light photons to catalyse the four-electron oxidation of two water molecules to form one O_2 molecule plus four H^+. The protons help establish a gradient across the membrane and are used for ATP generation by ATP synthase. The visible light photons initiate very rapid charge separation events (fs – ps), and much slower electron-transfer events (hundreds of ms) to reduce the quinone pool that are subsequently used for converting CO_2 into sugars.



O_2 bond formation within PS-II is catalysed by the oxygen evolving complex (OEC) that include a Mn_4O_5Ca cluster (see figure). When a photon is absorbed by the P680 chromophore within PS-II, it results in charge separation and electron transfer to the quinone site. The oxidised P680 is then reduced by the OEC, which advances one oxidation state with each photon absorption event. In the Kok cycle, the first photon promotes the S_1 to S_2 transition, the second photon S_2 to S_3, and the third photon from S_3 to S_4. The S_4 state catalyses the conversion of two water molecules into O_2 resulting in the S0 state of the OEC. Absorption of a fourth photon produces the stable S_1 starting state.

The Mn atoms within the cluster act as a redox “buffer” and each oxidation state has a unique $\mathrm{Kbeta}_{1,3}$ X ray emission spectrum (XES). Consequently, time-resolved XES collected simultaneously with time-resolved SFX provides complementary data on the electronic and atomic structures of the catalytic centre. Some recent results[3, 4] probed the $S_2 \rightarrow S_3$ transition with microsecond temporal resolution and SFX structures to 2 Å resolution that demonstrate motion of the Mn atoms and entry of a new solvent atom. The atomic models are correlated with oxidation of the Mn atoms within the OEC and an O_2 generation assays from crystal slurries. Ongoing studies at XFEL sources continue to probe each of the S-state transitions in the Kok cycle. Atomic resolution movies of the entire reaction coordinate will emerge; most importantly, the process by which two solvent molecules are transformed into O_2.

1. Orville AM, Recent results in time resolved serial femtosecond crystallography at XFELs, Curr Opin Struct Biol. 65:193-208 (2020) DOI: 10.1016/j.sbi.2020.08.011
2. Fuller F, Gul S, Chatterjee R, et al. Drop-on-demand sample delivery for studying biocatalysts in action at X-ray free-electron lasers, Nat Methods 14, 443-449 (2017) DOI: 10.1038/nmeth.4195
3. Ibrahim M, Fransson T, Chatterjee R, et al. Untangling the sequence of events during the $S_2 \rightarrow S_3$ transition in photosystem II and implications for the water oxidation mechanism, Proc Natl Acad Sci U S A 117(23):12624-12635 (2020) DOI: 10.1073/pnas.2000529117
4. Kern J, Chatterjee R, Young ID, et al. Structures of the intermediates of Kok’s photosynthetic water oxidation clock, Nature 563, 421-425 (2018) DOI: 10.1038/s41586-018-0681-2

With the emergence of XFEL-generated ultrashort X-ray pulses, powerful new techniques are being developed for coherent diffractive single shot imaging (CDI) of biological and non- biological structures, including imaging non-periodic, non-reproducible structures and nanocrystals. In the future, there is potential for these techniques to provide nanoscopic imaging of biological assemblies and molecular machines within the necessary time resolution under in vitro conditions.

Similarly, the application of SFX is enabling the study of otherwise inaccessible proteins, such as membrane proteins that frequently cannot be made to form macroscopic crystals and allowing structures to be studied free of radiation damage and potential cryo-artefacts. These techniques have the potential to expand the information on protein structures that have been a major success of synchrotron light sources over the past decade.

Future ultrashort pulse techniques open the possibility of studying the structural dynamics of light-activated proteins. Recent ground-breaking work has shown the possibility of using the snapshot imaging capability of an XFEL to study rare, but functionally critical, conformational changes in a virus .[xii]

Summary of the future light source requirements for life sciences

Research Areas	Source technical requirements
Healthcare technologies	• Non-invasive techniques such as SORS
Complex biomolecular structures and plant science	• Monomolecular resolution • Correlative microscopy/imaging methods
Engineering and biomaterials applications	• High brightness hard X-rays • Correlative microscopy/imaging methods
Structures at cellular and organism scales	• High resolution and brightness • Correlative microscopy/imaging methods • Low-dosage techniques that avoid damaging cells
Structures and dynamics at atomic and molecular scales	• Ultra-short pulses (<10 femtosecond)

6.3 Physical sciences challenges

Basic research in the physical sciences is a key driver of productivity and economic growth, enabling solutions to many of the health, environmental and technological challenges facing our society today. Addressing these challenges is key to realising technological innovations in many areas including:

- Solving material science challenges that are limiting the performance of new energy generation and storage systems, and restricting the lifetimes of critical engineering components
- Developing addressable antiferromagnetic semiconductors, which are critical as the underpinning technology behind extremely secure storage devices
- Probing the electronic states of nanoscale 2D materials and hetero-structures controlled by engineered strain or voltage gates, in order to open up new concepts in electronics and quantum computing
- Revealing the structure and operation of catalysts, so that new products can be manufactured for fuels, healthcare and environmental protection
- Understanding failure mechanisms in emerging optoelectronic device technologies, including solar photovoltaics and light emission diodes for displays.

Cutting-edge light sources are needed to reveal the structure and dynamics at atomic, molecular or electronic levels and can answer questions of fundamental importance including:

- How can we optimally exploit quantum mechanics in information and other technologies, so they can be harnessed for real-world applications?
- Can we fundamentally understand the operation and failure mechanisms on different length and timescales in new photovoltaic technologies that will play a critical role in meeting our net zero carbon needs?
- How can we identify and control states in quantum materials (e.g. superconductivity or charge transport in topological insulators) with light?
- How do liquids, like water, change and fluctuate at the nanoscopic scale?
- How do materials behave at the high pressures of planetary cores?
- What are the properties of matter in extreme and exotic conditions, such as at the centre of stars and galaxies, so we can realise safe fusion energy generation?

The UK science community is at the forefront in applying light source techniques in many areas of the physical sciences – over 3,200 researchers used Diamond in 2019.

6.3.1 Chemistry

Chemistry is a fundamental science to modern life that has been directly responsible for improvements in health (pharmaceuticals), agriculture (fertilisers and pest control) and energy (petrochemicals). Light source facilities have made major contributions to the development of chemical knowledge. The use of spectroscopy and scattering techniques, and more recently imaging, is providing a detailed understanding of the geometrical and electronic structures of the different species involved in chemical processes, and relating this knowledge to function.

Catalysis

Catalysis research is fundamental to the sustainability of our modern way of life. Catalysts are involved in the processing of more than 80% of manufactured products, most of them used by modern societies for fuels, chemicals, polymers, and pharmaceuticals, as well as for abatement of air and water pollution. Further improvement in the techniques probing the electronic, chemical and structural degrees of freedom is essential to developing a detailed mechanistic understanding of how catalysts work, to inform new strategies for materials design and synthesis.

The mixture of catalyst, support structure, microstructure and nanostructure, and the resulting correlations with selectivity, function and performance, remains a challenging multidimensional problem. A step change of at least four orders of magnitude in high brightness hard X-ray sources is needed to allow the time required for in situ studies of full particle imaging to be reduced from, typically, one day at present to seconds, so that the multi-parameter studies needed can be achieved in acceptable timescales. The next generation of synchrotron sources will be able to achieve this. Also, the advances being made in sources will increasingly allow real-time, operando measurements.

Time-resolved studies of liquid and gas phase chemistry are improving our understanding of chemical dynamics of relevance to catalysis, where X-ray emission spectroscopy has proved a decisive method in resolving research questions.

XFELs are increasingly being employed to access the fastest (sub-picosecond) timescales relevant to catalysis.

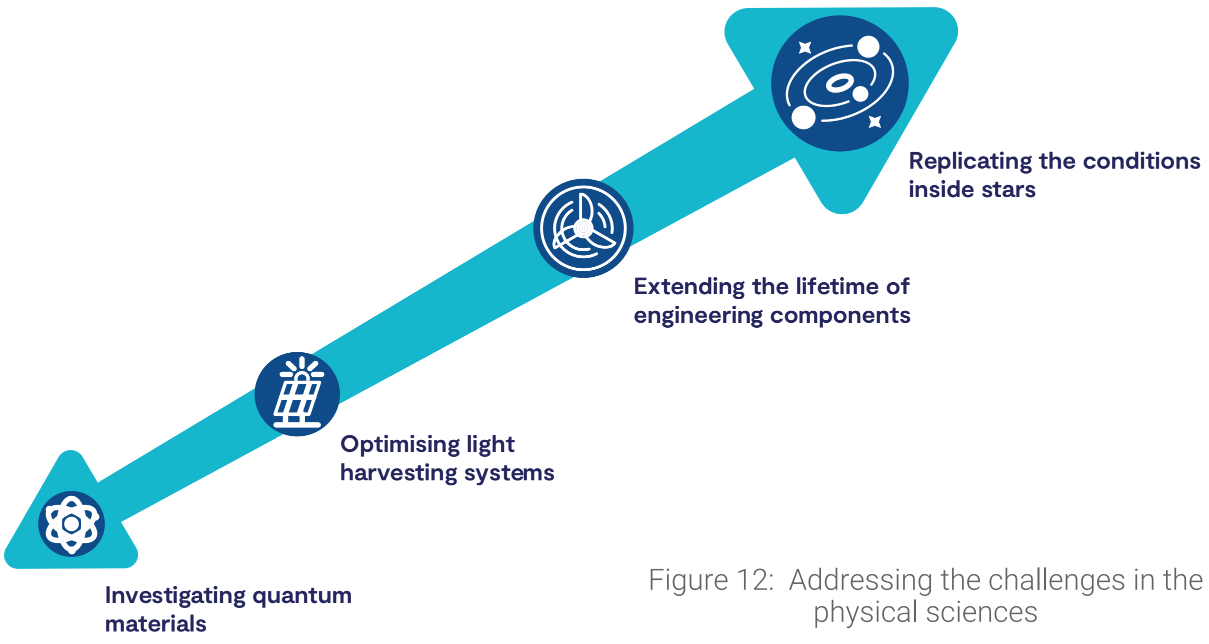
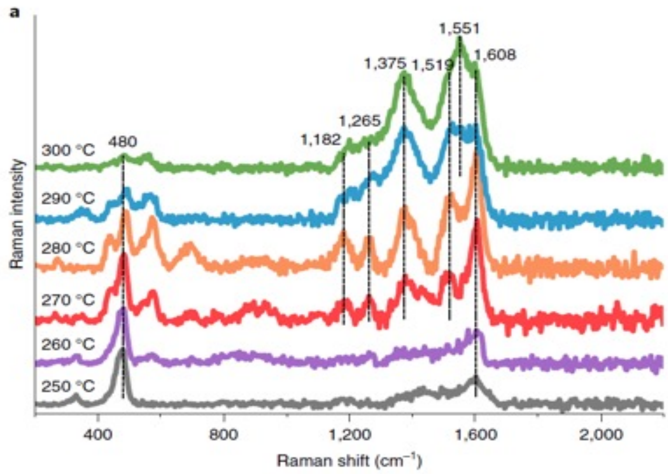


Figure 12: Addressing the challenges in the physical sciences

Case Study 7 – Ultrafast laser spectroscopy to understand catalyst deactivation

The deactivation of catalysts as a result of contaminant build-up on their surface has both economic and environmental impacts, as reactivation is a highly energy-intensive process. Time-resolved Kerr-gated Raman spectroscopy has been used at the CLF to study the build-up of contaminants on zeolite catalysts as reactions proceed. This has shown that the nature of the contaminant is different from previously thought, and has led to the proposal of a new catalyst design.



