Science and Technology Facilities Council

Next-generation XFEL Science and Technology Case Overview

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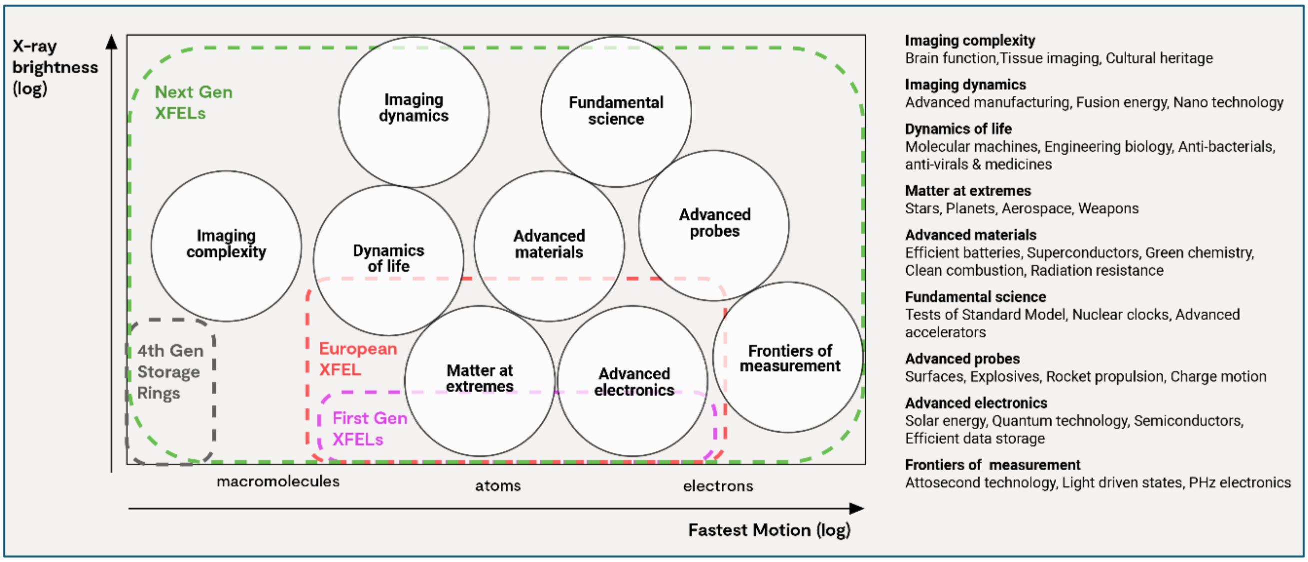
Overview of the UK's Next-Generation XFEL Science and Technology Case

UK scientists are amongst the leading users of pioneering X-ray free-electron laser (XFEL) facilities, which enable revolutionary atomic-level imaging and ultrafast time resolution far beyond other methods. The next generation of these machines will vastly enhance research productivity through higher data rates, increased throughput, and x-ray quality. There is a strategic opportunity for the UK to leverage its scientific leadership to drive deep and wide-ranging impact across all areas of science and technology and major sectors of the economy, including all of the IS-8 growth-driving sectors. Access to such capability is vital for any leading economy: the UK can secure global leadership by hosting a new facility or co-developing an international project.

Next Generation XFEL Opportunities for Research and Innovation

Next-generation XFELs will be the most advanced light sources the world has ever seen, with average x-ray brightness over a thousand times higher than fourth generation storage rings like Diamond-II, and a peak brightness a billion times higher. This will provide revolutionary **x-ray atomic-level structure determination and nanoscale imaging capabilities** that will benefit defence, biotechnology, batteries, solar energy and catalysis. Still more importantly, this will give access to the **intrinsic timescales for physical, chemical and biological changes in matter,** enabling studies of electron motion on timescales of a femtosecond (10^{-15} s) or less, and atomic motion on typical timescales of 100 femtoseconds, far beyond the nanosecond (10^{-9}s) limit of storage rings. Access to this unprecedented information will transform science and technology and be a driver for innovation, as summarised in the figure below and discussed in full in the **Next-Generation XFEL Science and Technology Case[1].**



The high x-ray average brightness coupled to extreme time resolution of a Next Generation XFEL enable new classes of measurement that will drive discovery in science and technology

The Case addresses how UK access to a next-generation x-ray free-electron laser (XFEL) facility can underpin future national economic growth and industrial competitiveness. The new science and technology enabled by a next generation XFEL will boost delivery of the **UK government's (2025)**

[1] It is anticipated that the full Next Generation XFEL Science and Technology Case will be published in March 2026

Industrial Strategy including advances in the **IS-8 growth-driving sectors**. This would be through directly addressing key technology challenges for **Advanced Manufacturing**, **Clean Energy Industries**, **Digital and Technologies**, **Life Sciences** and **Defence**. In addressing the Industrial Strategy, a next-generation XFEL will address key topics integral to the UK's broader science and technology environment:

- **Advancing the frontiers of knowledge** through the ability to probe quantum processes in matter and understand the couplings and interactions that underpin, for example, chemistry, materials science and life sciences, as well as through the potential to study matter at extreme conditions in the universe.
- **Advancing technology** through the boost provided by space- and time-resolved understanding, leading to the development of new energy, data, nuclear and materials technologies.
- **Furthering healthcare** by the profound advances in understanding of biochemical and biomolecular function, facilitating better guidance in developing drugs and therapies.
- **Underpinning net zero** goals by the space- and time-resolved data that is essential to developing sustainable approaches to catalysis, carbon capture, fusion energy and understanding the action of pollutants and particulates in the environment.

Next-generation XFELs will be among the world's largest sources of high-value scientific **data**, with a highly synergistic relationship with **AI and machine learning** that is critical to harness for the UK. Just as the highly successful AlphaFold protein structure prediction tool relied on ~200,000 experimentally determined protein structures, equivalent AI tools for predicting dynamics and mechanisms will require far larger datasets, which will be enabled by next-generation XFELs. Large numbers of scientists and engineers will hone their skills in this environment and ultimately join the workforce, thereby boosting all sectors including the other **IS-8 growth-driving sectors Creative Industries**, **Financial Services** and **Professional and Business Services**.

Access to the combination of next generation XFEL capabilities will boost **economic strengths** as well as providing vital **sovereign capabilities** for the defence and wellbeing of the nation. Moreover, the research enabled is critical to the missions of multiple **UKRI** research councils:

- **EPSRC** through impact in physics, chemistry, materials, advanced manufacturing, green energy, AI/Exascale computing and nuclear fission;
- **STFC** through impact in accelerator technology, astrophysics, dark matter searches and tests of the standard model;
- **NERC** through enabling new research impacting atmospheric chemistry, geophysics, geochemistry, and palaeontology;
- **BBSRC** through advancing biochemistry, structural biology and brain imaging;
- **MRC** through impact upon tissue imaging, drug discovery and drug interactions at the molecular level;
- **AHRC** through opening up new imaging capabilities for cultural heritage and archaeology.

