Science and Technology Facilities Council

UKXFEL
Science Overview and Conceptual Design Options Analysis

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Contents

Abstract

An advanced "next-generation" X-ray free electron laser (XFEL) facility would create key new opportunities across the sciences and in technology, help to answer pressing scientific questions, and contribute to solving societal challenges of major importance. The facility would generate myriad world-leading multidisciplinary advances. It would have a high impact in advancing technology, healthcare, frontiers of knowledge, net zero commitments and economic strengths, and provide a vital platform for creating a world-leading science and technology landscape in the UK. Following on from the Science Case (available at xfel.ac.uk), a three-year Conceptual Design and Options Analysis (CDOA) phase has begun; this is supported by the UKRI Infrastructure Fund and will run until October 2025. Here we highlight the opportunities emerging from the Science Case that inform the process and indicate the next steps and planned activities of the CDOA.

1. Introduction

Ultrafast X-rays from free electron lasers allow us to image the workings of matter at all relevant scales of both space and time. In common with neutron, synchrotron X-ray sources and electron microscopy, XFELs can establish the static structure of matter at the atomic scale. XFELs, however, are unique in that they can also allow us to follow the innumerable types of structural and electronic dynamics that are essential to understanding the workings of matter at the quantum scale, i.e. at their natural timescales of attoseconds to nanoseconds. They are therefore transformative in enabling the understanding and control of matter and technological processes at the quantum spatial and temporal scales.

In the Science Case we looked at how intense X-ray pulses from XFELs open new windows into the understanding of light and matter in the universe, making possible a range of new opportunities, such as: probing properties of matter in solar and planetary interiors; understanding the basic interaction physics between photons (i.e. X-rays and gamma rays) and matter; and even providing new tests of the Standard Model. High brightness X-rays can be used to develop new technologies, for example X-ray lithography to engineer devices on the nanometre scale. The energetic electron beam from the linear accelerator required to drive the X-ray laser can also be used directly to perform fundamental physics investigations, drive the world's brightest gamma ray source, and advance new accelerator technology.

Examples of big scientific questions that an advanced XFEL will be able to answer include:

- How do materials behave at the high pressures of planetary cores?
- How do enzyme-catalysed reactions occur in a living cell?
- How can we control states in quantum materials (e.g. superconductivity) with light?
- How do molecular machines efficiently cross energy barriers to drive biological processes?
- What are the charge dynamics during antibody-antigen molecular binding events?
- How do X-rays propagate in the interior of stars?
- How do liquids, like water, change and fluctuate at the nanoscopic scale?
- How can we optimally exploit quantum mechanics in solar and information technologies?

As well as underpinning a vast array of science, the capability and understanding delivered by an advanced XFEL will also be critical in advancing emerging technologies with great potential importance to UK industry and sovereign capability, including:

- developing fast, energy efficient, compact data storage
- optimising novel quantum sensors and quantum elements for quantum computing and information processing
- enabling quantum metrology of measurement science and powering the second quantum revolution
- advancing light harvesting, carbon capture with solar biofuel production, and energy storage technologies
- discovering advanced drugs, antibiotics and antivirals
- advancing catalysis and facilitating sustainable chemistry using Earth abundant elements
- designing advanced materials for use in defence, industry and nuclear energy

In the Science Case we explore how an XFEL facility with technically-leading **next-generation capabilities** could form an essential part of a science infrastructure landscape that serves the UK and ensures a vibrant, high technology, environment whilst building cutting-edge skills in the UK workforce. There is an excellent opportunity to internationalise the project, create a major global facility with capabilities and capacity to support ground-breaking science for the next half century. Below we briefly highlight some of the foreseen scientific advances that can be made with a next-generation XFEL capability.

2. The Science

2.1 Science Opportunities in Physics and X-ray Photonics

High intensity, ultrashort pulses of X-rays create new possibilities in physics and new potential in X-ray photonics that will find future application across the sciences. Here we consider new basic physics enabled by a transform limited high repetition rate XFEL, and the exciting science opportunities provided by the resulting innovative X-ray based measurement methods.

Frontiers in ultrafast chemical physics

Ultrafast X-ray probing using scattering and spectroscopy provides unprecedented insight into how energy and charge is transferred within and between molecules in processes such as photoexcitation or X-ray ionisation. Taking inspiration from non-linear optical spectroscopy techniques, and implementing them in the X-ray regime, will enable dynamic probing of electronic properties and how they couple to structural dynamics. These techniques will prove key in finding answers to questions such as how DNA responds to ionising radiation and how to control photophysical processes at the quantum level.