The spectral "fingerprint" shows the build-up of contaminants as temperature increases

https://doi.org/10.1038/s41563-020-0800-y

Biochemistry

Combining X-ray diffraction and X-ray emission from molecules of interest in biochemistry is proving very promising, leading to new insights on the photosystem II complex photocycle. Higher flux densities are needed to enable combining X-rays with spectroscopy from IR, Raman and UV-visible measurements to include NMR and electron paramagnetic resonance (EPR), so that biocatalysts can be studied under realistic operating conditions with more challenging environments.

Ultrafast laser spectroscopy can be used to study dynamic processes in biological molecules, for example light harvesting, enzyme catalysis, and protein folding. 2D infrared spectroscopy has the potential for investigating the interactions between proteins and drug candidate molecules and may prove valuable as a drug screening method. This is the subject of a joint Rosalind Franklin Institute and CLF project.

Case Study 8 – Two-dimensional infrared spectroscopy (2D-IR) as a potential tool for drug discovery

Pump-probe infrared spectroscopy tells us about the way molecular structures change with time following stimulation with a laser pulse (the pump). By varying the frequencies of both pump and probe pulses, we can obtain two-dimensional spectra. This technique provides information beyond linear infrared spectra, by spreading the vibrational information along multiple axes, yielding a frequency correlation spectrum. It is the optical analogue of multidimensional nuclear magnetic resonance (NMR) spectroscopy. One potential application of 2D-IR spectroscopy is investigating the interactions between potential drug molecules and their binding site on a protein.

The “LIFEtime” station on the CLF’s Ultra facility allows the collection of 2D-IR spectra in seconds. Combined with principal component analysis (PCA), this opens up the possibility of using 2D-IR as a screening tool for drug discovery.

A collaborative project between the Rosalind Franklin Institute and the CLF will develop instrumentation and analysis techniques, obtaining proof-of concept data to demonstrate the feasibility of using 2D-IR for drug candidate screening.

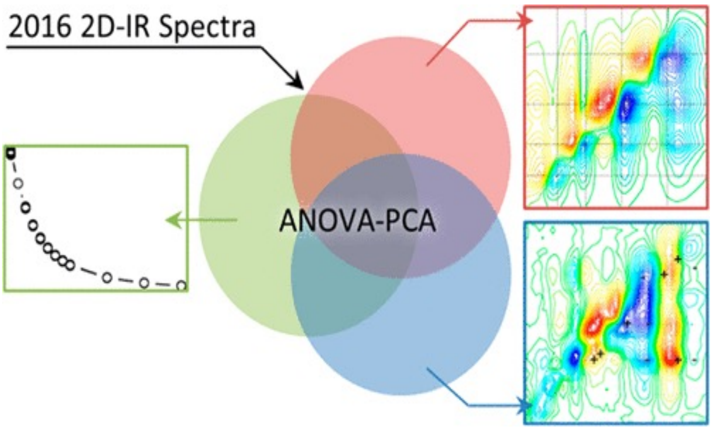


Figure reprinted from Fritzsch R, Donaldson PM, Greetham GM, et al. Rapid Screening of DNA-Ligand Complexes via 2D-IR Spectroscopy and ANOVA-PCA. Anal Chem. 2018;90(4):2732-2740. DOI:10.1021/acs.analchem.7b04727

Liquids and their role in chemistry

A key scientific goal for liquid phase experiments is to investigate the role of solvated electrons in water, which influence many aqueous reactions and could be responsible for many poorly understood dissociative properties from DNA to atmospheric chemistry. XUV photoelectron spectroscopy extends the technique of time-resolved photoelectron spectroscopy, which has proven to be a powerful tool to study and disentangle electronic and nuclear motion during chemical reactions. It increases the probe photon energy from ~6 eV to ~20 eV, giving the probe an unrestricted view of the entire reaction, including all intermediates and final products. This, along with other techniques such as transmission and emission X-ray spectroscopy, will allow inner valence and non-bonding electrons to be tracked as they respond to changes in nuclear geometry and valence electron density.

6.3.2 Advanced materials and engineering

The synthesis of new materials designed with specific properties for technological applications is one of the main research areas in chemistry and materials engineering. Collecting fast kinetic data across a range of timescales, from microseconds to attoseconds, will provide information about the mechanisms that govern the structural transformations in these materials, enabling the study of fast processes under real conditions of operation.

It is increasingly important to be able to search for new materials with specific, desirable properties. This can be efficiently achieved by, for example, preparing libraries of multicomponent materials in which the chemical composition is systematically varied – guided where possible with computational studies – and then studying their structure with high throughput crystallographic measurements. The speed and throughput will benefit greatly from next-generation sources.

New techniques to investigate novel materials, such as nano-porous materials, include X-ray Photon Correlation Spectroscopy (XPCS) which makes use of the coherence properties of the X-ray beam to measure dynamical processes through the variation of the speckle pattern in the measured diffraction image. New high brightness sources will provide access to dynamical processes occurring down to tens of nanoseconds. This will bridge the gap with other time-domain spectroscopy techniques, such as neutron spin-echo, and enable diffusion coefficient and jump parameters to be compared with the results of molecular dynamic simulations, helping to validate the accuracy of simulation techniques.

Microscopy techniques are being used to investigate the structure of advanced materials. Physics-based super-resolution techniques designed for imaging biological samples are now finding applications in the study of materials, a good example of the cross-fertilisation that occurs in the facility environment. For example, a combination of high-resolution imaging and optical trapping has been applied to the study of 3D block copolymers.

Pump-probe spectroscopy is a simple, but widely used technique that enables a temporal resolution much shorter than that achievable via electronic measurement of signals. The value of pump-probe laser spectroscopies in understanding material properties is recognised worldwide and it is one of the primary drivers for investment in infrastructures such as the European XFEL in Germany and ELI-APS in Hungary. However, scientists around the globe have only begun to scratch the surface of what is possible.

Advanced material engineering and processing

Advanced materials and manufacturing are areas of UK strength, and include advanced composites, high-performance alloys, low energy electronics and telecommunications, materials for energy and nano-materials for health. They present many significant engineering challenges; for example, designing and testing the materials needed for the first wall of a future fusion reactor that require long-term pulsed loading material studies to be undertaken.

Our ability to understand material physics and to link experiments and modelling is, in many areas, limited by our ability to fully probe the critical length and timescales of material processes. A gap exists between the nanoscale region in which many processes occur, and the microscale region that we can spatially probe using current generation sources and instruments, forcing compromises between time resolution, penetrating depth of X-rays, and signal-to-noise ratio. More intense, smaller beams will allow us to:

- probe the changes in composition and structure across surfaces and interfaces that are typically only a few micrometres in size (oxides, corrosion, welds)
- carry out high resolution chemical and structural probing of defects and precipitates
- achieve higher signal-to-noise results enabling rapid measurements
- use phase contrast to examine bubbles, cracks and voids
- use new imaging and coherent diffraction techniques to provide nano and microscale strain under real operating conditions.

In-operando studies at process timescales will help drive the next generation of materials, engineering and process development, including Additive Manufacturing techniques.

Laser peening (LP), or laser shock peening (LSP), is an important, but niche, industrial technique for surface treatment to increase substantially the component lifetime. It is currently limited to highly specialised applications, such as jet engine turbine blades. There is a need to cover much larger areas per pulse and deliver correspondingly large increases in throughput. LP could revolutionise the field by reducing costs in those industries that already use peening, and also significantly increasing the range of potential applications.

Designing and controlling quantum materials
Basic research in quantum materials is key to advancing knowledge and identifying applications for industry; for example, building devices that can exchange photonic to electronic signals and vice versa in quantum information processing.

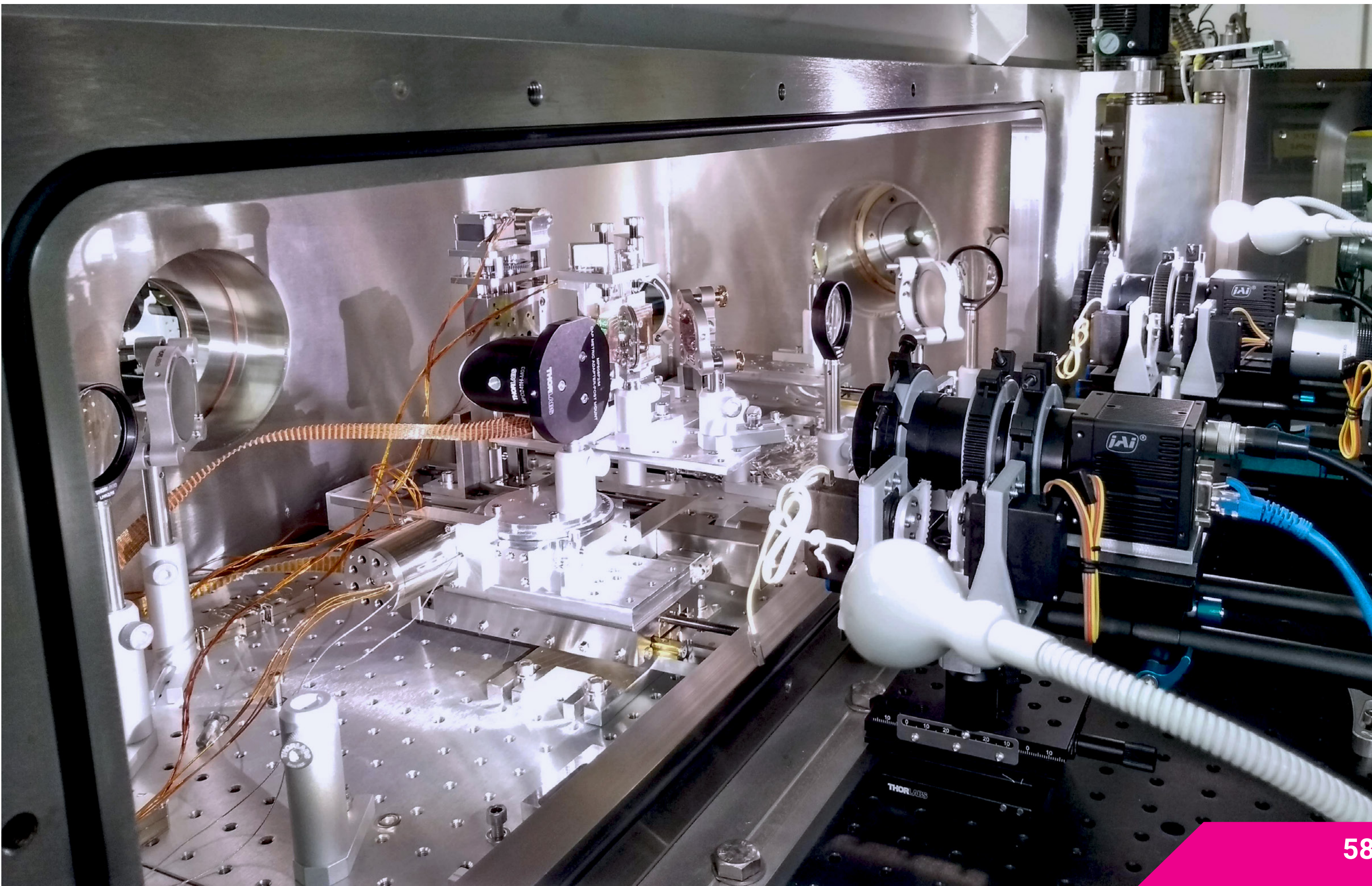
Quantum materials, however, present immense challenges to our existing understanding of material properties, and the development of new and advanced analytical tools is need to realise their full potential. Experimental probes based on polarised synchrotron Vacuum Ultraviolet (VUV), soft and hard X-ray scattering, resonant inelastic X-ray scattering (RIXS) absorption and spectroscopy are beginning to give unrivalled insights into quantum materials, unveiling a host of complex phenomena at the electronic and magnetic level, and from the atomic to the mesoscopic scale. For example, spatially resolved RIXS on the nanoscale offers the possibility of mapping the dynamic structure factor of quantum materials in real space to trace the origin of emergent phenomena, opening up the possibility of engineering new materials with technologically relevant properties.