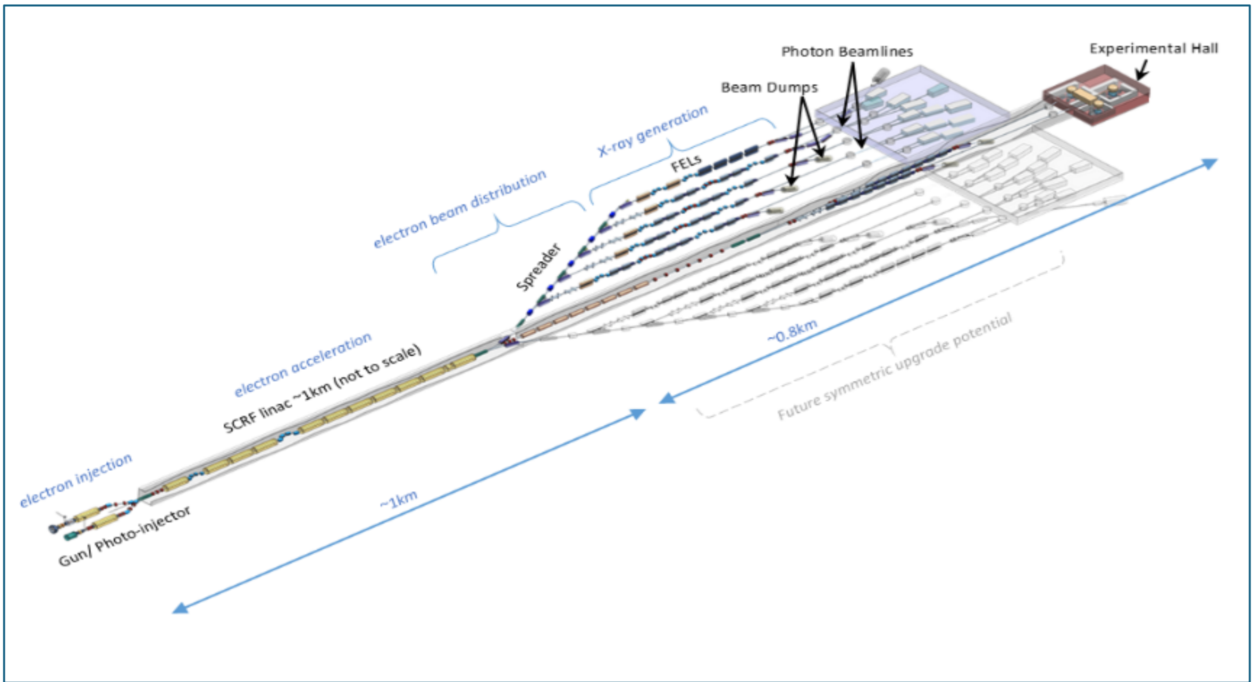
Other major agencies will also be direct beneficiaries, including **UKAEA** through the ability to image the processes in nuclear fusion energy including compression of material and radiation damage mechanisms, and **AWE/MOD** through advances in defence technology and matter at extreme conditions.

UK use of XFELs has grown rapidly over the last decade, with UK researchers now amongst the major users at the European XFEL and LCLS (see use survey figures in Chapter 10). A huge advantage can be gained through a next generation XFEL facility that massively boosts access opportunities and is optimised with the most advanced features matched to our needs, ensuring substantial access of the capabilities of direct benefit to the UK economy. The conceptual design would enable parallel operation of more than 10 scientific end-stations and rapid switching between experiments, to increase the amount of research access almost a hundred-fold compared to existing facilities. Ensuring ease of access for both established and new user communities is of critical importance to deliver the fullest range of the potential science, technology and industrial benefits.

In the Science and Technology Case we discuss the science and technology that will be enabled by access to a **next generation XFEL** and **specify the new capabilities** such a facility must have to maximise the research impact. Here we provide a brief overview of that Case, the Conceptual Design and select a few examples of that science and technology.

Strategic Case for UK Leadership of a Next Generation XFEL

In recognition of the growing importance of XFELs to current and future science and technology, leading industrial nations across the globe have established their own XFEL capability, with systems now in operation, or under construction, in the USA, Germany, Italy, Switzerland, Japan, Korea and China. XFELs are recognised as indispensable to the development of new technologies where the quantum scale structural dynamics of matter must be understood and exploited. The UK has the opportunity to play the leading role in next-generation XFELs and thus reinforce its place as a leading scientific and industrial power. Failure to do so could see strategic competitors grasping these opportunities ahead of us and reaping the benefits by outpacing our technology and science.



An outline of the conceptual design for a next-generation XFEL that would provide a unique combination of capabilities, able to deliver the opportunities discussed in this Case

The 2020 Science Case has already had a strong impact on the thinking of the international facilities in terms of their strategy and planning. A broad consensus has emerged at these facilities as to what a next generation XFEL capability should encompass that strongly aligns with the vision set out by the UK XFEL project. Since then long-term plans at SLAC for a successor facility to LCLS II have begun to form along similar lines of a next generation facility (see LCLS-X the name of this putative future project). The UK XFEL project is also influencing the thinking at European XFEL as they consider strategic directions beyond 2030 and also the SHINE facility in Shanghai that is currently being commissioned. It is likely that the current Conceptual Design and Options Analysis report, including the Next Generation XFEL Science and Technology case, will continue to be influential in informing policy across the globe.

The UK can leverage this position still further by maintaining a leadership role in the planning and implementation of a future international next generation XFEL facility – no matter which of the active options it chooses going beyond the *status-quo*. These options include **investment in, and partnering with, European XFEL and/or LCLS or hosting a new facility also in partnership with other nations.**

Here we briefly set out the reason that doing this can be so beneficial to the UK:

- Vital to future growth in Advanced Manufacturing, Defence, Clean Energy, Life Science and Digital Technology Sectors for which the next generation will provide the underpinning facility capability to the necessary research and innovation.
- There is a vibrant and growing community of UK scientists and technologists using XFELs for cutting edge research, with the right tools available they would drive major cross-disciplinary advancements in UK research and innovation
- The development of a facility with a substantial UK investment and activity will secure essential advanced skills in UK workforce through research, training and attracting global talent
- Economic growth will come from construction, new manufacturing capabilities and new supply chain opportunities
- As the investment will be spread over several decades from construction through operation and upgrades so that the direct boost to UK industry and technology will be ongoing over years
- An option that includes construction in the UK brings with it the potential for a huge regional development opportunity and economic boost
- The partnering in a facility built anywhere would be a catalyst for growth in the technology sector across the nation
- Playing a prominent role in the construction of a new facility will enhance national prestige and firmly signal that the UK is a science & technology superpower

So far in Europe and North America there are advanced superconducting XFEL machines, but no one has yet committed to developing a next-generation XFEL. The UK can thus perform a crucial role in bringing about these revolutionary machines by either playing a leading part with European XFEL or SLAC upgrades and/or spearheading the construction of a new international facility in the UK.