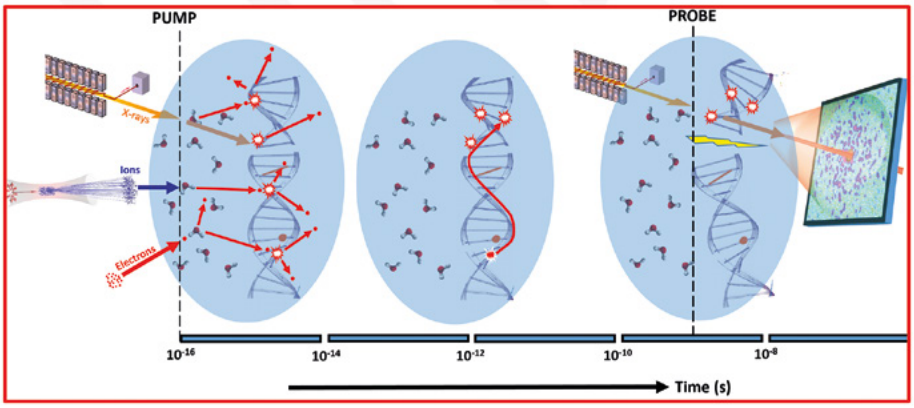

Figure 1: **Ultrafast X-rays** probe attosecond electron dynamics, radiation interaction with materials & biomolecules & elementary processes in chemical reactions

New concepts in scattering

The arrangement of atoms in matter and the motion of those atoms is fundamental for comprehension of the function of material systems. XFELs enable us to determine dynamic changes in structure, providing insight that will allow us to engineer molecular machines and devise new catalytic processes. By combining ultrafast X-ray scattering with novel ideas from quantum optics and scattering physics, we will be able to explore new physics, circumvent the phase problem that currently restricts imaging of matter, study samples that are too disordered or fragile for today’s technologies, and image important but elusive phenomena such as electron dynamics and coherent transport phenomena.

Attosecond science and non-linear X-ray spectroscopy

Electron dynamics, typically occurring on attosecond to femtosecond timescales, play a crucial role in a wide array of physical, biological and technological processes. High temporal resolution X-ray probes are essential to the understanding and harnessing of these processes, and will impact on knowledge and control of, for example, excitons in light harvesting systems, the primary steps in photocatalysis, advanced photodetectors and photodynamic therapy, and the development of future high speed electronic and photonic devices.

Capturing conformational dynamics and rare thermo-dynamic states

Chemical reactions catalysed by biomolecules and transformations between states of matter, such as crystallisation or phase transitions, progress via complex trajectories across rare thermodynamic states. Many of the transitions and fluctuations critical to these processes happen at timescales too fast to be captured by any existing methods. XFEL imaging methods, coupled to advanced data sorting algorithms, offer a unique way to capture these changes essential to understanding how, for instance, biomolecules function in their native state and deliver improved control of crystalline matter for the benefit of material science.

Non-linear X-ray physics and physics beyond the Standard Model with XFELs

With the development of high intensity X-ray lasers, we can explore new non-linear X-ray interaction physics in matter and with the quantum vacuum. The interaction physics of high intensity X-rays with matter is a largely unexplored problem and may open new avenues in nanoscale lithography and materials processing. High intensity X-rays open the door to using multi-photon interaction in ground-breaking precision tests of observables that are normally manifest only in very high-energy collisions. This may allow tests for deviations from the Standard Model of particle physics, while being far below the Planck scale of 10^{19} GeV that is beyond the direct reach of any particle accelerator.

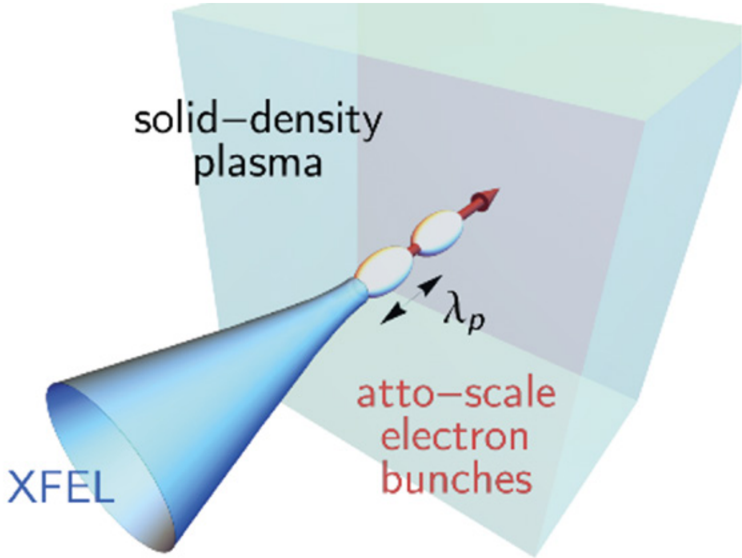

Figure 2: **High X-ray intensity and high data rate** allow exploration of fundamentals of X-ray matter interaction and new concepts in time resolved imaging at nanoscopic scale

High brightness relativistic electron beam science

Monoenergetic relativistic electron beams with low emittance, in addition to driving the XFEL, can also be used directly for new research. This research includes: electron beam-driven plasma wakefield acceleration (PWFA), a unique inverse Compton scattering gamma source, and opportunities to use the electron beam for fundamental physics experiments. The incorporation of plasma photocathodes in PWFA can boost electron energy and brightness, which can have a transformative impact on photon pulses produced by an advanced XFEL in a future phase. The gamma source would be a major research asset for nuclear science and the nuclear industry in the UK.

2.2 Science Opportunities for Matter in Extreme Conditions

Femtosecond X-ray pulses from XFELs coupled to state-of-the-art high energy/high power lasers enable the probing of the atomic and electronic structure of transiently produced extreme phases of matter in unprecedented detail. This provides new knowledge and understanding as to the behaviour and control of matter in widely diverse settings, including planetary interiors, stars, inertial confinement and in shocked engineering materials.