Quantum magnetism, data storage and superconductivity

Magnetism has fascinated mankind since its discovery over two thousand years ago. Although magnetic fields can be conceptualised using classical physics, the existence of magnetic materials can only be understood in terms of the fundamentally quantum mechanical nature of the world around us. Our ability to manipulate magnetism over very short timescales via ultrafast laser excitation has therefore attracted considerable excitement within the scientific community. In terms of applications, ultrafast magnetism provides routes to fast switching of electronic devices, which often store information in different magnetic states. Magnetic or spin degrees of freedom are also intimately tied to many of the most interesting emergent electronic properties of materials, such as high temperature superconductivity quantum spin liquids, colossal magnetoresistance,[xiii] etc. Understanding quantum magnetism is therefore important to nascent efforts to realise and manipulate such states transiently.

Ultrafast photoexcitation of quantum materials that exhibit intricate coupling between charge, spin and orbital degrees of freedom holds great promise for understanding and controlling the properties of non-equilibrium and hidden states. State-of-the-art time-resolved resonant measurements enabled by XFELs, such as inelastic X-ray scattering (trRIXS), are a means of measuring charge, spin and orbital excitations.

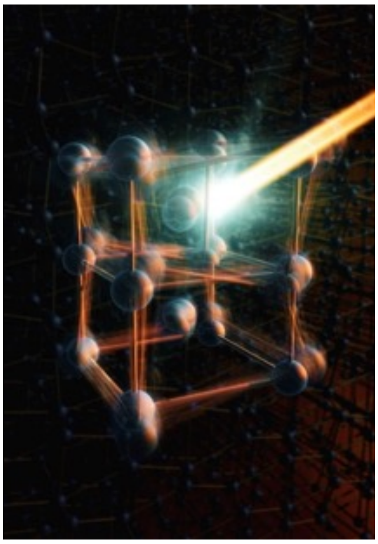
These excitations encode the correlations and interactions that determine the detailed properties of the generated states and may advance the technology of, for instance, fast, energy efficient, data storage.



Case Study 9 – Light-induced phase transitions in quantum materials

The structures of quantum materials can be transiently modified from their equilibrium state with the use of femtosecond pulses of laser light, inducing rapid phase transitions that are capable of changing a magnetic insulator into a metal or even a superconductor. This has led to a new field of research with the aim of controlling the properties of quantum materials "on demand". With the advent of XFELs, researchers now have the ability to observe how the atoms re-arrange themselves during such phase transitions, measuring multiple microscopic structural and electronic degrees of freedom simultaneously on ultrafast timescales.

Vanadium dioxide (VO_2) is an insulator at room temperature, but, when heated just above room temperature, undergoes a phase transition that increases the conductivity of the material by over five orders of magnitude. Using the advanced techniques unlocked by XFELs, researchers were able to observe, for the first time, a disorderly rearrangement of the atoms in VO_2 on ultra-fast timescales,[1] completely overturning previous orthodoxy on how such a transition could happen so quickly. This step-change opens the way to transforming our understanding of quantum materials, and how they might be exploited for applications in nanotechnology and optoelectronics.



Depiction of the insulator-to-metal transition of vanadium dioxide

1. Figure reprinted by permission from American Association for the Advancement of Science: S. Wall et al. "Ultrafast disordering of vanadium dimers in photoexcited VO_2," Science 362, 572-576 (2018). DOI: 10.1126/science.aau3873

Optical and terahertz (THz) field dressing of quantum materials probed by XFEL pulses is leading to the discovery of hidden phases of significance to high Curie temperature (Tc) superconductivity and other functional properties. [xiv]

6.3.3 Energy materials

Many challenges remain to realising the global energy revolution needed to improve aspects of energy conversion, storage, transmission and low-power device efficiency, in order to limit the detrimental effects on the planet. Light source enabled investigations are crucial to understanding details of the structure, chemical nature and electronic states of energy materials, not only in their pristine state, but as they evolve during a reaction or process.

Battery research

The 2019 Nobel Prize for Chemistry was awarded for the development of lithium-ion (Li-ion) batteries. Akira Yoshino created the first commercially-viable lithium-ion battery in 1985 and, since they first entered the market in 1991, they have revolutionised our lives. The ever-increasing need for portable electronics and electric vehicles places heavy demands on battery capacity, calling for further improvements in energy density, as well as cost reductions.

Case Study 10 – How short circuits can lead to thermal runaway in Li-ion batteries

From mobile phones to electric vehicles, Li-ion batteries are ubiquitous in today's society. These devices have, however, been known to fail, sometimes in spectacular fashion, as seen as seen in 2016 with the recall of Samsung's Galaxy Note 7 devices. Now, in a paper published in Energy and Environmental Science, a team of researchers has investigated the nature of this failure in an effort to improve the safety and reliability of Li-ion batteries.

The team, led by UCL, used a device developed by NASA and the National Renewable Energy Laboratory to induce short circuits in Li-ion batteries at a specific and pre-determined time and location. As battery failure takes place in millisecond time frames, they used high speed X-ray imaging at Diamond Light Source and the European Synchrotron Radiation Facility to track how failure propagates through Li-ion batteries.

Their work has enabled them to look inside the 'black box' of commercial Li-ion batteries and determine why failure happens. They now plan to investigate different safety devices to determine which work best. Ultimately, they hope their work will help to develop new safety devices and materials for future generations of Li-ion batteries.

Finegan, D.P. et al. Characterising thermal runaway within lithium-ion cells by inducing and monitoring internal short circuits, Energy Environ. Sci., 10 , 1377 —1388. (2017) DOI:10.1039/C7EE00385D

A range of spatial resolutions – from atomic up to micron – is required to understand the processes that limit battery performance, such as capacity, power, charging speed, lifetime and degradation mechanisms.

Monitoring the formation and changes that occur in real time and during operation with chemical sensitivity (for example, tuning to X-ray absorption edges) will give new and important structural information. Time-resolved operando experiments using X rays and infrared lasers will provide key information on dynamic and kinetic processes during charging and discharging of real devices.

High-flux and high-energy X-rays with a micrometre-sized beam are required to enable the combined in situ imaging and diffraction mapping for operando studies of large devices. The combination of high time and spatial resolution, using techniques such as X-ray diffraction computed tomography (XRD CT) and X-ray fluorescence computed tomography (XRF CT), allows real-time investigation of the evolution of spatial inhomogeneities that contribute to battery degradation. Rapid acquisition of lensless imaging techniques, such as ptychography and Bragg coherent diffraction, can be used to identify the instigation of defect-driven failure modes, such as cracking crystallographic defects that increase the impedance of Li-ion mobility. The sensitivity of battery materials and electrolytes to air and moisture requires advanced operando cell environments that should mimic the real cells as closely as possible, and increased brilliance, energy and flux will all aid in the improvement of these cell environments allowing for truly 4D studies.

Photovoltaics

The ability to convert solar radiation, which delivers a vast amount of power to the Earth's surface, is limited by several factors such as efficiency, ability to withstand long-term exposure to solar radiation, materials degradation, toxicity of the materials used, and cost. Addressing these challenges involves understanding the device structure, composition and dynamic processes over a wide range of length scales and timescales, in particular for new families of materials such as halide perovskites.

A combination of imaging and diffraction techniques with smaller spot sizes, together with grazing incidence XRD and X-ray reflectivity, would enable detailed analysis of the material structure including the distribution of defects (which dictate device performance) during formation of thin film absorbers throughout solution- or vapour-based processing and drying.

As the charge generation processes are ultrafast, and complex power loss mechanisms such as carrier trapping and recombination happen at these fast timescales, time resolved information is also now recognised as critical to achieving advances in photovoltaics. There is heterogeneity in the structural, chemical and optoelectronic properties of emerging photovoltaic materials on micro- and nano-metre length scales, and high spatial resolution will also be required to elucidate these variations. Operando measurements enable these processes to be visualised under typical device operating conditions, and be connected with longer term power losses and failure mechanisms.

Femtosecond stimulated Raman spectroscopy (FSRS) can be used to study charge transfer in photovoltaic devices and measure molecular rearrangements on the hundreds of picosecond timescale. This provides valuable insights into the design of new plastic photovoltaics for optimal efficiency.

6.3.4 Properties of matter in extreme conditions

A broad range of science requirements rely on the high energy densities, high fields, high pressures and ultrashort pulse characteristics of light sources, in particular high- power lasers and FEL systems, to explore novel and extreme states of physical systems and the underlying science.

Fusion energy research and hot electron transport studies

Lasers are the main driver in inertial confinement fusion (ICF) and attempts to produce inertial fusion energy (IFE). Investigating and developing the underlying science behind advanced ignition routes is key to achieving fusion energy.

As well as being central to fast fusion ignition studies, the transport of hot electrons in plasma is of fundamental importance to the field of high-power laser plasma interactions and relativistic beam physics. Understanding the interplay of the various physical mechanisms involved during the transport, collimation and scattering of high densities of hot electrons in relativistic laser plasma is essential, as in many cases it is the primary mechanism for energy transport in high energy density conditions.