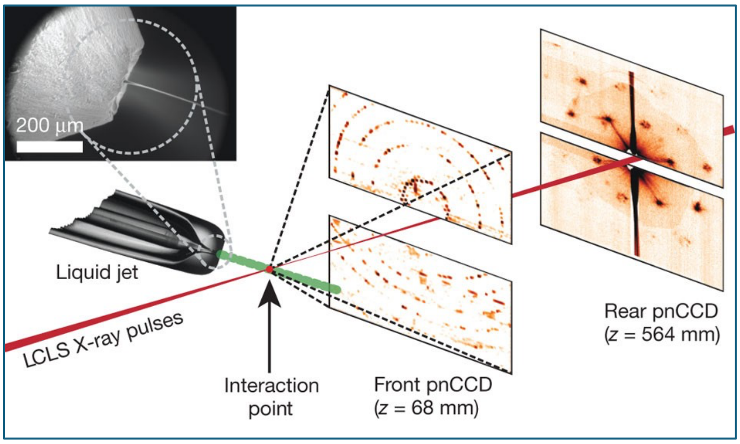
In summary, the pursuit of a next generation XFEL capability for the UK is a strategically important and future facing action that will yield wide ranging scientific, technological, industrial, societal and economic benefits.

Recent High Impact Science with Current XFELs

The opportunities afforded by XFELs in time-resolved studies have already advanced research in the **chemical and physical sciences** and in the **life sciences.** To illustrate this impact we consider a very small sample of high profile research that has been published in recent years, a comprehensive survey can be found in the full next-generation XFEL Science and Technology Case.

Advances in methods

"Femtosecond X-ray protein nanocrystallography" published in Nature, February 2011,[2] used extremely short x-ray laser pulses from LCLS, each lasting less than 100 femtoseconds (100 x 10^{-15} s), to take rapid diffraction "snapshots" of millions of tiny protein crystals in a flowing stream, before the intense X-rays could damage them. They demonstrated this by studying Photosystem I, a complex membrane protein involved in photosynthesis, using nanocrystals far too small for traditional x-ray methods (*below*). By combining over three million individual diffraction patterns, they reconstructed a detailed three-dimensional structure without growing large crystals. This "diffraction before destruction" technique works because the x-ray pulse records data before any damage occurs, effectively outrunning the damage problem that has limited protein imaging in the past. Their breakthrough opened a new way called Serial Femtosecond Crystallography (SFX) to study important, hard to crystallize, fragile proteins, like those found in cell membranes, at high resolution under realistic, hydrated conditions.



Advances in physics and X-ray photonics

"Attosecond-pump attosecond-probe X-ray spectroscopy of liquid water" published in Science, February 2024,[3] used the attosecond x-ray method at LCLS to probe the very fastest dynamics of ionized water (*below right*). The x-rays with a pulse duration of ~300 attoseconds act like a super-fast camera to watch how electrons in liquid water react. In this measurement, they sent two of these x-ray bursts through water, one to kick out an electron and the second, almost immediately after, to check what happened next. Because the second burst arrives so quickly (within a few hundred attoseconds), the atoms themselves do not have time to move, effectively freezing the motion of the water molecule. They discovered that a mysterious feature in a specific x-ray spectral signal, seen in earlier longer timescale measurements, was caused by water molecules moving on femtosecond timescales that were eliminated in the current attosecond measurement. This powerful snapshot

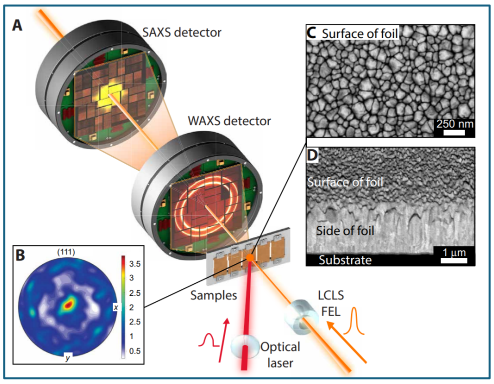
2 H.N. Chapman *et al.* « Femtosecond X-ray protein nanocrystallography" *Nature* 4**70**, 73–77 (2011) DOI: 10.1038/nature09750

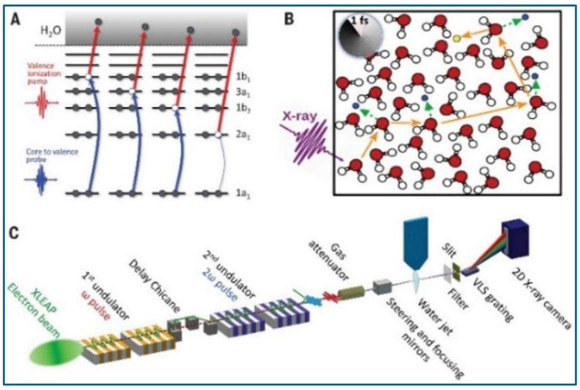
3 Shuai Li *et al.* "Attosecond-pump attosecond-probe X-ray spectroscopy of liquid water" *Science* **383**, Issue 6687 1118-1122 (2024) DOI: 10.1126/science.adn6059

settled that longstanding puzzle and demonstrated how attosecond x-ray spectroscopy can reveal how electrons behave in liquids and solids and gives access to the earliest events of radiation damage.

Advances towards industrial applications

“Femtosecond quantification of void evolution during rapid material failure” published in Science Advances, December 2020,[4] reports the use of x-ray scattering from the LCLS XFEL (*below left*) to capture how tiny voids form and grow inside materials as they break under extreme stress. This process happens on a picosecond timescale, so the team used femtosecond imaging to observe it in real time. Understanding this rapid failure will help researchers predict when and how materials will break, especially in high-speed impacts like car crashes or explosions. These insights could lead to stronger, safer materials for use in aerospace, defence, and construction. Ultimately, this research may help design materials that resist breaking under sudden, intense forces.



