Science and Technology Facilities Council

UK XFEL Science Case

Executive Summary

The production team for the UK XFEL Science Case was as follows:

Editor: Jon Marangos

STFC Sponsor: John Collier

Production: Tracey Burge, Andrew Collins, James Green and Jon Marangos

Authors from the Science Team:

Andrew Burnett, Marco Borghesi, Andrew Comley, Mark Dean, Sofia Diaz-Moreno, David Dye, Jason Greenwood, Andrew Higginbotham, Adam Kirrander, Jon Marangos, Malcolm McMahon, Russell Minns, Marcus Newton, Allen Orville, Thomas Penfold, Anna Regoutz, Ian Robinson, David Rugg, Sven Schroeder, Jasper van Thor, Sam Vinko, Simon Wall, Justin Wark, Julia Weinstein, Amelle Zair and Xiaodong Zhang

Facility Science and Technology

Jim Clarke, John Collier, Louise Cowie, David Dunning, James Green,
Neil Thompson and Peter Williams

Additional contributing authors

Massimo Altarelli, Frederico Alves Lima, Moatez Attallah, Shakil Awan, Stuart Bartlett, James Baxter, Uwe Bergmann, Tom Blackburn, Rebecca Boll, Stefano Bonetti, Christian Bressler, Bill Brocklesby, Colin Brown, Will Bryan, Phillip Bucksbaum, Richard Catlow, Roy Chantrell, Aina Cohen, Simon Coles, James Cryan, Georgi Dakovski, Sarnjeet Dhesi, John Dyke, Daniel Eakins, Gwyndaf Evans, Michael Foerst, Leszek Frasinski, Gianluca Gregori, Markus Guehr, Fahim Habib, Dave Hall, Samar Hasnain, Thomas Heinzl, Bernhard Hidding, Simon Hooker, Nils Huse, Olof Johansson, David Keen, Premysl Kolorenc, Adrian Mancuso, Stuart Mangles, Mattias Marklund, Steve Matthews, Stewart McWilliams, Martin McCoustra, Paul McKenna, Christopher Milne, Henrike Mueller-Werkmeister, Shaul Mukamel, James Naismith, Keith Nelson, Abbas Ourmazd, Robin Owen, Foivos Perakis, Paolo Radaelli, Dave Riley, Alex Robinson, John Rodenberg, Nina Rohringer, Kai Rossnagel, Marco Ruberti, Christopher Russo, Charlotte Sanders, Marcus Scheck, Paul Scherkl, Christopher Schofield, Robbie Scott, Edward Snell, Emma Springate, David Stuart, Geoff Thornton, Joachim von Zanthier, Martin Walsh, Mark Warren, Peter Weber, Philippe Wernet and Junko Yano

Contents

Appendices

Glossary

ARPES	Angle-resolved Photoemission Spectroscopy
CDI	Coherent Diffractive Imaging
CLF	Central Laser Facility
Cryo-EM	Cryogenic Electron Microscopy
ESCA	Electron Spectroscopy for Chemical Analysis
EUV /XUV	Extreme Ultraviolet (20 - 200 eV)
EXAFS	Extended X-ray Absorption Fine Structure
HAXPES	Hard X-ray Photoelectron Spectroscopy
HED	High Energy Density
HHG	High Harmonic Generation
HXR	Hard X-ray (4 keV - 100 keV)
ICS	Inverse Compton Scattering
IR	Infrared
Linac	Linear Accelerator
LWFA	Laser Wakefield Acceleration
MX	Macromolecular Crystallography
NC	Normal Conducting
ODL	Orbital Degeneracy Lifting
PDF	Pair Distribution Function
PWFA	Plasma Wakefield Acceleration
QED	Quantum Electro-Dynamics
RAL	Rutherford Appleton Laboratory
RIXS	Resonant Inelastic X-ray Scattering
SASE	Self-amplified Spontaneous Emission
SC	Super Conducting
SCO	Spin-crossover
SFX	Serial Femtosecond Crystallography
STFC	Science and Technology Facilities Council
SXR	Soft X-ray (200 - 4 keV)
THz	Terahertz (10^{12} Hz)
UED	Ultrafast Electron Diffraction
UKRI	UK Research and Innovation
UV	Ultraviolet
VUV	Vacuum Ultraviolet (10 - 20 eV)
WAXS	Wide Angle X-ray Scattering
WDM	Warm Dense Matter
XANES	X-ray Absorption Near Edge Structure
XAS	X-ray Absorption Spectroscopy
XES	X-ray Emission Spectroscopy
XFEL	X-ray Free Electron Laser
XFELO	XFEL Oscillator
XPCS	X-ray Photon Correlation Spectroscopy
XPS	X-ray Photoelectron Spectroscopy