Plasma Accelerators

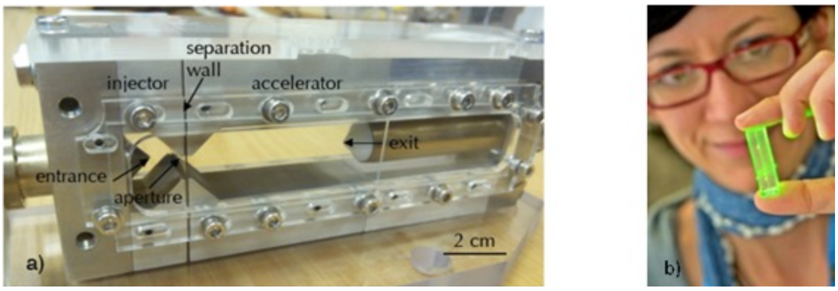
An emerging application of intense lasers is their capability to drive plasma-based accelerators, either of electrons or of ions (also positrons and neutrons as well). The acceleration mechanisms are different in both cases, but, common to both, the plasma acts as a transformer of the transverse fields of the laser into the ultra-high longitudinal fields capable of accelerating particles to high energies over very short distances.

High energy density physics (HEDP)

HEDP encompasses the study of material properties at densities from normal up to a hundred-times solid density, and temperatures up to around one million Kelvin. Such material occurs in fusion plasmas, in stellar interiors and (at the lower temperature range) in planetary cores. These states of matter can be produced by high power lasers. High energy density physics also encompasses material in astrophysical plasmas, although some of the more extreme degenerate plasmas have not yet been reproduced in the laboratory.

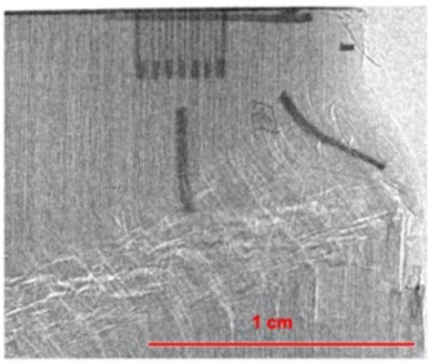
Case Study 11 – Laser driven particle acceleration

The CLF's Gemini facility, commissioned in 2008, was a major advancement for laser-driven particle acceleration. It provided a relatively high-repetition rate of 1 shot every 20 seconds, compared to the few shots per hour shot rates of the petawattscale laser facilities available until then. This step-change allowed Gemini to convert the curiosity-driven science of plasma acceleration into applications, making it one of the preeminent centres for laser-driven acceleration in the world. Gemini can yield stable electrons beams with high energy (> 2 GeV) and high charge (~ 0.5 nC) from high-gradient plasma accelerators that are only a few centimetres long, as opposed to the kilometre-long structures based on conventional accelerator technology.



(a) and (b) Centimetre-scale plasma accelerators used in Gemini

These compact laser-driven accelerators can produce spatially coherent femtosecond X-ray pulses, which have been used for a multitude of applications – from tomographic imaging of medical samples[1] to probing matter in extreme conditions such as those found in giant planetary cores.[2] These synchrotron-like X-ray beams enable micron-scale phasecontrast imaging that can distinguish even small changes in material densities, opening up imaging applications in high value manufacturing.[3] The Extreme Photonics Applications Centre (EPAC) will exploit these applications.



Radiograph of kink band failure in a composite material, obtained with the laser-betatron source. Individual carbon fibre tows are visible.[3]

1. Cole J, Wood J, Lopes N, et al. Laser-wakefield accelerators as hard X-ray sources for 3D medical imaging of human bone, Sci. Rep. 5, 13244 (2015) DOI: 10.1038/srep13244
2. Kettle B, Gerstmayr E, Streeter MJV, et al. Single-shot multi-keV X-ray absorption spectroscopy using an ultrashort laser-wakefield accelerator source, Phys. Rev. Lett. 123(25), 254801 (2019) DOI: 10.1103/PhysRevLett.123.254801
3. Gruse J-N, Streeter MJV, Thornton C, et al. Application of compact laser-driven accelerator X-ray sources for industrial imaging, Nuclear Inst. And Methods in Physics Research, A 983 (2020) 164369 DOI: 10.1016/j.nima.2020.164369

Warm Dense Matter

Warm Dense Matter (WDM) is an important part of the HEDP parameter space, ranging in density from normal solids to around 10-times compression, and in temperature from 0.1 eV to 100 eV. The study of WDM is directly relevant to the understanding of Earth and planetary interiors. The Earth's core is still not well understood. For example, the mechanisms of geomagnetism remain mysterious other than a broad understanding that it involves phenomena in the outer core. However, the effects of a geomagnetic reversal (which occur irregularly, every fifty thousand to one million years) may have a huge impact upon communications and electricity transmission systems, as well as high levels of ionising radiation reaching the ground. Understanding the material properties of the core is thus vital in building robust models to predict how, when, and with what consequences, these reversals occur.

WDM is of central importance in fusion science, laser plasma science, laboratory astrophysics, and in modelling the cores of large planets and exoplanets. Creating WDM states in a wide range of materials within a laboratory environment enables the study of its formation and properties, for example performing ultra-fast X-ray spectroscopy and scattering to probe the local structure, density and other physics properties, and to study the structural dynamics of the solid-to-plasma phase transition.

Ultrafast photon sources have the potential for dynamical studies of condensed matter with ultrafast time-resolution, using techniques such as time- and angle-resolved photoemission spectroscopy (Tr-ARPES) with femtosecond XUV or harder X-ray pulses. This enables researchers to track (in the electron momentum space) the mechanisms behind ultrafast photo-excitations. Furthermore, this technique has great potential to explore ultrafast switching of devices in the sub-picosecond domain.

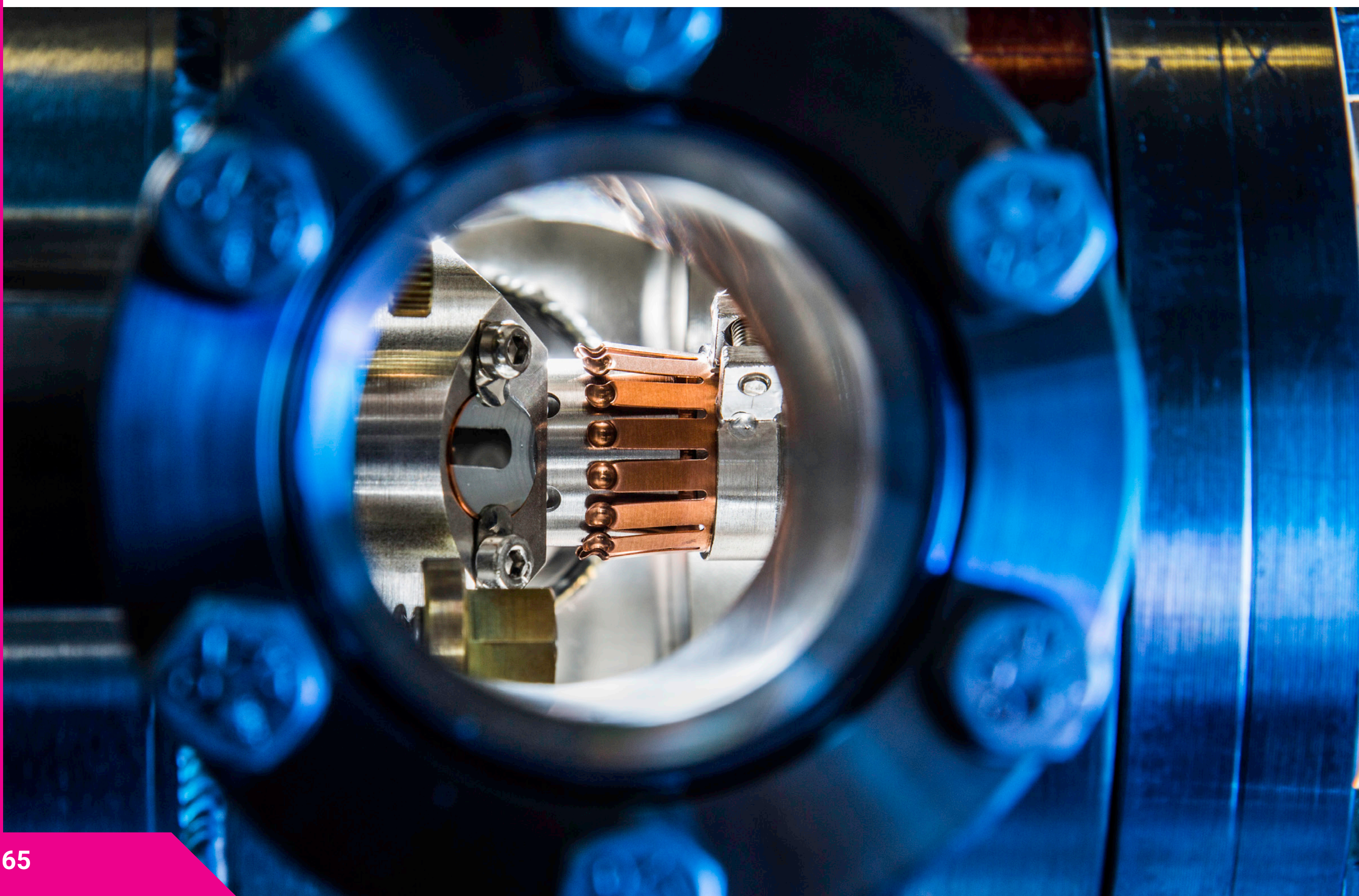
Time- and spin-resolved photoemission is a promising route to directly observe electronic spin dynamics on an ultrafast time scale. The spatial coherence of the XUV source will enable imaging of magnetic structures with nanoscale spatial resolution to be combined with ultrafast time resolution. Possible imaging techniques include coherent diffractive imaging, which has recently reached sub-25 nm resolution with an ultrafast XUV source.

Laboratory Astrophysics

The intrinsic high energy densities of laboratory plasmas mean that laser produced plasmas are often a suitable analogue system to astrophysical objects. Laser-plasma experiments have the potential to model a variety of situations such as supernova expansion, collision-less and radiative shock waves, the instabilities of jets flowing into the interstellar medium, and magnetic field generation in colliding plasmas.

The observation of a shock velocity instability, along with measurements of X-ray emission in several wavelength ranges in laser produced plasmas, has provided valuable data to compare to simulations and analytical calculations, with a view to designing scalable laboratory astrophysics experiments.

Shocks and gas jet streams found in interstellar media are often associated with giant magnetic fields. When integrated over the whole universe, this magnetic energy represents a sizeable component of the cosmic energy budget. At present, the origin and the distribution of the magnetic field is far from being understood.