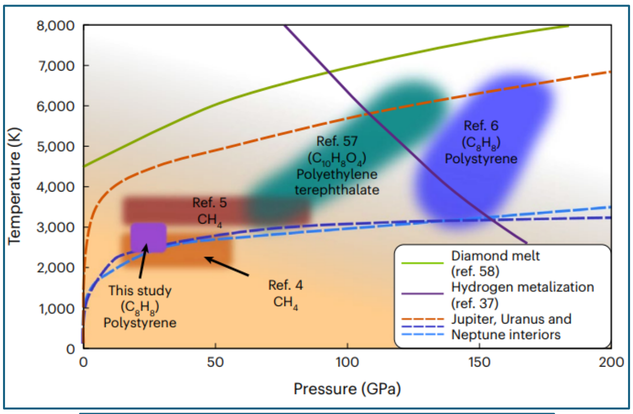


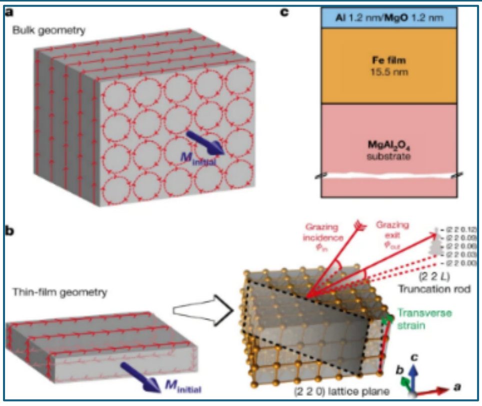
Advances in matter at extreme conditions

In “**Diamond precipitation dynamics from hydrocarbons at icy planet interior conditions**” published in Nature Astronomy, January 2024,[5] a thin film of polystyrene was squeezed between diamond anvils and exposed to ultra-fast x-ray pulses from the European XFEL, duplicating the pressures (190,000 – 270,000 times Earth’s atmospheric pressure) and temperatures (>2,500°C) that exist a few thousand kilometres inside Neptune and Uranus (*below left*).

4 Coakley *et al*., “Femtosecond quantification of void evolution during rapid material failure,” *Sci. Adv*. **6**: eabb4434 (2020) DOI: 10.1126/sciadv.abb4434

5 Frost *et al*. “Diamond precipitation dynamics from hydrocarbons at icy planet interior conditions,” *Nature Astronomy* **8**, 174-181 (2024) DOI: 10.1038/s41550-023-02147-x



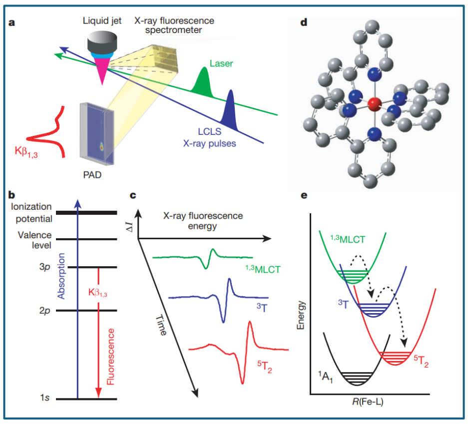


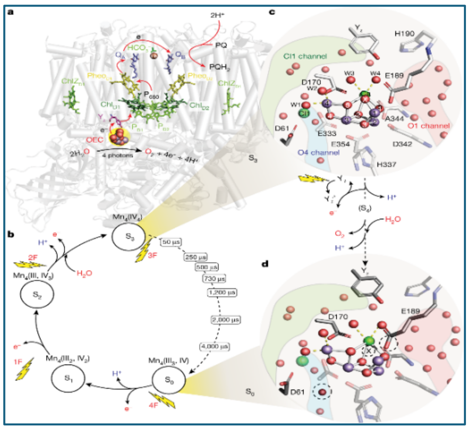
Within 30-40 microseconds they directly observed carbon atoms separating from hydrogen and crystallising into diamond. This leads to the phenomena of “diamond rain” thought to occur in giant planets. The study showed that it can begin sooner and at much lower pressures than earlier nanosecond shock-wave experiments had suggested. This work resolved a decade-long experimental discrepancy and reset the boundary conditions for carbon-hydrogen demixing in planetary interiors. Because newly forged diamonds are heavier than the surrounding ice, they would sink, releasing gravitational energy and stirring conductive fluid layers; the team argues that this extra heat and convection help explain the unusual magnetic fields of Neptune and Uranus, and suggests that the same process could operate in the abundant class of exoplanets dubbed “mini-Neptunes,” where it would begin at even shallower depths than previously assumed. The refined pressure-temperature map for diamond formation will now feed directly into interior-structure, heat-flow and dynamo simulations, improving our understanding of how icy giant planets and their extrasolar cousins evolve over time.

Advances in chemical sciences

“Tracking excited-state charge and spin dynamics in iron coordination complexes” published in Nature, May 2014 [6] is a landmark study that employed femtosecond x-ray emission spectroscopy to directly track, in real time, the excited-state charge and spin dynamics of an archetypal metal complex, Fe(II) polypyridyl. By launching a charge transfer excitation between the metal and surrounding parts of the molecule (ligands), and monitoring the highly spin-sensitive x-ray emission, the researchers revealed that spin state change proceeds not as a simple two-state jump but involves a critical intermediate triplet state (*below left*). This clear identification of a transient intermediate species – bridging the initial and the ultimate high-spin state – resolved longstanding debates about the mechanistic pathway. The work not only showcases a powerful new spectroscopic tool with sub-100 fs time resolution, but also provides unprecedented molecular-level insight into the ultrafast interplay of charge, spin, and structure in light-activated 3d transition-metal complexes critical in emerging quantum technologies.

[6] W. Zhang, R. Alonso-Mori, U. Bergmann *et al.* “Tracking excited-state charge and spin dynamics in iron coordination complexes” *Nature* **509**, 345 (2014) DOI: 10.1038/nature13252





Advances in life sciences

"Structural evidence for intermediates during O_2 formation in photosystem II", published in Nature, May 2023,[7] employs SFX to address a key cycle in biology (*above right*) – photosynthesis, which is responsible for nearly all O_2 generation on Earth. Photosystem II is a very large protein complex in plants and photosynthetic microbes in the oceans, that helps turn water into oxygen during photosynthesis. Scientists have long wondered exactly how photons from the Sun drive oxygen (O_2) formation during this process. This paper, and other recent XFEL-related work[8], provides experimental data showing the steps the protein goes through as it sequentially absorbs energy from the Sun (four photons in total) to eventually "split" two water molecules and transfers the four electrons and four protons to other biological processes. However, in the end the enzyme brings the two oxygen atoms together to make one dioxygen molecule and thereby resets itself for another round of reaction. These snapshots capture several photon-driven, sequential, and short-lived "intermediates" – temporary states that the molecules pass through during the catalytic cycle. Understanding these steps also helps explain how nature uses energy from the sun to separate charge (preferential electron flow) that is already inspiring new ways to produce clean energy such as improved photovoltaic panels.