Shocked materials and matter at extremes

The experimental study of matter at extreme density, where ion cores overlap significantly and the electronic structure is unique to the high-density regime, holds the promise of breakthroughs in our understanding of both solid and liquid phases. The creation and study of such matter will enable us to describe, understand and predict what electrons and ions will do in other condensed matter systems, with direct relevance to exoplanetary science and engineering materials. It will also enable us to determine how matter might be manipulated in the future, to design new and improved materials that cannot be predicted by more traditional "evolutionary" methods.

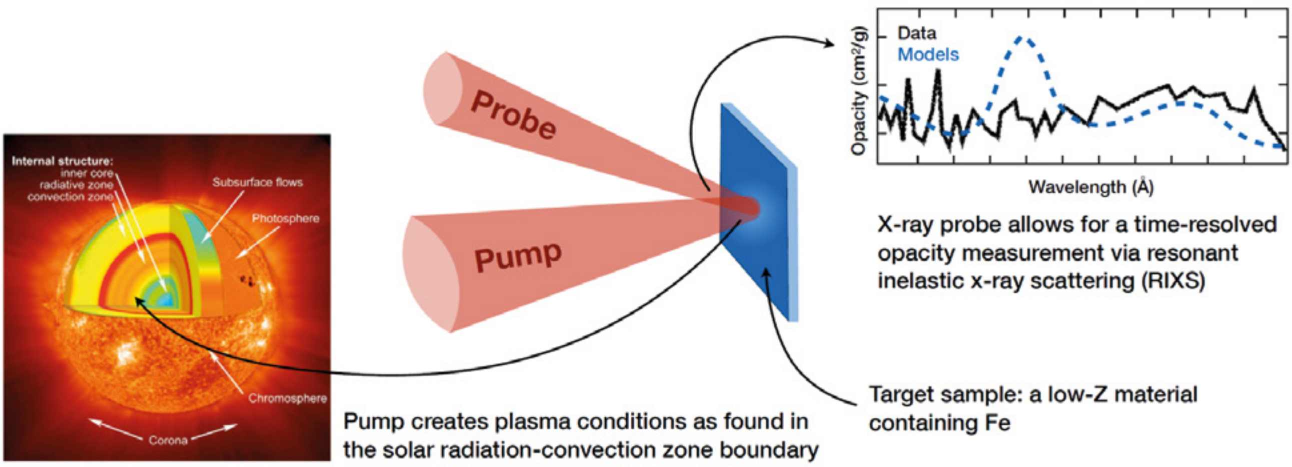

Figure 3: **High energy/power optical lasers and bright X-rays** access the conditions inside planets, stars and shocked materials in engineering, defence and fusion energy

Quantum plasmas: warm and hot dense matter

The overwhelming majority of the visible universe is in the plasma state, and extreme states of matter are routinely found in all astrophysical bodies from (exo)planets to stars. A comprehensive understanding of the structure and dynamics of such high energy density plasmas is thus of fundamental physical interest in its own right, but also forms the basis for progress in planetary physics, astrophysics, applications using laser-plasma interactions to generate compact radiation sources, and in providing the foundation to laser-based fusion energy. High temporal resolution X-ray probes, synchronized with high-energy drivers, will allow us to create these extreme conditions in a controlled laboratory setting and probe them on the fundamental temporal and spatial scales.

X-ray interactions with laser accelerated electrons

By utilising compact, laser-driven, plasma-based accelerators we can generate X-ray and gamma ray sources synchronised with the X-rays available from the XFEL. Combining relativistic electron and XFEL sources would enable new science, for example allowing us to probe warm dense states, to access the extreme science of fundamental particle interactions, and to test the fundamental theories of quantum electrodynamics.

Coupling an XFEL to a laser-driven spherical compression facility

The potential coupling of a laser-driven spherical-compression facility to a sufficiently hard X-ray FEL would enable the diagnosis of extreme states of matter in unprecedented detail, leading to further advances both in the optimisation of fusion energy and our understanding of the universe. This would be a transformative marriage of technologies that would be globally unique, enabling the UK to attain a leadership position in the associated science, technology, and engineering.

2.3 Science Opportunities in Quantum and Nanomaterials

Quantum and nanomaterials represent an important class of materials that contain fascinating new physics and have the potential to enable disruptive technologies for devices and in energy applications. Transform limited, high repetition rate X-ray pulses, coupled to optical sources from the deep UV to the THz, will uncover the physics and harness these technology opportunities.

Magnetic materials and control of ultrafast magnetisation

Ultrafast photo-excitation 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. For example, the method of time-resolved resonant inelastic X-ray scattering (trRIXS) is a powerful way of measuring charge, spin and orbital excitations. These excitations encode the correlations and interactions that determine the detailed properties of the generated states and the deeper understanding that can be obtained will advance the technology of, for instance, fast, energy efficient, data storage.