Case Study 12 – Cosmic magnetic fields

Magnetic fields are a ubiquitous feature of astrophysical plasmas. They are likely to have originated from so called “primordial seed fields” that were created in the early universe. The origin of this primordial magnetic seed field is not completely understood. Seed fields can be generated by a variety of different physical processes in plasma. In the early universe, before stars and galaxies formed, possible seed magnetic fields could form due to misaligned density and temperature gradients in the primordial plasma, the Biermann battery mechanism. Similar seed fields also occur in laser-produced plasmas where gradients of density and temperature are often misaligned, resulting in the generation of a magnetic seed field. If a turbulent plasma contains a weak seed magnetic field, the stochastic motions of the plasma will stretch and fold this field, amplifying it until it becomes dynamically significant. This is the basis of the plasma turbulent dynamo.

Since the theory of hydrodynamics of plasma is highly scalable, a new field called laboratory astrophysics has emerged to become an important branch of plasma physics. Using powerful lasers and the hydrodynamic scaling relations, laboratory experiments can investigate astrophysical environments. The scaling makes these experiments relevant, thus coupling large astrophysical scale events to very small laser plasma scales. In a number of experiments carried out using high power lasers, such as the Vulcan laser at the CLF, generation and amplification of seed magnetic fields by the turbulent dynamo action was demonstrated. One particular laser experiment carried out at Vulcan[1] investigated magnetic field generation of a seed and amplification by the turbulent dynamo, aimed at explaining why magnetic fields in the supernova remnant Cassiopeia A were much higher than those in the surrounding interstellar plasma.

Supernova remnant Cassiopeia A

Image: NASA

1. Meinecke J, Doyle H, Miniati F et al. Turbulent amplification of magnetic fields in laboratory laser-produced shock waves, Nature Phys 10, 520–524 (2014) DOI: 10.1038/nphys2978

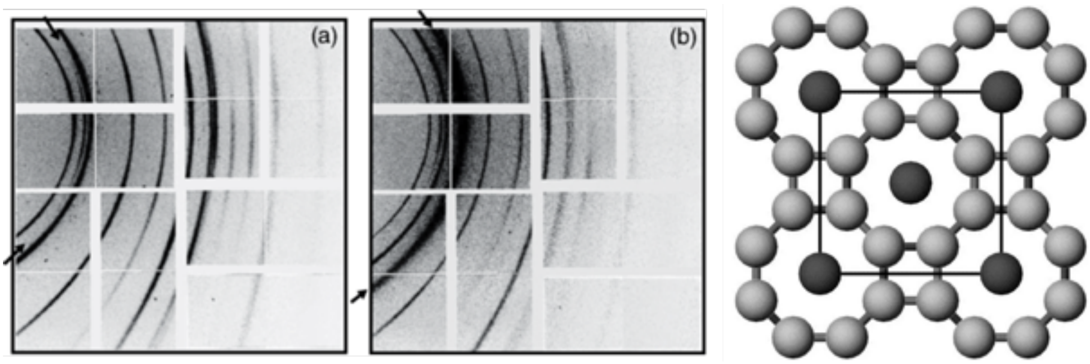
Materials under extreme conditions
The Equation of State of materials at multiple-Mbar shock pressures is required to allow understanding of important processes. The study of the formation of defects and their evolution, how fast different phase transitions occur under shock compression, and how well equations of state are understood at ultrahigh pressures, all require access to high energy photon sources.

New pump-probe methods are allowing the interrogation and study of dynamics in states only transiently accessible, for example, high pressure shocks, hot dense matter, matter dressed by lasers, and matter in extreme electric and magnetic fields.

Case Study 13 – Shock-induced phase changes

The dynamic compression of matter using the impact of a projectile, the detonation of explosives, or a high-energy laser pulse has a long pedigree, dating back to the Manhattan Project. Laser compression can generate extreme pressures and temperatures otherwise found only deep within giant planets, but merely for nanoseconds. It has long been very difficult to make X-ray studies of matter under such conditions, because laser-plasma X-ray sources were insufficiently bright. The billion-fold increase in brightness afforded by XFELs, and their ultrashort X-ray pulse length, is, however, perfectly matched to the needs of obtaining high-quality X-ray diffraction and spectroscopy data from laser-generated high-pressure states.

UK researchers from Edinburgh and Oxford have been pioneering detailed structural studies of high-pressure phases of elemental metals at the LCLS XFEL in Stanford, USA. In a series of high impact papers they have described the complex phase transition sequences, including melting, seen in antimony, bismuth and scandium on compression. Of most note was the observation of a transition to an incommensurate "host-guest" structure in scandium above 45 GPa.[1] That this complex structural form – comprising a 3D "host" lattice with interpenetrating 1D chains of "guest" atoms – could form in less than a nanosecond was unexpected, as was the fact that the chains were disordered and liquid-like. Such complex structural arrangements can only be discerned using the highest-quality X-ray data that XFELs can now provide.



(Left) 2D diffraction images collected from the LCLS XFEL on a single CSPAD detector from (a) uncompressed (hcp) scandium and (b) scandium compressed to 51.1 GPa. (Right) The "host-guest" structure in scandium at 51.1 GPa

1. Figure reproduced from R. Briggs et al. "Ultrafast X-Ray Diffraction Studies of the Phase Transitions and Equation of State of Scandium Shock Compressed to 82 GPa" Phys. Rev. Lett. 118, 025501 (2017), American Physical Society. DOI: 10.1103/PhysRevLett.118.025501

Strong Field QED

Strong Field Quantum Electrodynamics (QED) physics is based on fermions interacting with a quantised radiation field and the QED vacuum not being empty but containing virtual electron-positron pairs, whose fleeting existence makes a small correction to the predictions of Maxwell's equations. QED processes can be accessed in laser-electron beam and laser-plasma interactions, as well as laser- vacuum interactions.

Pair production (creation of electron-positron or other matter-antimatter pairs from the vacuum) could be investigated using the high photon flux. Collective photon effects, such as four-wave mixing, will make it possible to produce new photons from the quantum vacuum, and the structure of these photons would shed light on QED and the possible corrections to standard quantum field theoretical particle models. The large number of photons is also likely to give a means for investigating dynamical quantum vacuum effects, such as laser pulse compression in external fields, an area that, to date, it has not been possible to examine experimentally.

Summary of the future light source requirements for physical sciences

Research Areas	Source technical requirements
Chemistry and catalysts	• Ultrafast time resolution • High spatial resolution • High flux densities • Tuneable energies
Energy materials and systems	• High flux and high energy X-rays • High spatial resolution
Advanced materials and engineering	• High energy pho stons capable of penetrating dense materials • Point sources for high-resolution imaging
Fusion and high energy density physics	• Very high power • Very high pulse energy for fusion drive • Short pulses of intense light • Photon pulse shaping (to control fusion implosion dynamics) • Tight focusing (point sources) to enable high-resolution radiographic imaging • Frequency tunability for off-fundamental frequency probing
Materials in extreme conditions	• Very short pulse (extremely bright) • Very high intensities • High energy photons (X-ray) for probing dense media • High repetition rate pulses for temporally resolving probes • Pulse synchronisation for pump- probe platforms • Tight focusing (point sources) to enable high-resolution radiographic imaging

6.4 Underpinning functions

In common with other research infrastructures, light sources need a range of underpinning functionality and support services in order to be able to deliver the science and innovation outputs, including:

- Detectors
- Data handling and analysis
- Sample preparation and environments
- Specialist engineering.

This strategic vision does not directly address these support functions, but it is critical that the important roles they play is recognised. Their intrinsic importance to future light source developments is illustrated in the following examples.

6.4.1 Detectors

The performance of any source is ultimately decided by the efficiency of the detection systems that are deployed. Building higher flux sources will only be beneficial if the additional photons can be detected. Light sources use a wide range of detector types that can be embedded components of the infrastructure, or independent systems built by users and brought to a facility. The UK leads in many areas of detector technology; for example STFC's Technology Department has built and installed one of the world's fastest detectors, capable of capturing images in billionths of a second, for use at the European XFEL[xv] .

6.4.2 Data handling and analysis

Modern light source facilities generate extremely large amounts of data that needs to be handled, analysed and stored efficiently. Applying big data and machine learning techniques will be needed to help realise many of the opportunities that new sources can bring. For example, using large and robust datasets from high-throughput experiments can help develop computational algorithms for protein engineering and the rapid development of new drugs. UKRI's Ada Lovelace initiative[xvi] is one approach to enabling this scientific computing capability for users of the UK's national facilities.

6.4.3 Sample preparation and environments

Many techniques used at light source facilities need complex samples to be prepared and held in specific conditions, such as crystals for X-ray diffraction studies, living cells in *in vivo* conditions for life science investigations, and complex microscopic targets for inertial confinement and high energy density physics experiments. Highly accurate and reproducible sample systems are needed, especially for rapid multi-parameter studies. *Operando* battery and electrochemical cells, which work well with the beam conditions and produce reliable electrochemistry, are key. These have traditionally been developed for each experiment by users. Increased collaboration has the potential to make these systems available "as standard" for other users.

6.4.4 Specialist engineering

Modern science infrastructures require a vast array of specialist engineering capability to operate efficiently and safely. For light sources this includes:

- high precision mechanical engineering
- optics design
- semiconductors
- superconducting electromagnets
- cryogenics.

7. Future light source options

7.1 Option categories

As the science and innovation challenges evolve and progress, the requirements for science facilities will also change. In order to be able to plan the optimal mix of capacity and capability, it is important to map out the range of feasible options, building on the infrastructures currently available. These options fall into several categories as follows:

- Maintain the status quo
- Upgrade capacity and/or capability
- Build or access new capacity and/or capability
- Decommission/exit from current infrastructure.

The following section outlines the possible options in these categories for each of the primary light source types.

7.2 Option details and analysis

Tables 9 to 12 capture the options for each of the main current light source types (synchrotrons, FELs and lasers) and potential new source types. For each option there is:

- A short description
- A commentary on the potential consequences/benefits of the option
- A high-level analysis of how the option could form part of the future strategy, where possible noting where there are complementary/ alternative options.

Table 9: Synchrotron Source Options – Maintain status quo

Maintain status quo		
Opportunities	**Comments/Consequences**	**Options Analysis**
Diamond		
Option i: "Maintenance only" option is replacing like for like on beamlines and other infrastructure when they fail or in anticipation of failure. Option ii: Incremental upgrades to beamlines to enhance performance. Current Diamond capital budget about £20M/year, of which at least £5M needed for essential maintenance and the rest for incremental upgrades.	Preserves an important UK infrastructure with no extended loss of availability. Users will have to go overseas to access new capabilities. Facility will decline progressively compared to the best internationally. Risk of losing users and staff in medium to long term (5 years plus) with negative impact on UK science competitiveness.	If there are no further upgrades to Diamond (Option i), it can only continue to support world-class science in the short term. Incremental upgrades at modest cost (Option ii) is the current approach, but by 2030 Diamond would be very uncompetitive with any other major synchrotron and at the end of its productive life.
ESRF		
UK continues as a full member at 10.5% (£8.9M/year) contribution. This covers operations and maintenance.	A major upgrade (EBS) was completed in 2020, giving UK academic and industry users access to a world leading synchrotron at high energy for the next 10 to 20 years.	ESRF provides access to a world leading 4th generation synchrotron, with some capability complimentary to Diamond, and even Diamond-II, as well as providing additional capacity, and should remain a core element of the UK's light source plan.
Other international		
Maintain the mutual access arrangements with partner national facilities for small amounts of beam time via their access panel peer review mechanisms.	Helps promote collaboration and can give access to specific (unique) capabilities but access levels available are modest. Typically relies on established relationships.	Access to national synchrotrons in other countries is a useful supplement to the core access plan.