Next-Generation Capabilities

Through the development of the Science and Technology Case, we have identified the key capabilities required of a next-generation XFEL to drive future research and innovation. These capabilities are in reach with moderate technical advances as confirmed by the Conceptual Design:

- **Near transform-limited operation across the x-ray range using modes going beyond conventional noisy XFEL emission**
- **A high-efficiency facility, with a step-change in the simultaneous operation of multiple end stations**
- **Evenly spaced, high repetition rate pulses to match samples, lasers, and detectors**
- **New AI approaches for operation, data acquisition, analysis and interpretation of the vast volumes of data generated**
- **Improved synchronisation/timing data with external lasers to < 1 fs**
- **Widely separated, multiple colour x-rays to at least one end station by combining the outputs from two FELs**

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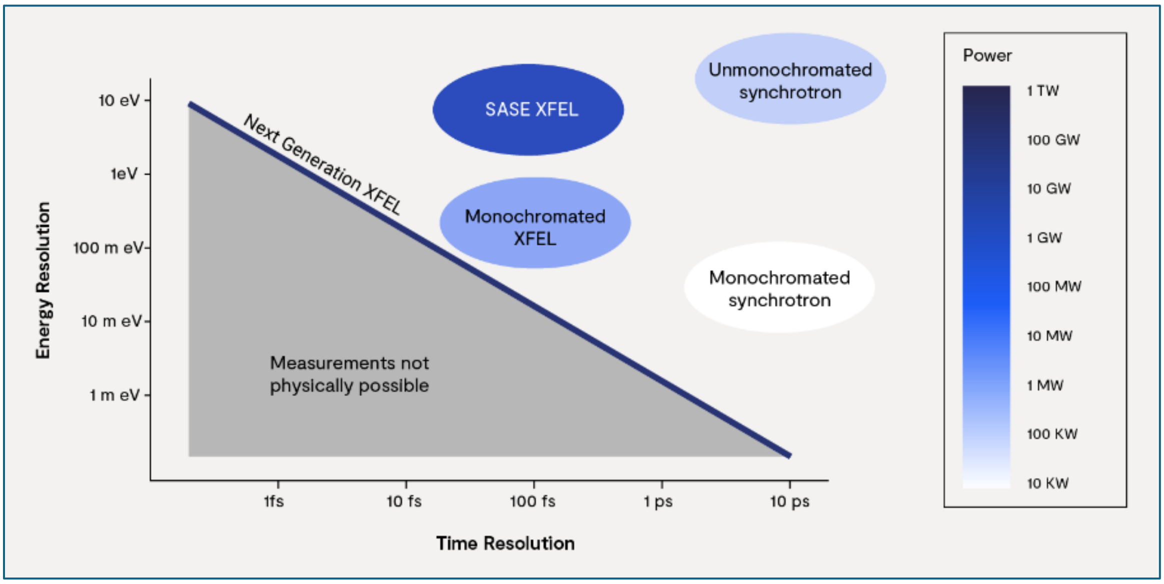
[7] A. Bhowmick *et al*. "Structural evidence for intermediates during O_2 formation in photosystem II" *Nature* **617**, 629-636 (2023) DOI: 10.1038/s41586-023-06038-z

[8] Li, H. *et al*. Oxygen-evolving photosystem II structures during S1–S2–S3 transitions. *Nature* **626**, 670-677, doi:10.1038/s41586-023-06987-5 (2024)

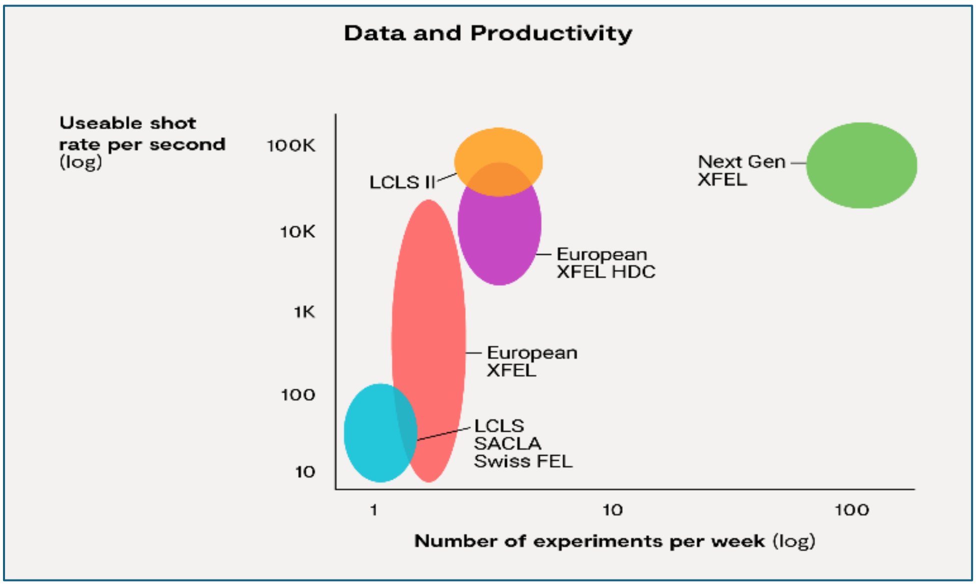
- **Full array of synchronised sources including optical lasers and non-linear optical conversion across the electromagnetic spectrum from XUV – THz, charge particle beams, high energy and high power lasers**
- **A sustainable facility meeting Net Zero targets**

The transformative benefits of each of these new capabilities are discussed briefly below:

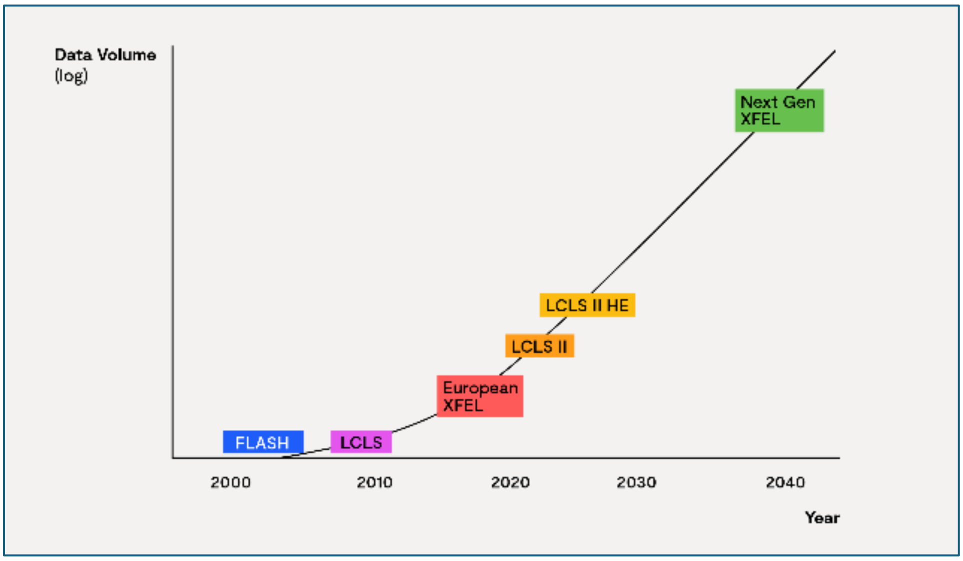
Near transform-limited operation across the x-ray range will permit measurements at the physical limit of combined temporal and energy resolution. In addition, a whole array of as yet untapped non-linear x-ray methods will only be made possible with high quality and reproducible transform-limited x-ray fields. These non-linear x-ray methods include: second-harmonic generation with surface sensitivity, hard x-ray Raman methods to measure chemical dynamics in dense environments, impulsive stimulated x-ray Raman to enable attosecond measurements of electronic dynamics within complex systems. Moreover, the improved x-ray properties, compared to the current stochastic properties, will vastly increase the useful data rate and so, combined with high repetition rate, enable measurements that previously took weeks and days to be completed in hours and minutes.