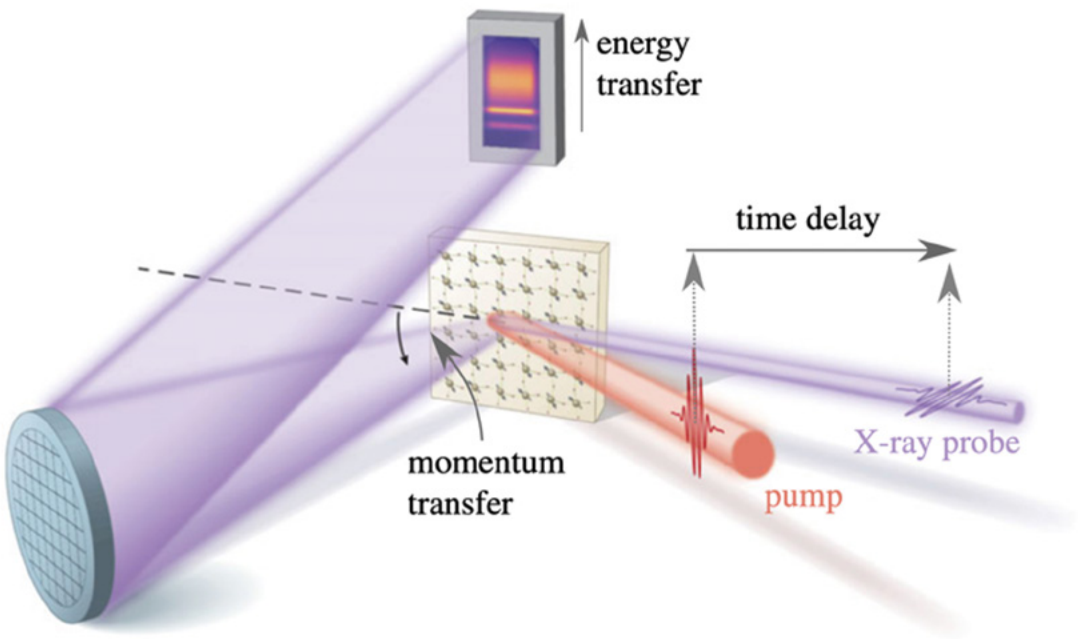

Figure 4: **Transform limited X-rays and high data rates** enable probing and optimisation of quantum materials, ultrafast magnetisation and functional materials

Structural dynamics and light induced phases in quantum materials

The transient modification of structure in quantum materials by femtosecond pulses of laser light can induce new properties that do not appear in equilibrium. Coupling with an ultrafast X-ray probe can provide unprecedented insight into how electrons, phonons and spins interact to determine the properties of materials, such as magnetism, insulator-metal transitions and superconductivity. Light can be used to manipulate these interactions effectively and efficiently, and ultrafast X-rays used to probe the outcome in order to control material properties, with high potential impact.

Imaging dynamics in nanomaterials

The ability to directly image, in three-dimensions, time varying phenomena in nanoscale materials at the surface and in the bulk can greatly increase our understanding of how novel phases develop and how they influence the material properties. Coherent diffractive imaging (CDI) is a form of microscopy that can permit high resolution imaging, where the use of conventional optics is not feasible. When combined with ultrafast X-rays, time-resolved Bragg CDI provides a novel and robust means to image ordered material systems with sub-ångstrom sensitivity. Such insight will greatly aid our understanding of the dynamical response of nanomaterials and will serve as a platform to develop next-generation materials and devices.

Electronic dynamics in quantum materials

Ultrafast photoelectron spectroscopy (PES) is an enabling technique to provide insight into spin, orbital and charge degrees of freedom of chemical bonding characteristics in quantum materials. PES and other spectroscopy techniques with ultrafast X-rays will provide much needed answers to questions related to localised quantum state dynamic behaviour on the femto- and attosecond timescale, capturing electronic behaviour in real time and allowing access to the real-time function of materials and high-speed electronic devices.

Time resolved pair distribution functions

Persistent disorder in quantum materials can appear in various forms, including chemical, electronic, magnetic and geometric. Correlations present within the disorder often give rise to novel phases in the physical and chemical properties of quantum materials. Pair Distribution Function (PDF) measurements are able to probe disorder and, when performed with ultrafast X-rays, provide a potent method to identify the symmetry breaking transitions.

2.4 Science Opportunities in the Chemical Sciences and Energy

Virtually any chemical reaction, regardless of the means of its initiation, is enabled and accompanied by simultaneously occurring structural changes. These changes range from the complete dissociation of a chemical bond to subtle fluctuations in local geometries accompanied by changes in electronic structure and spin-state. XFELs operating across the X-ray energy range, coupled with tightly synchronised optical, EM field and particle sources, will give unique and incisive access to these dynamics, which is vital to scientific understanding and myriad applications of chemistry to real-world applications.

Fundamentals of reaction dynamics: Coupling between nuclear, electronic and spin degrees of freedom

Chemical dynamics encompasses the entanglement of phenomena across multiple timescales, from femtoseconds (a vibrational period of a chemical bond) to seconds (full cycle of photosynthesis), involving structural, electronic and spin states evolving together. An advanced XFEL source will bring a combination of sufficiently short pulses of photons, with energies tuneable from THz to X-ray, sufficiently high repetition rate of > 100 kHz, high spectral purity, and high brightness of 10^{12} photons/pulse, to enable a comprehensive interrogation of chemical reactions, non-equilibrium processes, and transformations.

Exploring complex energy landscapes through chemical activation

Physical, chemical and biological processes are all governed by interactions across complex potential energy surfaces. Understanding these surfaces is fundamentally important for everything from chemical reactivity and protein folding, through to crystal structure prediction and developing new materials and pharmaceuticals. Ultrafast X-rays synchronised with a variety of excitation modes (optical, THz, electrons) will enable us to understand these surfaces in ever greater detail, across multiple length and time scales, and will permit us to demonstrate control over the electronic, spin and ionic degrees of freedom of a material, to engineer transient states of matter far from equilibrium, regulate transitions across barriers, and explore new phases and materials with exotic and novel properties.