Units

Time

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

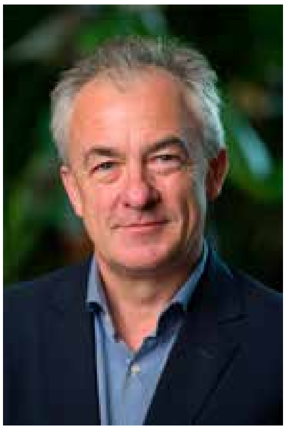
Ångstrom	1 Å = 10^{-10} m
Nanometre	1 nm = 10^{-9} m

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}

> “The question that the current UK XFEL Science Case seeks to address is how, over the coming decades, will the technological and scientific opportunities enabled by XFELs develop and what specific impact might there be from a UK machine aimed at offering new capabilities beyond those that exist today.”

Foreword



The world's first X-ray free electron laser (XFEL) began operation in 2009 at Stanford, USA. In the following decade these machines have proven a powerful new tool for science. Using time resolved X ray methods, spectroscopy and scattering, they give a unique window into the structural and electronic dynamics of matter at the nanoscopic scale, imperative to further our understanding of critical natural processes in diverse settings from stellar and planetary cores, to biomolecules and chemical reactions, and to the development of new technologies based upon this understanding. There are now five XFELs operating in the world that have pioneered the application of new techniques across life, physical, chemical and material sciences, and generated important and transformative results. The UK is partner with one of these machine, the European XFEL in Hamburg operating since 2017, and UK users are active at all the other facilities. Although already proving highly impactful, XFELs are only at the beginning of their trajectory, and new capabilities are emerging that may prove still more significant. The question that the current UK XFEL Science Case seeks to address is how, over the coming decades, will the technological and scientific opportunities enabled by XFELs develop and what specific impact might there be from a UK machine aimed at offering new capabilities beyond those that exist today.

The process of preparing this Science Case began around a year ago with a broad-based community consultation that gathered data and ideas through a series on workshops involving key national and international scientists. The science team, comprising 25 scientific experts across a wide spectrum of fields and led by Prof. Jon Marangos of Imperial College, then distilled this input to form the current case. They were assisted by the expertise of 80 additional authors from the UK and overseas who contributed to the document. The intention is to look forward to what new capabilities a machine operating from around 2030 might be able to deliver. In the process the team drew on the expertise of the UK accelerator science and laser communities to identify a feasible set of advanced specifications that go beyond those currently available. The present case will now be shared with the UK scientific community and will be reviewed by external experts to establish whether or not there is a scientific "Mission Need" for such a machine. The establishment of "Mission Need" would then initiate a conceptual design study to examine the technical and financial feasibility of a UK XFEL.

The UK XFEL Science Case was developed through interaction with the UK scientific and technology communities and so it is natural now to share this output with those communities. It is hoped that this will enable further discussion informed by the substantial case now available for public examination and engagement. It is also hoped that this report will help to broaden the discussion to include other potential stakeholders in industry, academia, learned societies and government. A series of webinars will be held over the coming few months to present the main features of the case and to promote discussion. It is hoped that this will add to the Science Case and build a wider community support as well as promoting the wide benefits to science and technology that can be delivered by XFELs.

Professor Mark Thomson

Executive Chair, Science and Technology Facilities Council

1. UK XFEL Science Case – Executive Summary

An advanced X-ray free electron laser facility in the UK 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 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 in creating a world-leading science and technology landscape in the UK, which will support advanced innovation. The facility would prove a vital resource for achieving step-changes in science and technology that address urgent societal challenges, e.g. in combating viral pandemics and attaining carbon neutrality and sustainability.