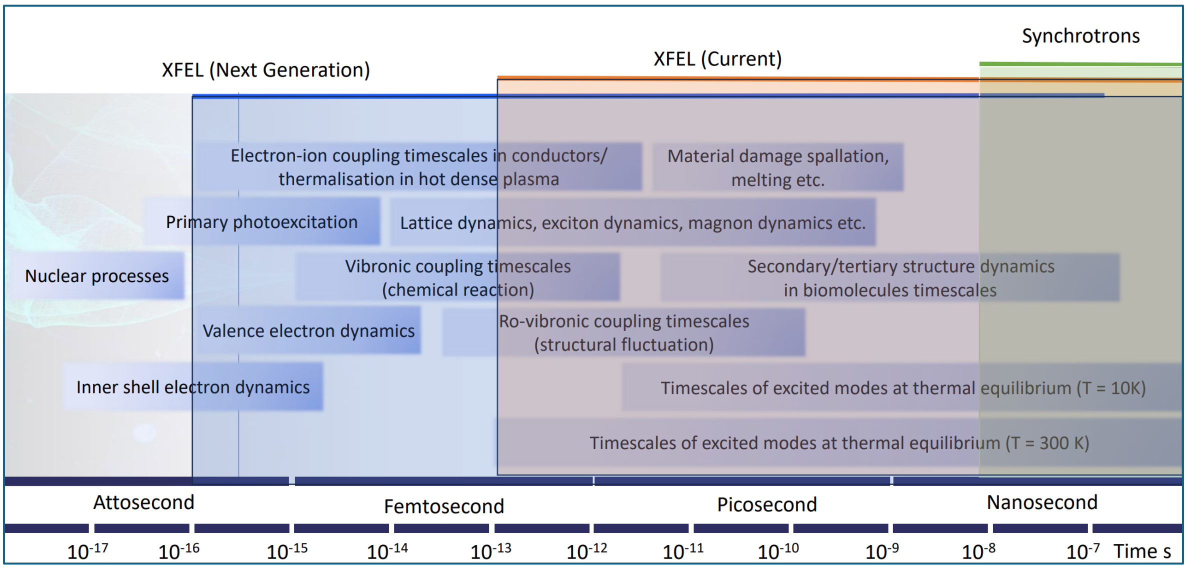
A high efficiency facility, with a step-change in the simultaneous operation of multiple end stations in parallel, will open XFEL measurements to many new branches of science and technology, by dramatically lowering the barriers to access. Multiplexing along with the high useful data rate will enable more than an order of magnitude increase in the number of measurements that can be completed every week. Moreover, some scientific programmes of high potential impact (see Flagship Programmes in **Section 9**) will only be feasible with extended and repeated beamtime access (as is the case at Synchrotron facilities).



Evenly spaced, high repetition rate pulses are an essential prerequisite for many measurements that need to reach high signal-to-noise, or for which the signals are inherently weak (e.g. measurements of chemical dynamics in low concentration, as might occur in nature). This capability would also unlock enormously high average spectral flux, which will enable entirely new dynamic and chemically-sensitive imaging capabilities that are impossible with current light sources. The huge data volumes generated will require the most ***advanced AI tools*** for efficient acquisition, analysis and interpretation to deliver the best possible research outcomes. This will also act as a driver for innovations in the use of AI in science and technology.

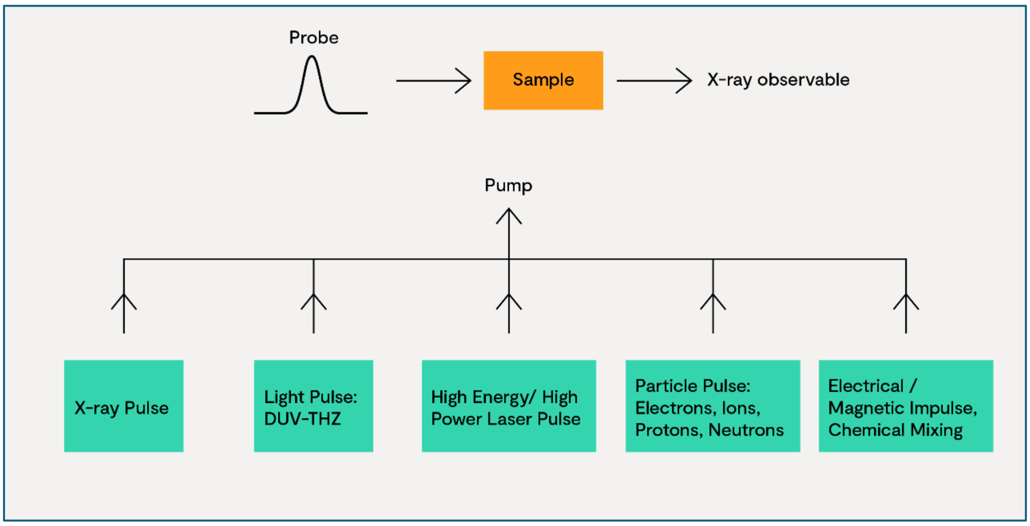


Improved synchronisation/timing data to ~ 1 fs between optical lasers and the x-ray pulses will enable the fully resolved study of the dynamics of electronically excited states that underpin solar energy, solar fuel generation, photodetectors, optoelectronics devices and photosynthesis, and will offer a major advance over the current status.



Access to the fastest dynamics – important in nanoscopic processes in science and technology – is enabled at a next-generation XFEL by having pump-probe pulse timing tools with 1 fs fidelity (optical - X-ray) and 0.1 fs fidelity (X-ray - X-ray)

Having a ***full array of synchronised sources*** will unlock the measurement of photodynamics initiated across the electromagnetic spectrum from deep UV to mid IR. In addition, the use of THz directly to drive lattice motions is vital in the study of quantum materials, and for providing precise temperature jumps to trigger dynamics in many systems. Pulsed particle beams including electrons, protons, neutrons and ions will open the way to measuring the dynamics in a vast array of radiolysis and radiation damage situations. ***Widely separated, multiple colour x-rays to at least one end station*** will provide a unique set of measurement possibilities, where the sample is first pumped by soft x-rays and then probed by hard x-rays (or vice versa) to time resolve the effects.



Based upon these next generation capabilities and the end-stations identified for a future XFEL we have developed 11 high impact Flagship Research Programmes with a strong applications driven focus that would become possible from day one. These are introduced below as we discuss the impact of a Next Generation XFEL to Industry.

Industrial Impact

Here we highlight a few case studies to illustrate the wide benefits to industries across multiple sectors of significantly enhanced access and dedicated end-stations enabled by a next-generation XFEL.