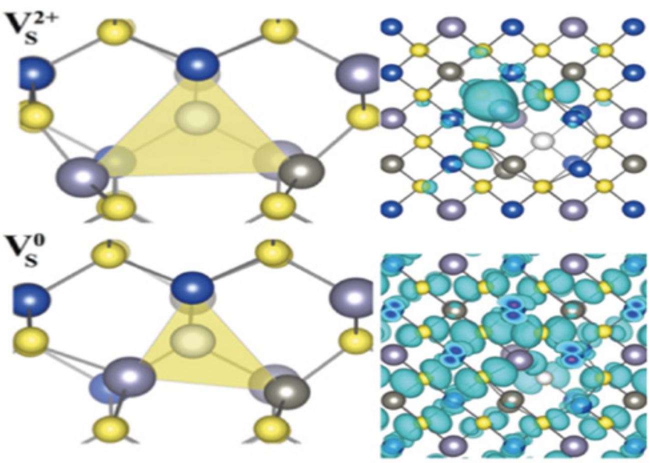

Figure 5: **X-rays synchronized to ultrafast lasers, THz and electrons** uncover the fundamentals of chemical dynamics in the environment, space and energy materials

Energy materials and devices: Solar cells and batteries

Our energy systems are rapidly evolving, driven by the challenges associated with decarbonisation, an ageing infrastructure, geopolitical pressures, and shifts in societal expectations. Achieving a radical shift in how we supply, manage and consume energy calls for new materials and a detailed understanding of how they function. Yet in many energy technologies there remain fundamental processes related to function that we simply do not understand, and this is severely impeding progress. Ultrafast X-ray probing will provide unprecedented insight into the function of materials on the atomic scale of time (femtosecond) and length (ångströms), leading to a greatly improved understanding of structure-function relationships in materials for optimisation of energy applications.

Understanding catalysis

Although catalysts are often the key to invaluable chemical and biochemical processes, their complex and elusive nature has by and large defied our current abilities to characterise and understand their microscopic action. This situation has partly arisen from the very fast timescales involved in their role as agents of chemical action, which are faster than conventional characterisation capabilities. The recent developments in femtosecond XFEL technology and instrumentation have finally opened the door on this fascinating research area, and we now have an unprecedented opportunity to capture the behaviour of catalysts in their active state. These developments are now expected to deliver on the long-standing dream of catalyst by design, as opposed to trial and error.

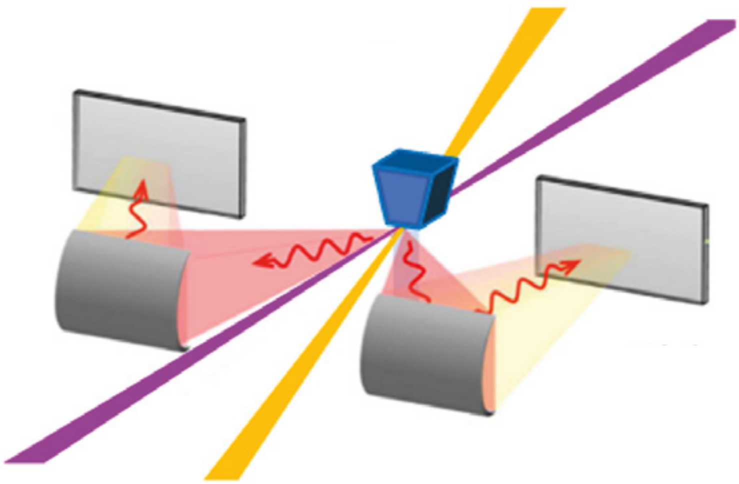

Figure 6: **High rep-rate multi-colour ultrafast X-rays** provide powerful approaches to systematic advances in catalysis

2.5 Science Opportunities in the Life Sciences

XFEL uses in the life sciences include serial femtosecond crystallography (SFX), time-resolved SFX and time-resolved single particle imaging. In many cases, especially with metal-dependent systems, complementary spectroscopic information can also be collected from the same samples and X-ray pulses, providing even more detailed mechanistic insights. Structure-functional results will translate into better drugs and treatments impacting human health, and better catalysis for clean energy and agriculture. A frontier opportunity made possible by high repetition rates of X-rays, samples and detectors is to extend single particle imaging methods of biomolecules in solution, so that nearly all dynamic processes in biology can be studied with high temporal and spatial resolution.

Serial femtosecond crystallography enabled by XFELs – a new era in structural biology

Serial crystallography presents a revolutionary opportunity to solve structures from slurries of nano- to micron-size crystals. The high brightness and tight focus of the XFEL beam enables a diffract-before-destroy methodology that rapidly reveals structures from samples at physiological conditions.