In this Science Case we address how construction of a UK X-ray free electron laser (XFEL) facility would create a national economic and industrial stimulus, forming an essential part of a science infrastructure landscape that ensures a vibrant, high technology environment, and helping to build and retain cutting-edge skills in the UK workforce. A UK XFEL will uphold national competitiveness in science, secure sovereign capabilities and grow new technologies of key importance to industry, healthcare and defence. We identify a path to create an XFEL infrastructure delivering a step-change in capability that will thrust UK science and technology ahead internationally in many vital areas.

The chief motivations for building a UK XFEL are:

- Unique X-ray and coupled capabilities can be optimised to create an ambitious, world-leading, UK XFEL for tackling emerging scientific and societal challenges
- Reinforces the UK as a centre for the most advanced science and innovation and will attract the best minds and boost skills in the national workforce
- Secures direct benefits to the UK economy from construction, procurement and operation, with high potential for levelling up R&D across the UK
- The UK will retain full control over the science and technology programme, and safeguard future sovereign capabilities and advances for industry, healthcare and defence.

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 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.

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, at their natural timescales of attoseconds to nanoseconds. They are therefore transformative in enabling the understanding and control of matter at the quantum *spatial* and *temporal* scales.

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 in the UK 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?
- 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 UK XFEL will also be critical in the advancement of 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 information processing
- 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.

The new science and technology enabled by an advanced UK XFEL will boost delivery of the **UK government's Industrial Strategy**, through addressing the key challenges of **AI & Data Economy**, **Clean Growth**, **Future of Mobility** and an **Ageing Society**. For example, this facility will generate vast amounts of data that will require the development of cutting edge concepts to efficiently process, and so the UK XFEL will be a pioneering environment and incubator for new ideas in **Data, AI and Machine Learning** that can quickly propagate into the wider economy, along with the large numbers of highly trained scientists and engineers whose skills will be honed at the facility. In parallel to the Industrial Strategy, it will also address the themes integral to the **UKRI Strategy**. **Advancing technology** is addressed through the boost provided by space and time resolved understanding, leading to the development of new energy, data, nuclear and materials technologies. **Healthcare** is furthered by the profound advances in understanding of biochemical and biomolecular function, which allows better guidance in developing drugs and therapies. **Frontiers of knowledge** are advanced 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. **Net zero commitments** are underpinned by the space and time resolved data that is essential to developing sustainable approaches to catalysis, optimised combustion, carbon capture, and understanding the action of pollutants and particulates in the environment. In this latter area, the UK XFEL's mission resonates directly with the **UK government's Clean Growth Strategy**. Together these capabilities combine to boost **Economic strengths** as well as provide vital sovereign capabilities for the defence and the wellbeing of the nation.

In this Science Case, we explain these far-reaching science and technology opportunities, and detail how an advanced UK XFEL would deliver these opportunities. We outline ambitious XFEL facility options of realistic scale for the UK that would achieve this. The outline design options (an example is shown in **Figure 1.1** below) incorporate a wide array of unique features, in terms of the X-ray and accompanying capabilities, which will ensure a facility that will be both world-leading and able to tackle the most challenging research problems.

The international landscape of X-ray sources – synchrotron and XFEL – has seen rapid advances in the last decade. XFELs are now established in the USA, Germany, Switzerland, Italy, Japan, South Korea and China, with multiple sources being planned at other locations. Similar growth has been seen with high brightness synchrotrons and, with the planned Diamond-II, the UK will maintain a strong presence in that technology and its application to increase understanding of the static structure of matter. What the UK must also secure is the capability for performing the most advanced time-resolved science that goes beyond the partial capabilities offered by ultrafast lasers, ultrafast electron diffraction and petawatt lasers. For this we will need extensive access to the very best XFEL facilities. A survey of research groups in the UK indicates that over 500 UK scientists have had active involvement in XFEL science in the last decade and the number is growing steadily. A huge advantage can be gained by developing a UK 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.