Additive manufacturing

Laser additive manufacturing via laser bed fusion is an industrially important method but involves complex processes on multiple spatial and temporal scales. Residual strain and the complexity of the process are large challenges to our understanding of how to improve the product quality. Given that important components of the process take place on sub-microsecond to picosecond timescales, XFELs are a critical technology. Understanding how the laser penetrates the material is a key example of how XFEL-based dynamic imaging can be incisive. Cracking can also arise due to the high thermal gradients and large residual strain can build up in the material. Time-resolved x-ray imaging and diffraction of the cracking mechanism are an excellent opportunity to progress the issues. Likewise, imaging melting dynamics in laser machining for drilling and cutting is a critical issue that only an XFEL can resolve. The **Flagship Programme "Understanding magneto-hydrodynamic stability and fluid mixing"** is indicative of some of the capabilities that can be used to boost this research.

Batteries

Batteries are a critical technology in the green transition, and gains from increased efficiency and options to reduce reliance on a supply of a single element, lithium, are seen as strategically important. The timescales of interest in batteries range from femtoseconds/picoseconds (electron transport), nanoseconds/milliseconds (polaronic transport), redox (milliseconds to minutes), degradation (weeks to years). To get a picture of the full operation of a battery, over its whole cycle, requires access to all these timescales as well as probing of large-scale analogues of a real battery. See **Flagship Programmes "Ion-conductor solid state electrolytes"** and **"Probing and controlling elementary steps in batteries"** in **Chapter 9**. Transformative impacts would come from resolving the ultrafast structural dynamics accompanying structural rearrangement under battery operation, identifying intermediate species in the battery operating cycle, determining ion dynamics, and diffusion mechanisms. With XFELs, all measurements will become much faster compared to conventional x-ray sources (due to brightness) with the unique possibility of focusing on the fastest timescale-critical processes.

Biotechnology and Engineering Biology

A next-generation XFEL will have major impacts on our understanding of the mechanisms underpinning biochemistry and molecular machines by opening to measurement the crucial sub-picosecond timescales – to reveal the true *dynamics* at a molecular level as opposed to the ensemble averaged kinetics. This will give not only deep understanding of the essential processes of life, but has huge implications for biotechnology and medicine. The importance of G protein-coupled receptors (GPCRs) in cell membranes for the development of many drugs is a particular current area for XFEL-based serial nano-crystallography approaches and key players in the Pharma sector are advocating for more access to XFELs for the Pharma industry. Moreover the high average brightness provided by a next-generation XFEL opens unprecedented opportunities in the x-ray imaging of tissue to reveal the biochemical and biophysical processes in the context of the whole system see **Flagship Programme "Nano-bioimaging in tissues and organs – wiring diagrams for whole brains"** in **Chapter 9.**

Catalysis

Around 80% of manufactured products, including fuels, fertilisers, food and drink, cars, mobile phones and medicines, rely upon catalysts for their production. Catalysis research is already a big user of Diamond Light Source, using x-ray spectroscopy to focus in on the atomic sites at which catalytic activity is occurring within a larger molecular complex, and diffraction to observe the accompanying structural changes. The high average brightness and temporal resolution of a next-generation XFEL will enable access to the full temporal range of catalytic mechanisms, from femtoseconds to microseconds, and at realistic concentrations. Chemical imaging XRD-CT scans probing atomic structure over mesoscopic scales would become possible, a high brightness XFEL would enable this to be measured on timescales of minutes. With accompanying capabilities for *in operando* studies, a wide range of measurements will become possible, with the goal of making catalysis greener and more sustainable by systematically replacing some of the rarer materials currently used with Earth-abundant elements see **Flagship Programme "Enabling routes to greener chemical synthesis"** and **"New chemical dynamics induced by sudden ionisation"** in **Chapter 9**.

Engineering materials

The response of engineering materials to shocks and stresses is vital to the engineering industry, as well as to our safety (e.g. the integrity of aeroengines). Advances in understanding this are closely connected to the scientific efforts in MEC with, for instance, the pioneering SAXS/WAXS studies of laser shocked metals resolving void formation and failure at high strain rates by UK researchers. Residual stress from the manufacturing process is an important factor leading to failure of materials. Some processes are too fast to be captured by other methods (e.g. neutron scattering) and require access to sub-millisecond timescales only available at an XFEL. Mitigation methods to relieve residual stress include laser shock peening, widely used in aeroengine components, but to understand this requires fast temporal resolution as recently applied at the SACLA XFEL. See **Flagship Programme "Measuring the dynamics of materials far from equilibrium"** in **Chapter 9**.

Fuel additives and lubricants

Fuel additives and lubricants are vital to the mechanical efficiency, energy consumption and lifetime of combustion engines. Even with the green transition, such engines will remain essential to society for decades to come. XFELs enable studies of the dynamics of barrier-crossing in the complex network of reactive nucleation processes (e.g. sulphonate stabilised calcium carbonate nanoparticles used as detergents in engine lubricants) that are vital for the control of product properties; x-ray reflectivity studies of self-assembly dynamics at the interfaces of the polymers used to reduce friction between components; ultrafast dynamical studies of the mechanistic basis of friction modifiers; and understanding the molecular basis of the kinetics of component interactions (e.g. of detergents and dispersants) via time-resolved ultrafast spectroscopy and imaging.

Fusion technology

Fusion energy will benefit from the availability of XFEL measurements in both understanding and mitigating radiation damage within the first wall materials of the fusion reactor. Further they can, for example, advance understanding of radiation induced quenching of High Temperature Superconducting (HTS) magnets, efficient lithium isotope enrichment strategies, radiation damage in structural materials and coolants, and diffusion of hydrogen isotopes through interfaces, which are all of importance in magnetic confinement technology. For inertial confinement, the same methodologies used in MEC science can be used to study dense plasmas. Dynamic tomographic imaging will provide unique insights into instabilities, vital to understand for ensuring efficient compression. XFELs are becoming an essential component in ongoing developments. See **Flagship Programmes "Tracking the fastest dynamics of radiation damage in materials for nuclear and space technology"** and "**Exploring extreme material conditions in current driven X-pinch implosions"** in **Chapter 9**.