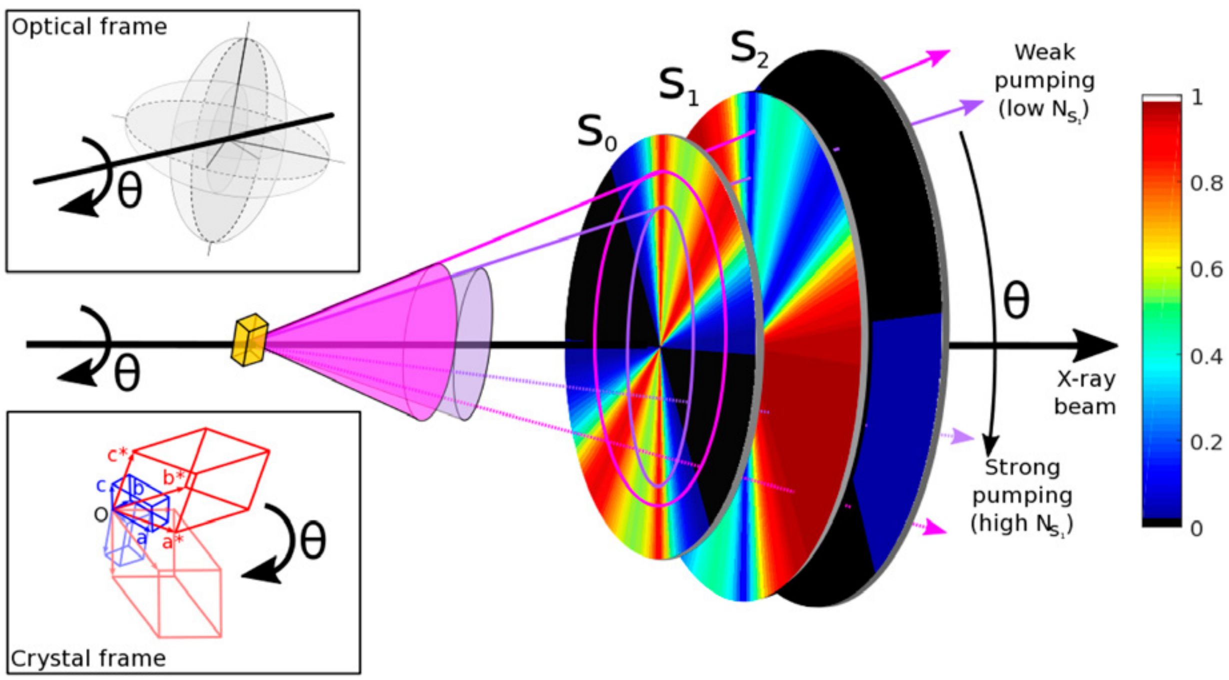

Figure 7: **Controlled X-rays and samples** will extend the power of serial femtosecond nanocrystallography for advancing knowledge and drug discovery

Dynamic structural biology: Photosensitive systems

A remaining frontier challenge of structural biology is to determine time-resolved structures at atomic resolution directly from systems engaged in function, at physiological temperatures and pressures. XFEL methods coupled with pump-probe strategies are making important advances towards this goal.

Dynamic structural biology: Molecular movies of enzyme catalysis

Dynamic structural biology applies a set of tools to collect as much data as possible, from every sample and every X-ray pulse, at physiological temperature and pressure, with an aim to create time-resolved molecular movies of macromolecules engaged in function. Time-resolved SFX studies exploiting mixing methods are generalisable and have significant potential for revealing the dynamics of enzyme catalysis in broad context across biology.

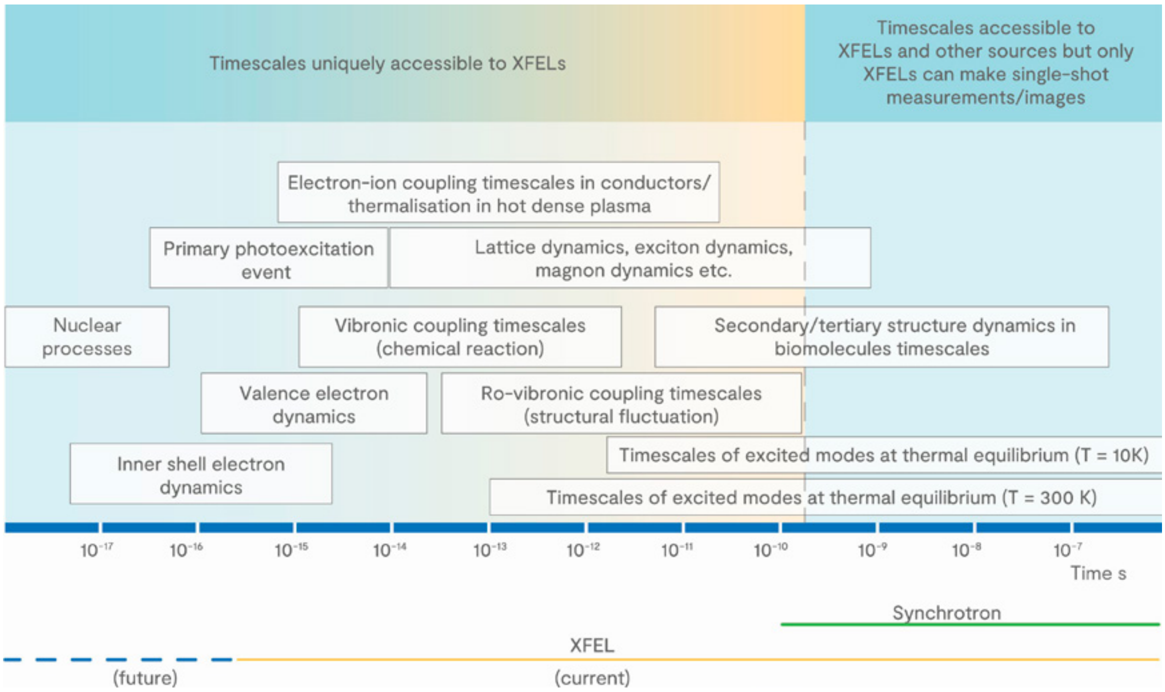

Figure 8: XFELs provide unique access to the structure and dynamics of matter at the quantum scale: nanometre spatial and ultrafast temporal scales