Table 9: Synchrotron Source Options – Upgrade capacity and/or capability

Upgrade capacity and /or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
Diamond		
Major upgrade to achieve a step change in beam characteristics (brightness and divergence) and instrumentation, including for data and computation. Options are: (i) Machine upgrade plus movement of critical beamlines (£250M); (ii) Machine upgrade plus new beamlines and data capabilities (£518M).	Keeps UK at the leading edge creating the potential to achieve new science and boost innovation in areas tailored to UK research strengths and priorities. 5 to 7 year timescale from approval to commissioning. Dark period of about 18 months (small risk that some users may establish elsewhere and not return). Based on largely tried and tested design and technology so low risk of not delivering predicted performance and/or outcome gains.	The most cost effective and timely upgrade option, delivering greatly increased capability and capacity part-way through the 2020s (as opposed to partway through the 2030s for the option of building a wholly new synchrotron), while reusing most of the existing infrastructure. Potential to establish MX beamline abroad for the dark period - important for pharma industry and research.
ESRF		
Negotiate an increase in the UK's contribution and associated access. A major upgrade has been completed so only likely to be incremental changes in the next 10 years. Need agreement from all partners for any changes.	More beamtime available for UK users at the upgraded source but might not be possible to secure a significant increase because of competition from other countries. UK share of future decommissioning costs would also increase.	It will be very difficult to achieve a significant increase in access so this should not form part of the core plan. It is a potential, partial mitigation measure if Diamond were closed.
Other international		
Opportunities may arise for the UK to partner with another facility to share the costs of a major upgrade.	Can be useful option to mitigate against dark periods for critical capabilities. Capital and operational costs likely to exceed £10M per beamline. Opportunities are likely to be very limited and timescales may not fit with UK needs.	This may be a useful mitigation measure but would only cover a limited range of science areas. It may be harder to manage access for industrial users (e.g. legal frameworks for proprietary use).

Table 9: Synchrotron Source Options – Build or access new capacity/capability

Build or access new capacity and/or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
Diamond		
Build a completely new facility - accelerator, storage ring and a full complement of 30 or more beamlines (£1.4Bn).	Design unconstrained by the current machine. Timescale of at least 15 years to complete. Avoiding a prolonged dark period would mean maintaining the existing machine for an extended time with significant implications for costs and staff resources.	The UK science community, including industry, would not have access of any significant capacity to a 4th generation synchrotron for approximately 15 years from approval for Diamond-II. Inward investment would be a way to reduce capital costs but with a likely loss of capacity for the UK.
ESRF		
Complete rebuild to add new capabilities.	A major upgrade to the ESRF synchrotron has recently been completed and taken it close to the physical limits for a machine of this energy so the benefits from replacing ESRF are minimal for the foreseeable future.	Not a realistic option.
Other international		
Opportunities may arise for the UK to partner with other countries to share the costs of a new facility. Buy beam time at another international facility.	Hard to plan for as the opportunities are likely to be very limited and with scope and timescales outside the UK's control. Depends on the availability of beam time at a suitable source.	In the unlikely event of significant opportunities, they should be considered to see if they would bring significant benefits.

Table 9: Synchrotron Source Options – Decommission/exit from current infrastructure

Decommissioning/exit from current infrastructure		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
Diamond		
Mothballing - stop user experiments but maintain facility. Close and decommission.	Loss of UK capability and expertise - major impacts on science and innovation. Mothballing allows for possible restart or even provides basis for future upgrade, but only for a short time. Closure (immediate or after mothballing) requires decommissioning costs to be covered.	The only benefit of mothballing is if there is a reasonable prospect of initiating an upgrade and restart within 1-2 years. Closure would have a major impact on UK ability to service key industry needs, particularly in pharma.
ESRF		
Negotiate a reduction in membership (<4%), then become an associate member with significantly reduced influence.	Could compromise UK science advances. Still responsible for historic share of decommissioning costs.	This could be an option if a new build UK project is pursued, as there would likely be significant overlap in capabilities, but not for approximately 15 years.

Table 10: FEL Source Options – Maintain status quo;
Upgrade capacity and/or capability

Maintain status quo		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
European XFEL		
Continue as a shareholder member at 2.1% level (share of future costs is likely to be linked to access levels so costs will increase if UK usage stays higher than this).	Ensures a minimum underpinning access to FELs. Risk of UK falling further behind competitors in science and technology gains that FELs can unlock.	The UK currently uses about 7% of European XFEL time. This is key to continuing to build the UK FEL user community, so should be a continuing element of the core access plan.
Other facilities		
Continue arrangements with national facilities for small amounts of beam time via their access panel peer review mechanisms. Facilities include: LCLS/LCLS II, SACLA, PAL FEL (Korea), FELIX, FERMI and Swiss FEL	Helps promote collaboration and can give access to specific (unique) capabilities but access levels available are modest. Relies on established relationships.	Access to national FELs is a useful supplement to the core access plan and helps build international links and grow the UK FEL user community.

Upgrade capacity and/or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
European XFEL		
Negotiate an increase in access %	Enables growth of UK user base and FEL expertise at modest cost (10% access would cost ~ £10M/year)	As the UK community grows this may be an important option to enable science objectives to be met.
Other facilities		
Buy beam time at another international facility.	The limited number of FELs means they all have high demand so may not be possible.	If opportunities arise then they can be considered to see if they would bring significant benefits.

Table 10: FEL Source Options – Build or access new capacity/capability

Build or access new capacity and/or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
UK FEL		
Build a limited scale pilot facility as a test bed for a future full facility. This could be an extension to the CLARA test facility at Daresbury at a cost of ~ £40M.	A test facility would keep UK accelerator/FEL science "match fit" for future opportunities. Capability would be limited to optical / UV so science range limited.	Some critical UK XFEL design R&D could be tested and optimised.
Build a full-scale facility, options are: (a) A national facility with limited capacity and capability at a cost of ~£500M. (b) An internationally competitive facility with world-class capabilities at a cost of >£1Bn	Build time for a facility matching current specifications (e.g. like the Swiss FEL) could be accelerated with near "off the shelf" designs and technologies. Could achieve first light in 6 - 8 years. Low technical risks, but could become obsolete after a couple of decades. UK can be a world leader across a swathe of opportunities. Some technical risks, but these can be mitigated by preparatory R&D and close relationship to other XFELs. 9 - 11 years to first light.	Option (a) could capture a minority share of the science opportunities identified in the UK XFEL Science Case, offering UK competitiveness into the late 2030s. Option (b) would capture most of the science opportunities identified in the UK XFEL Science Case. Lasting UK leadership across an expanded range of science and technology. UK capital costs could be reduced by seeking partners to invest in the facility.
Other facilities		
Opportunities may arise for the UK to partner with another facility to share the costs of a major upgrade such as building a new beamline. Costs for a UK "owned" beamline: ~ £10M - £50M capital depending on beamline type; and ~£2M - £4M / year operating costs.	Needs a suitable and willing partner. Costs likely to be higher than an increase in European XFEL% but with the opportunity for guaranteed UK access. Costs would be reduced if the new capacity is shared with another country. Likely to only benefit one or two disciplines depending on the choice of investment.	If opportunities arise then they can be considered to see if they would bring significant benefits. It is a potential alternative option to building a UK national FEL but would limit scope for a broader scientific and technology impact and for the wider economic benefits.

Table 10: FEL Source Options – Decommission/exit from current infrastructure

Decommission/exit from current infrastructure		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
European XFEL		
Negotiate a reduction in access or full exit.	Access is already at a low level, so reducing access risks becoming unviable. Likely to lead to outflow of scientists from UK and compromise science goals.	This should only be considered if a UK FEL is built.

Table 11: Laser Source Options – Maintain status quo

Maintain status quo		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
CLF facilities		
Vulcan Maintain current operations	Vulcan has been maintained with no major investment since 1998. Continued status quo will mean an inevitable decline with the resulting impact on the high energy density science community.	If there is no major upgrade soon, Vulcan can only continue to support good science in the short term.
Gemini/EPAC Maintain current operations	EPAC will be the successor facility to Gemini.	Gemini's future will be determined by future EPAC development.
Imaging and dynamics facilities (Octopus, Artemis and Ultra) in the Research Complex at Harwell (RCaH) Maintain current operations	Imaging and dynamics technology and science are areas of rapid development and progress. Status quo for more than 1-2 years and they will slip behind major international competitors, harming UK competitiveness in many priority science areas.	With no development, the imaging and dynamics systems will have a limited productive lifetime.
Other laser facilities		
Extreme Light Infrastructure (ELI) The UK is not a member of the ELI ERIC.	The UK has no formal guaranteed access to ELI, other than through goodwill and/or collaboration with researchers from member countries. The ELI sites are in differing states of completion with various systems undergoing commissioning.	Collaborative projects could give the opportunity to access some new capabilities. Experience with these may help inform decisions on other options.
ORION (AWE) Up to 15% available for academic access (10% used currently)	ORION is a defence asset and can only be used for defence related purposes. As a result, this excludes some science topics and researchers. It is unlikely the 15% limit can be increased.	ORION is a useful complement to Vulcan for a restricted range of research areas.
University-based laser systems Systems that complement some CLF capabilities exist at Strathclyde, York, Imperial and Queen's University Belfast.	These systems help support the research community and are excellent training capabilities, but limited operational resources limits their capability to support wider user access.	University based systems are a valuable complement to the CLF capabilities.

Table 11: Laser Source Options – Upgrade capacity and/or capability

Upgrade capacity and/or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
Vulcan		
Upgrading Vulcan to 20PW/10kJ (x100 in intensity) combined with existing HEPW (1kJ, 1PW) facility and a 6-fold increased shot rate would create the most flexible and highest power facility in the world. ~£60M capital over 5-year build time (+£3M resource per year).	Maintain world lead for the UK in High Energy Density / Extreme Field & Conditions science and sustain the science community for the next decade. A Vulcan upgrade has been suggested for several years and has a high degree of support from the UK user community.	The upgrade specification is not scalable - it would need to be implemented in full to achieve its aims. Investment in Vulcan ensures UK leadership in an increasingly competitive area of science. Not to invest means accepting the inevitable decline of HED UK science in the UK and reliance on national facilities elsewhere in the world that we have no control over.
Imaging and Dynamics (RCaH)		
Upgrade the CLF's three facilities in the RCaH. ~ £30M capital (could be split by project) and £2M resource per year	Keeps UK at the forefront of fast changing multi-disciplinary science and innovation areas. Increases capacity, especially for industry. An extension to the RCaH whilst not necessary for upgrades, would be highly desirable to address capacity issues.	Dynamics - studies how systems (atoms, molecules, proteins, cells etc.) evolve in time which in the main gives rise to their functional properties. Upgrades will give greater time resolution, sensitivity and spectral coverage allowing a wider range of systems to be covered. Imaging - studies how complex systems (e.g. cells, drugs, catalysts, plants etc.) interact spatially. Using optical light, rather than X-Rays or electrons, doesn't kill living cells and has chemical specificity meaning living processes can be observed in real time. Upgrades will focus on increasing spatial resolution to be comparable with electron microscopy and AI systems to correlate optical and electron images.
ELI		
UK joins the ELI ERIC as a full member securing dedicated access ~£2-7M / year depending on negotiation and level of access	Guaranteed access to the CZ and HU elements of ELI capabilities. The ELI RO node is not currently part of the ELI ERIC so would need a separate agreement.	Options are to join ELI ERIC and / or partner with ELI - NP, subject to securing suitable terms.