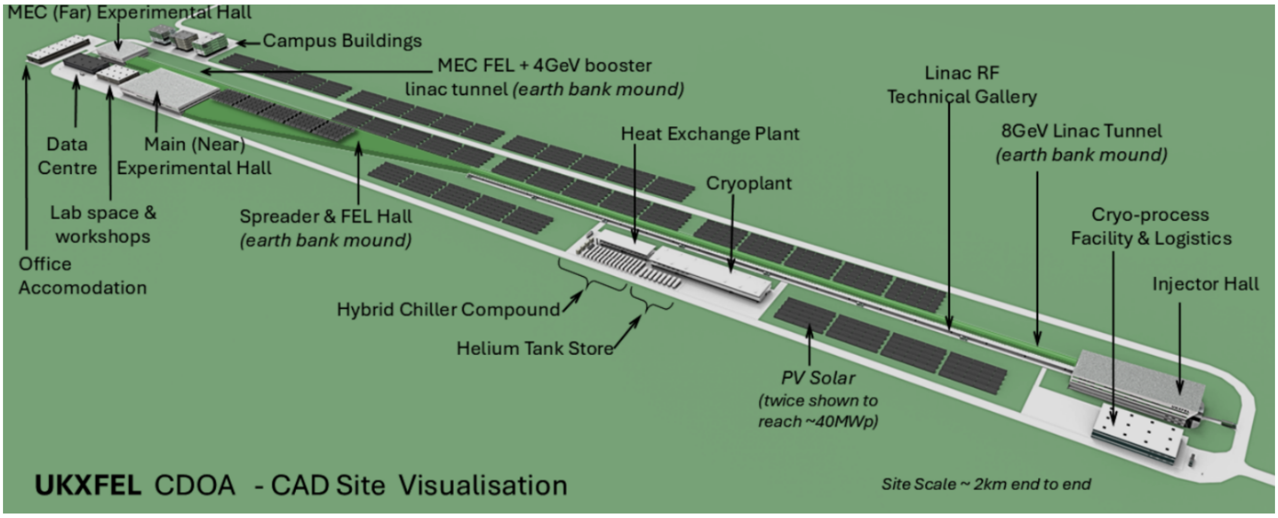
Semiconductors

The smooth supply of semiconductor wafers for chip manufacture is strategically essential for the economy. In the fabrication of semiconductors, full control over the integrity of the process is essential. Defects in semiconductors are a critical impediment and, for certain classes of defects that may be light or current induced, there is a need to track their formation and transport *in operando* on picosecond/femtosecond timescales. XFELs could play a crucial role here and in resolving the connection between carrier lifetimes and crystal defects in semiconductors. Again, it would be important to have the appropriate end-station instrumentation to do this under *in operando* conditions. See **Flagship Programmes “Probing THz electron transport in graphene”** and **“Probing exciton and spin dynamics in optoelectronic materials”** in **Chapter 9**.

Conceptual Design of a Next-Generation XFEL

Since the late-2000s, XFELs have proven to be a radical technology breakthrough, delivering X-rays that are many orders of magnitude brighter than other sources. **XFELs are now ready to enter a new era of capability and maturity in which they deliver world-leading, societally-relevant science at scale.** Looking to the future for the UK community, the UK XFEL project has developed a conceptual design for a next-generation XFEL that can deliver a true generational step in research productivity through enhanced data rates, throughput, and x-ray quality.

The design couples extremely high repetition rate operation (100 kHz – 1 MHz) developments of a range of accelerator, laser and end station technologies with the emergence of artificial intelligence and significantly increased multiplexing capabilities. The resulting vision for an internationally leading XFEL facility is applicable to both a new facility build and the upgrade of an existing facility. It can be scaled in capability and delivered across a phased construction pathway.



Site visualisation of the next-generation XFEL facility.

Next-generation XFEL features

A core feature is extremely high repetition rate (100 kHz - 1 MHz) operation and how the design couples rapid advances in various accelerator, laser, and end station technologies with the emergence of artificial intelligence and exascale computing. Proven MHz electron gun technology is integrated within a novel dual-injector configuration for optimal beam quality, redundancy, and double-bunch capability. Using superconducting linear acceleration, it achieves a 10,000× pulse-rate increase over normal-conducting XFELs, while lasers, detectors, and sample delivery systems are all developing toward similar rates. By connecting these features to a comprehensive data pipeline, including integration with national exascale and AI capabilities, **next-generation XFELs will be among the world's largest sources of high-value scientific data.**

The next generation XFEL is designed to deliver a step-change in capacity and throughput, to accelerate progress across many fields. It expands from current facilities that operate only 1-3 simultaneous experiments to support 10 or more, to reduce wait times and cost per experiment to enable rapid, related studies. The facility is highly modular and robust in terms of design and civil engineering. Critical front-end systems prioritise reliability and high technology readiness, while AI, digital twinning and robotics will drive efficiency throughout.

A comprehensive set of end stations has been developed through an extensive community-guided process - each has been associated with a particular FEL and has its own unique capabilities and direction to world-class science. Increased throughput will support internationally pioneering experimental programmes, while translating today's state of the art methods into on-demand measurements for industrial applications. By branching out into its separate lines and experimental areas, the facility is designed to progressively engender increased specialisation and experimentation.

Advanced FEL techniques will deliver extreme X-ray pulse qualities, including near transform-limited, 'laser-like' pulses at up to ~100 kHz across ~10 independently operable FEL lines, as well as a specialised capability for widely separated two-colour pulses (e.g. soft + hard X-ray). These high-quality X-ray pulses will be coupled with **a comprehensive suite of lasers and other sources** to trigger and probe a wide variety of ultrafast effects. The design features a normal-conducting electron energy booster in the straight-ahead FEL lines, enabling extreme photon energies and pulse powers for two end stations combining X-rays with high-energy lasers. **This will be a cutting-edge platform for studying matter in extreme conditions, for a range of applications.**

Emerging accelerator technologies such as plasma wakefield acceleration are integrated to ensure a long-term competitive edge beyond the initial design. An electron beam R&D line is included to provide a continuous source of novel electron and photon beam enhancements. The design also has potential to re-use the electron beam to efficiently support high energy physics studies.

Environmental sustainability has been built into the project from the start, giving the greatest opportunity to lock in long-term benefits. Over the course of the conceptual design study, work packages for each technical area have identified the most promising candidate technologies and techniques to improve environmental sustainability, feeding into a holistic study, which integrates and assesses all these factors.

Options analysis

Alongside the conceptual design, an options analysis has been undertaken to evaluate different options that could deliver UK access to next-generation XFEL capabilities by the 2040s. A comprehensive review of previous UK strategic exercises and the present XFEL landscape leads into identification and analysis of the primary investment routes. It includes:

- Assessment of the essential criteria
- A landscape analysis of XFEL activities, both national and international
- Definition and evaluation of possible investment options: (i) no additional investment, (ii) investment in an existing facility, (iii) investment to create a new facility
- A report on the socioeconomic impact of the investment options above

Summary

Next-generation XFELs present a strategic opportunity for the UK to leverage its scientific leadership to drive deep and wide-ranging impact across all areas of science and technology and major sectors of the economy, including all of the IS-8 growth-driving sectors. Access to such capability is vital for any leading economy: the UK can secure global leadership by hosting a new facility or co-developing an international project

While this project is a UK initiative, the aim of realising the next generation of XFELs is a truly international endeavour, towards which our many international collaborators are engaged. With their support, this set of documents set out a roadmap to an ambitious new generation of XFEL facilities that is robust and technically feasible. **Access to such sources would be transformational for the existing international light source user community, while attracting new generations of researchers across academia, industry, medicine and defence to solve emerging challenges.**

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