Controlling and measuring nuclear and electronic coherence within biological systems

Some photo-induced biochemical processes are so fast that nuclear and electronic quantum coherence are believed to have a role. XFELs are offering a new incisive window into this behaviour.

2.6 Opportunities for UK Industry, Society and Defence

Measurement of processes at their essential length and time scales made possible by an advanced XFEL is immensely important to advancing technology, as well as science. Key sectors of industry and manufacturing, such as engineering, advanced materials, chemicals, medicines/pharmaceuticals, consumer/household products, food, automotive, energy, agriculture and electronics, will substantially benefit from these advances, with societal impact in healthcare, environment, transport and defence.

Properties of shocked materials for engineering and defence

The properties of materials under shock loading conditions are both of fundamental scientific interest and important across a wide range of engineering domains, from aerospace through to defence. XFEL technology is driving rapid progress in the underpinning science in this area, and represents an accelerated pathway for the manufacturing and qualification of the next generation of engineering materials and processes.

Nucleation, solidification and crystallisation in soft-matter

Consumer product, chemical and pharmaceutical manufacturing are part of the chemistry-using industries and make a gross value-added (GVA) annual contribution of more than £65 billion to the UK economy. The properties of organic crystalline solids in particular present enormous industrial R&D challenges, because key transformations are poorly understood at the molecular level. These include, for example, nucleation, crystal growth, dissolution and agglomeration. For decades, the science of these phenomena has been slow due to the experimental challenges of localised spatiotemporally rare events. The time and imaging capabilities afforded by XFEL scattering and spectroscopies now open up a realistic perspective to progress in this area.

Dynamic processes in additive manufacturing, combustion, laser machining and photolithography

Various advanced technologies vital to the manufacturing base, including friction welding, additive manufacturing and laser machining, require an understanding of microstructural phenomena frequently occurring at fast timescales. XFELs offer probing capabilities that surpass the current state-of-the-art and allow these processes to be followed from milliseconds to sub-picosecond timescales. Soft X-ray/extreme UV pulses of high brightness from a high repetition rate XFEL may lead to new prospects in matching Moore's law with nanometre scale resolution photolithography.

Industrial inspirations from deeper insights into biology: Pharma to clean energy

Industrial XFEL users in life science want faster, better structures from smaller samples. They demand reliability and automation, especially for proprietary R&D efforts. Industry is already using Diamond and eBIC extensively, and starting to explore options at XFELs. They are watching for developments in cryo-EM, serial crystallography and time-resolved studies that couple structure and function from the same sample. New opportunities for drug discovery impacting human health are profound and progress has recently been demonstrated with serial femtosecond crystallography (SFX) results on several membrane proteins involved in cell signalling. Time-resolved SFX results targeting photosystem II, hydrogenases, and nitrogenases promise molecular level insights that will inspire the next generation of solar and full cells, and green catalysts to convert N_2 into fertilizer.

Gamma source application in nuclear security and materials in nuclear industry

With the globally unique quality and quantity of gamma production from an inverse Compton scattering source as part of the facility as outlined in the Science Case, a number of techniques of great value to nuclear security and industry sectors will become possible. Impact would be in the fields of nuclear waste management, nuclear forensics such as active nuclear materials and contraband detection, and medical isotope production. Further applications may include treaty verification and stockpile stewardship.

3. A Next-Generation XFEL

The key capabilities identified in the Science Case for a next-generation XFEL are:

- transform limited operation across entire X-ray range (pulse durations ranging from 100 as to 100 fs)
- even spaced high-rep rate pulses to match samples and detectors (rep-rates > 100 kHz in SXR, > 1 kHz HXR)
- improved synchronisation/timing data with external lasers (to < 1 fs)
- multiple colour X-rays to deliver simultaneously to one end-station or in parallel to multiple end-stations
- full array of synchronised sources and detectors: DC to mm-waves, mm-waves to THz, XUV - THz, e beams, high power and high energy lasers at high rep-rate

The Science Case explains the far-reaching science and technology opportunities that would be delivered with an advanced XFEL. The purpose of the conceptual design process beginning now is to establish a self-consistent technical solution that will deliver the challenging next-generation capability whilst incorporating a wide array of unique features, which will ensure a facility that will be both world-leading and able to tackle the most challenging research problems.