Table 11: Laser Source Options – Build or access new capacity and/or capability

Build or access new capacity and/or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
EPAC Phase 2		
Full completion of the EPAC Facility ~£20M	Three operating areas. Install 2nd gas beamline Completion of 2nd laser area and install 100 Hz driver laser system. Completion of labs and offices in shell and core	Completes the EPAC Facility 2^{nd} beamline allows for easier balancing between experiments, especially between academia, defence and industry who will have different interests. 100Hz driver gives greater opportunity for transitional research e.g. real time CT. Completion of labs and shell and core will allow academia and industry to be based long term in the building.
Other facilities		
Mutual access exists to different types of facilities with different capabilities at low additional cost to UK. Limited opportunities for greater access on a fee-paying basis.	Laserlab arrangement enables 10% access to a wide range of sources in Europe, including French LULI and Apollon systems. US (NIF) and French (LMJ) defence systems have 20% access by peer review, unlikely this access could be increased. The number of actual shots available is extremely limited. US OMEGA system access can be purchased on a shot day basis.	Access to overseas facilities is a useful supplement to the core access plan, particularly where this is to unique capabilities such as the NIF.

Table 11: Laser Source Options – Decommission/exit from current infrastructure

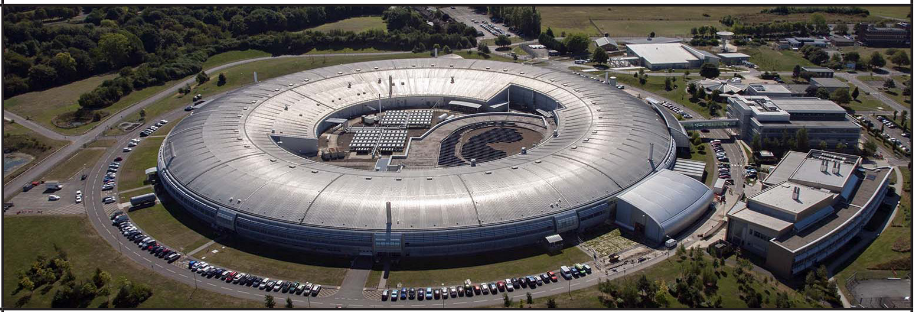
Decommission/exit from current infrastructure		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
Vulcan - decommissioning	HED science in the UK would decline without a national facility. Closing the largest CLF system would significantly affect the support resources (e.g. engineering) available to the other CLF systems. Significant loss of UK expertise.	An alternative to decommissioning would be to break it apart and give the useful components to universities and other facilities around the world that could use them.
Gemini - decommissioning	Once the first phase of EPAC is operational then Gemini could either be absorbed into EPAC or closed.	Gemini could also be absorbed into an expansion of EPAC.
Imaging and dynamics systems (RCaH) - decommissioning	Loss of unique national multi-disciplinary assets that would impact on a large academic community and result in significant loss of expertise.	If the imaging and dynamics capabilities do not keep pace with technical developments and science needs, then the systems are likely to fall out of use.

Table 12: New Source Type Options

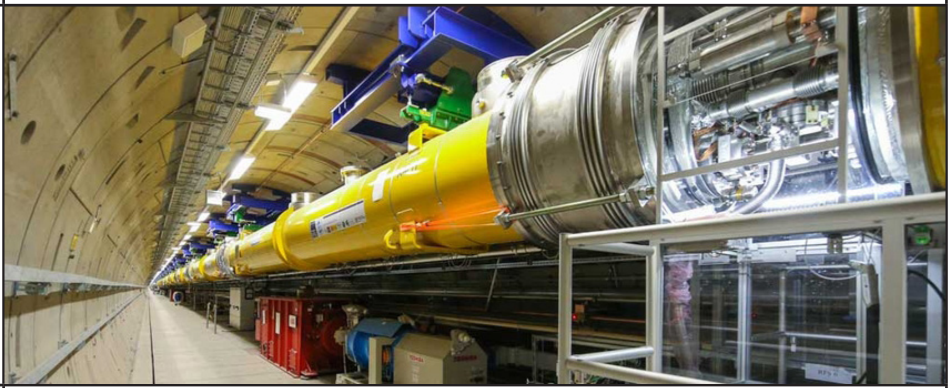
Build or access new capacity and/or capability		
Options and Opportunities	**Comments/Consequences**	**Options Analysis**
Terahertz		
New source technologies needed to fill the THx (20 micron) source gap.	Electron beam based sources are an option and could be developed as part of an XFEL system. This is identified in the UK XFEL Science Case as an attractive option.	The options for developing a source should be considered in FEL design studies. High power lasers produce the brightest sources of THz radiation.
Gamma ray		
High spectral brightness gamma ray sources have applications in basic nuclear physics and the nuclear industry	The ELI-NP source will offer an inverse Compton scattering source up to 17MeV energy. A high rep-rate XFEL system could also be used as a gamma ray source. This is discussed in the UK XFEL Science Case and appears feasible.	Once there is experience at ELI-NP the benefits of securing greater access should be considered. The options for developing a source should be considered in FEL design studies.
Plasma accelerator		
EuPRAXIA is a European Union funded consortium that has produced a design study for a European facility for plasma accelerator research. £5M-40M UK contribution depending on scope and partnering agreements	Internationalisation of EPAC with significant cost sharing opportunities (up to £60M co-funding). A dedicated plasma accelerator research end-station is discussed in the UK XFEL Science Case and strongly endorsed.	This option would create an opportunity to establish the UK as leaders in plasma accelerator technology. It could be considered as an element in the EPAC expansion option.
Electron diffraction		
The structural dynamics of complex macromolecular crystals can be studied using electrons if electron bunches of sufficient coherence and charge can be generated	Studies have shown that ultracold electron sources can be created using femtosecond near-threshold photoionization of a laser-cooled atomic gas.	An electron diffraction source has the potential to compliment conventional light sources.

Annexes

Annex 1: Profiles of some principal sources

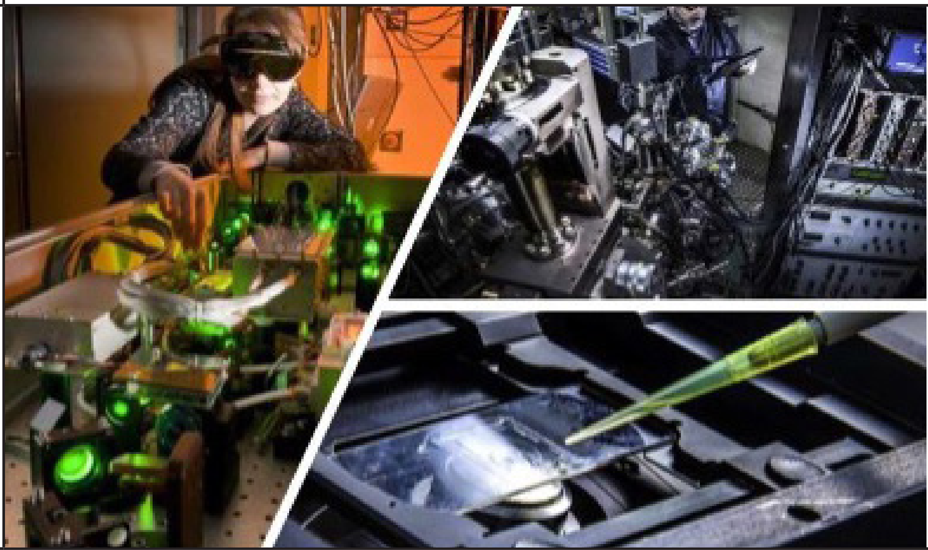
Source	Diamond Light Source
	
Nature of source	Third generation electron synchrotron Electron energy is 3 GeV Pulse length is 17 – 25 ps Operational in 2006
Capacity	33 beamlines and 39 instruments (including eBIC, ePSIC, XFEL Hub) supporting 5,500 user visits and 3600 remote user visits (17/18). Proposals exceed capacity by 50%.
Capability	Small Angle X-ray Scattering (SAXS), Grazing Incidence SAXS, X ray Powder Diffraction, X-ray Absorption Near-Edge Structure (XANES), Extended X-ray Absorption Fine Structure (EXAFS), Resonant Inelastic X-ray Scattering (RIXS), X-ray Emission Spectroscopy (XES), Single-Crystal Diffraction, Infrared spectroscopy, X-ray atomic pair distribution function (XPDF), energy-dispersive diffraction (EDXD), X-ray tomography, X-ray Fluorescence (XRF)
Access	Open access for published research selected on merit by peer review. Commercial use (unpublished) on a fee basis ~ 3%; industrial access with academic partners for lower TRL; publishable work is of the order of 20 – 30%.

Source	European Synchrotron Radiation Facility
	
Nature of source	Fourth generation electron synchrotron Electron energy is 6 GeV Pulse length is 100 ps Resumed operations in 2020 after major upgrade
Capacity	44 beamlines; 6548 user visits, 1735 experimental sessions, 36% of proposals allocated beamtime (2018)
Capability	Powder diffraction, Macromolecular crystallography, Surface diffraction, X-ray microtomography, X-ray fluorescence microscopy, Small- and wide-angle X-ray scattering (SAXS and WAXS), X-ray Absorption Spectroscopy
Access	Open access for published research selected on merit by peer review. Commercial use (unpublished) on a fee basis (~ 2.5 M€ of commercial income in 2018).

Source	European XFEL
	
Nature of source	14 GeV, 1.5 μA electron beam
Capacity	Three beamlines
Capability	Femtosecond X-ray experiments; High energy density experiments; Materials imaging and dynamics; Single particles, clusters, and biomolecules and serial femtosecond crystallography; Small quantum systems experiments; Spectroscopy and coherent scattering experiments.
Access	Open access for published research selected on merit by peer review.