A next-generation XFEL can be designed to be a world-leading facility by integrating, in an optimised way, some of the exciting new developments emerging across the accelerator and X-ray science landscape. This will ensure the highest quality and most versatile X-ray specifications, e.g. by moving beyond conventional X-ray generation schemes and exploiting developments in laser seeding, attosecond operation, and high brightness modes, to approach transform limited X-ray pulses of high spectral purity and brightness, and unprecedented temporal resolution. High repetition rate in the soft X-ray range, and moderately high repetition rate over the hard X-ray range, is a powerful combination and this would be both world-leading and cost effective. Access to the most advanced radiation sources (e.g. terahertz (THz), ultrafast laser and high harmonic generation (HHG)), relativistic electrons (from laser wakefield acceleration (LWFA)) and other charged particle beams to arrive synchronized to the X-rays at the interaction point, will allow for a wide range of unique science. Direct use of the high-quality relativistic electron beam can be harnessed to advance accelerator science (e.g. plasma wakefield accelerators) and deliver a gamma source brighter than any in the world, with substantial benefits to nuclear science and UK industry. Detector and sample delivery of the highest calibre will be developed alongside the light sources to provide best-in-the-world performance, with the best data handling and data science developments available to support the most advanced analysis. There is a timely opportunity to develop a world-leading XFEL facility with beyond state-of-the-art capability, to innovatively tackle vital science and technology challenges.

4. National and International Context

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, South Korea and China. XFELs are now recognised as indispensable to the development of new technologies where the quantum scale structural dynamics of matter must be understood and exploited. A primary driver for the Linac Coherent Light Source (LCLS) II in the USA has been its fundamental contribution to the Department of Energy's mission, most critically in Basic Energy Sciences, but also in National Security Science and aspects of the missions of other major agencies within the USA, including the National Institutes of Health (NIH) and the National Science Foundation (NSF). Similarly, the other international XFELs are seen as making essential contributions to science and to future economic and national strength. The new science and technology enabled by an advanced UK XFEL will boost national research priorities, through addressing the key challenges in the AI & Data Economy, Clean Growth, Future of Mobility and an Ageing Society. A strong alignment to the highest priorities in the UKRI strategy is identified in the Science Case.

The transformative capabilities brought about by an advanced XFEL are in real-time imaging and measurement at the quantum scale that will underpin many future technological and scientific advances and developments in human health. No single technology, however, will solve all scientific problems. The solution to the challenges we face now, and the yet unforeseen challenges we will face in the future, will inevitably require a combination of technologies. An XFEL should be seen as an essential component in a wide-suite of capabilities that includes for example; lasers, spectroscopy, mass spectrometry, cryo-EM, synchrotron X-rays, ultrafast electron diffraction and neutrons. We further discuss these synergies in the Science Case.

A survey of research groups in the UK in 2019 indicated that over 500 UK scientists have had active involvement in XFEL science in the last decade and that number is growing steadily. A huge advantage can be gained by developing a UK-based XFEL facility optimised with the most advanced features matched to our needs, ensuring long-term access and control, as well as direct benefits to the UK economy. To allow the facility to deliver the fullest range of the potential science and technology, ease of accessibility for individual users, and for new user communities, is a critically important issue.

We are, through the CDOA, engaging with leading XFELs around the world to explore how the ambitious science identified in the Science Case can be delivered fully or in-part by partnering in future developments with them, whilst in parallel developing a conceptual design for a wholly new next-generation XFEL facility.

5. Conceptual Design and Options Analysis

In the Science Case, we discuss the main scientific opportunities as currently foreseen and identify the capabilities required to realise these opportunities.

An important part of the work of the current phase of the project, funded by the UKRI Infrastructure Fund, is to deliver a **Conceptual Design** for an advanced "next-generation XFEL" that can deliver on all of the science opportunities identified in the Science Case. This will be coupled to an **Options Analysis** that will undertake a rigorous study of all options to deliver the scientific opportunities identified in the Science Case. This includes building a unique new XFEL in the UK, as well as looking at what can be done through partnerships with existing XFEL facilities around the world, e.g. European XFEL, Germany, and LCLS, USA, to provide the technical capability to satisfy the greater part of the scientific need identified in the Science Case. Included in this analysis is the potential to develop the "next-generation XFEL" as a globally integrated facility that satisfies both future UK and international need.

The CDOA Project Sponsor is Professor John Collier, Director of the Central Laser Facility at the Rutherford Appleton Laboratory; to deliver the detailed technical work, we have formed a team of accelerator and X-ray scientists primarily based at the Daresbury Laboratory, led by Professor Jim Clarke with Dr Paul Aden as the Project Manager. Members of this team are already engaged in detailed technical discussions with, for example, European XFEL and LCLS. In parallel we have expanded the science team, and with Professor Jon Marangos as the science lead, they are charged with producing an updated Science Case to be delivered in 2025. We are seeking to broaden consultation and engagement with the full diversity of UK/overseas scientists, industry and institutions. This will be accomplished in part through a series of workshops on Science and Technology that will be held around the UK over the next two years.

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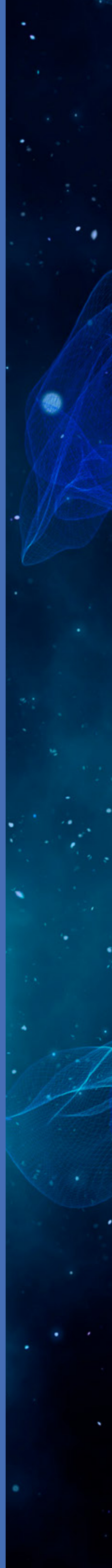

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