Source	Vulcan (Central Laser Facility)
	
Nature of source	Vulcan is a versatile high power laser system that is composed of Nd:glass amplifier chain
Capacity	Eight beam lines. Two of these beam lines can operate either short pulse mode or long pulse mode, the remaining 6 operate on a long pulse mode. The short-pulse and long-pulse systems operating jointly can be directed to three different target areas enabling sophisticated interaction and probing experiments.
Capability	2.6 kJ of laser energy in long pulses (nanosecond duration) and up to 1 PW (10^{15} W) peak power in a short pulse (500 fs duration) at 1054 nm. Interaction of super-high intensity light with matter Physics of fusion energy research Photo-induced nuclear reactions. Electron and ion acceleration by light waves Astrophysics in the laboratory Exploration of the exotic world of plasma physics dominated by relativity.
Access	Open access for published research selected on merit by peer review. Confidential proprietary access is available.

Source	Gemini (Central Laser Facility)
	
Nature of source	High power, ultra-short pulse, high repetition-rate laser. It uses titanium-doped sapphire (TiS) as its active material, and works at 800 nm in the near infra-red part of the spectrum.
Capacity	Main target area has access to both Gemini beams (15 J, 35 fs) which can be focused using f/20 or f/2 parabolic mirrors at a rate of one shot per 20 seconds. Plasma mirrors are optional in one beamline. The maximum intensity is of order 2 x 10^{21} W cm^{-2}. TA2 has access to a lower power beamline from the Gemini front end (0.5 J, 35 fs) at 1 Hz which can be focused to an intensity above 10^{19} W cm^{-2}. A second compressed beam is used as a pump for two independent probe beams generated in a hollow fibre pulse compressor and a tuneable optical parametric amplifier.
Capability	High power, ultra-short pulse laser system delivering dual beams of 15 J, 30 fs laser pulses, at a rate of one shot every 20 seconds generating bright, coherent X-ray sources, or energetic beams of electrons and protons.
Access	Open access for published research selected on merit by peer review. Confidential proprietary access is available.

Source	Central Laser Facility Imaging systems
	
Nature of source	A range of ultrafast light sources provide unprecedented flexibility to combine multiple beams, multiple colours (UV to mid-IR), mixed timing patterns (fs-ms) and pulse length (40 fs, 50 fs, 120 fs, 2 – 3 ps, 0.8 ns and continuous wave).
Capacity	Multiple flexible experimental stations.
Capability	Octopus offers a range of imaging techniques including multidimensional single molecule microscopy, 3- and 5-colour single molecule tracking systems, super-resolution microscopy (PALM, STORM and SIM), and advanced confocal microscopy (FLIM, PLIM, FRET, Anisotropy and multiphoton). As multiple light sources are linked to multiple imaging stations, combination of techniques can be brought to bear on the samples under investigation. Experiments on Artemis use high harmonics to investigate ultra- fast electron dynamics in condensed matter and gas-phase molecules, and for coherent lensless imaging.
Access	Open access for published research selected on merit by peer review. Confidential proprietary access is available.

Source	Extreme Photonics Applications Centre (Central Laser Facility)
	 
Nature of source	EPAC is a new national facility to support UK science, technology, innovation and industry. It's a partnership between UKRI, MoD, academia and industry. It will bring together world-leading interdisciplinary expertise to develop and apply novel, laser based, non-conventional accelerators and particle sources which have unique properties.
Capacity	Phase one of EPAC will be two target stations
Capability	EPAC will provide a step-change in capabilities for laser-driven accelerator research in the UK, enabling a plasma wakefield accelerator facility with multi-GeV electron beams and spatially coherent X-ray and gamma-ray beams for cutting-edge experiments in plasma physics, laboratory astrophysics and condensed matter and material science. The versatile experimental areas in EPAC can drive high-energy protons, ions, neutrons and muons by merely changing the target geometry, enabling multi-modal capability for probing highly dynamic processes in for example nature or industrial components. The unique capabilities of EPAC, combining near-light speed particles and synchronised ultra-intense electromagnetic fields, would provide a world-leading platform capable of generating extreme states of matter and the tools to probe, control and manipulate them, enabling exploration of some key fundamental questions in nature including those in quantum electrodynamics.
Access	EPAC is designed to support a mix of peer-reviewed academic research and application-focused industrial research.

Source	Orion (AWE)
	
Nature of source	Nd:glass laser system
Capacity	Single target chamber
Capability	Orion has 10 long-pulse beamlines (500 J, 1 ns @ 351 nm) with two synchronized infrared petawatt beams (500 J in 500 fs). One of the petawatt beamlines is operated in ultra-high-contrast mode by frequency doubling two square 300 mm sub-apertures to operate in the green, giving 200 J in <500 fs, 400 TW, with nanosecond contrast levels of $>10^{18}$.
Access	Up to 15% of time available for collaborative academic research. Selection is via the CLF access panel.

Annex 2: Glossary

Acronyms	Meaning
AI	Artificial Intelligence
CDI	Circular Dichroism
CDI	Coherent Diffractive Imaging
CLEM	Correlative Light and Electron Microscopy
CLF	Central Laser Facility
Cryo-EM	Cryogenic Electron Microscopy
CT	Computed Tomography
eBIC	Electron Bio-Imaging Centre
EM	Electron Microscopy
EPR	Electron Paramagnetic Resonance
ePSIC	electron Physical Science Imaging Centre
EPSRC	Engineering and Physical Sciences Research Council
ESFRI	European Strategy Forum on Research Infrastructures
ESRF	European Synchrotron Research Facility
EUV /XUV	Extreme Ultraviolet (20 - 200 eV)
EXAFS	Extended X-ray Absorption Fine Structure
FEL	Free Electron Laser
FLIM	Fluorescence Lifetime Imaging Microscopy
FLImP	Fluorescence Localisation Imaging with Photobleaching
FRET	Förster Resonance Energy Transfer
HED	High Energy Density
HEDP	High Energy Density Physics
HHG	High Harmonic Generation
IR	Infrared
LEAPS	League of European Accelerator-based Photon Sources
LP	Laser Peening
LSP	Laser Shock Peening
LWFA	Laser Wakefield Acceleration
MBA	Multi-Bend Achromat
MD	Molecular Dynamics
NMR	Nuclear Magnetic Resonance
PW	Petawatt
QED	Quantum Electrodynamics
RAL	Rutherford Appleton Laboratory
RFI	Rosalind Franklin Institute
RIXS	Research Infrastructure
RIXS	Resonant Inelastic X-ray Scattering
SEM	Scanning Electron Microscopy
SFX	Serial Femtosecond Crystallography
SESORS	Surface Enhances Spatially Offset Raman Spectroscopy
SORS	Spatially Offset Raman Spectroscopy
SR	Synchrotron Radiation

Acronyms	Meaning
SRS	Synchrotron Radiation Source, Daresbury
STFC	Science and Technology Facilities Council
THz	Terahertz (10^{12} Hz)
UKRI	UK Research and Innovation
UV	Ultraviolet
VUV	Vacuum Ultraviolet (10 - 20 eV)
WDM	Warm Dense Matter
XFEL	X-ray Free Electron Laser
XPCS	X-ray Photon Correlation Spectroscopy
XRD	X-ray Diffraction
XRF	X-ray Fluorescence
XUV/EUV	Extreme Ultraviolet (20 - 200 eV)

Units	
Attosecond	1 as = 10^{-18} s Attosecond range 1 - 1000 as
Femtosecond	1 fs = 10^{-15} s Femtosecond range 1 - 1000 fs
Picosecond	1 ps = 10^{-12} s Picosecond range 1 - 1000 ps
Nanosecond	1 ns = 10^{-9} s Nanosecond range 1 - 1000 ns
Length	
Ångstrom	1 Å = 10^{-10} m
Nanometre	1 nm = 10^{-9} m

Metric prefixes		
exa	E	10^{18}
peta	P	10^{15}
tera	T	10^{12}
giga	G	10^{9}
mega	M	10^{6}
kilo	k	10^{3}
hecto	h	10^{2}
deca	da	10^{1}
		10^{0}
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	µ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}
atto	a	10^{-18}

Annex 3: References

i. The UK government's R&D Roadmap was published in July 2020: UK Research and Development Roadmap (publishing.service.gov.uk)

ii. UKRI published the Research Infrastructures Roadmap in 2019: UKRI infrastructure roadmap - Progress report

iii. The UK Photonics Leadership Group published its report UK Photonics: The Hidden Economic Engine in 2018: UK_Photonics_The_Hidden_Economy.pdf (photonicsuk.org)

iv. STFC has produced strategies for:

Detectors and Instrumentation https://stfc.ukri.org/files/corporate-publications/detectors-and-instrumentation-a-strategic-review/

e-infrastructure https://stfc.ukri.org/files/e-infrastructure-strategy/

Accelerators https://stfc.ukri.org/files/2017-accelerator-strategy-review-report/

v. UKRI's first Delivery Plan was published in 2019: https://www.ukri.org/wp-content/uploads/2020/09/UKRI-250920-DeliveryPlan2019.pdf

vi. The European Strategy for Research Infrastructures (ESFRI) published a Roadmap in 2018: http://roadmap2018.esfri.eu/

vii. The UK government's modern industrial strategy forms part of the BEIS single department plan published in 2019 https://www.gov.uk/government/publications/department-for-business-energy-and-industrial-strategy-single-departmental-plan/department-for-business-energy-and-industrial-strategy-single-departmental-plan-june-2019#deliver-an-ambitious-industrial-strategy

viii. The Science Case for the Diamond II project was published in 2019: https://www.diamond.ac.uk/Home/About/Vision/Diamond-II.html

ix. ESRF published the Technical Design Study for the upgrade programme in 2014 : http://www.esrf.eu/Apache_files/Upgrade/ESRF-orange-book.pdf

x. The National Academy of Sciences report on Opportunities in Intense Ultrafast lasers was published in 2018: https://www.nap.edu/catalog/24939/opportunities-in-intense-ultrafast-lasers-reaching-for-the- brightest-light

xi. STFC published the Science Case for a UK XFEL in October 2020: CLF UK XFEL - Scientific Case Project (stfc.ac.uk)

xii. A. Hosseinizadeh, G. Mashayekhi, J. Copperman et al. "Conformational landscape of a virus by single-particle X-ray scattering," Nat Methods 14, 877-881 (2017) DOI: 10.1038/nmeth.4395

xiii. US Department of Energy Grand Challenges: EFRC Grand Challenges | U.S. DOE Office of Science (SC) (osti.gov)

xiv. R. Mankowsky, A. Subedi, M. Först et al. "Nonlinear lattice dynamics as a basis for enhanced superconductivity in YBa2Cu3O6.5," Nature 516, 71-73 (2014) DOI: 10.1038/nature13875

xv. STFC's Technology Department built the world-leading Large Pixel Detector for the European XFEL: https://www.technologysi.stfc.ac.uk/Pages/LPD-for-European-XFEL.aspx

xvi. Ada Lovelace – An inspiration to the next generation, the first computer programmer - Science and Technology Facilities Council (ukri.org)

Science and Technology Facilities Council

Science and Technology Facilities Council
Polaris House
North Star Avenue
Swindon
SN2 1SZ

stfc.ukri.org