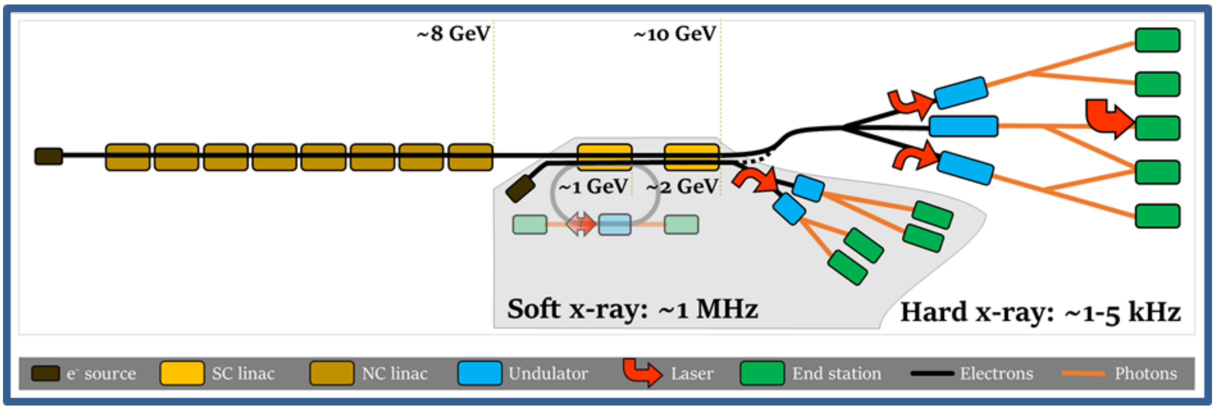


Figure 1.1: An outline design of one potential configuration with a unique combination of capabilities, able to deliver the science discussed in this case

We show that a UK 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 ensures 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 world-leading 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.

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. In part, this can be addressed by designing appropriate technical configurations of instruments, end stations and data systems into the facility from the outset. The possibility of conducting experiments solely via user supplied samples, without on-site users, will be developed in scientific areas that are currently at an advanced level of technical maturity, such as serial nano-crystallography. This approach will significantly boost throughput and lower the threshold to access. The second part of the solution to lowering barriers to access will lie with offering improved training and support for new users, in order to develop, and widely propagate, the required expertise to use the facility effectively. We recommend that work on this should start now, building on the actions already undertaken by the Life and Physical Sciences Hubs at Harwell that currently support UK access. Related actions, such as establishing dedicated Centres for Doctoral Training across a variety of science areas, should be undertaken with urgency. These measures are important to ensure readiness for a UK XFEL facility, but equally will allow UK science to successfully compete in using the existing international XFELs.

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.

The UK benefits from membership of the European XFEL in Hamburg. We must continue as a full member of this organisation, as this facility will remain one of the world's premier XFELs. In the longer term, the planned UK XFEL would deliver new capability beyond that at any existing facility and would remain complementary to the European XFEL. UK engagement with European science is likely to be maintained, but not substantially grow, over the coming decades. Clearly, we are now having to rethink strategies for protecting our best interests across a wide range of science and technology capabilities as geopolitical alignments evolve. **Secured access to the best XFEL facilities** is vital for ensuring, in the long-term, **sovereign** and **industrially critical capabilities**. A key advantage of building a UK XFEL infrastructure of international class is that it will ensure UK access to that capability, whilst being **a beacon to scientists from around the world** and a **catalyst for growing international collaborations**.

The direct national economic benefits of constructing and hosting a large scientific infrastructure in one's own country are substantial and well documented. Further benefits lie in opportunities for **greatly expanding the skills base in the UK workforce**, from PhDs and engineers, to technicians and apprentices. A UK XFEL would boost skills and attract and retain talent in areas critical to the economy, such as advanced electronics and control systems, optics, hardware and software for handling unprecedented data volumes, precision engineering and advanced manufacturing. The importance to future **key sovereign and industrial capabilities**, only available if we have **full control** on all decisions, must be at the core of making our plans. Without a UK XFEL programme, there is high risk of lost science and technology opportunities and, worse still, of a loss of skills in academia and industry and an accelerated brain drain. Building an XFEL is an essential part of a national strategy that ensures **we remain a technology maker**, and do not become merely a technology taker.

We should compare the current situation to that of the New Light Source (NLS) project in 2008-10, where high technical risks (*will XFELs work*?) and scientific risks (*will XFELs make a significant scientific impact*?) were seen. This encouraged a risk averse strategy, and led the UK to do nothing at the time. Now the situation is reversed. Today, the technical and scientific risks are looking low: these machines *work* and they *produce copious quantities of great science*. A 'do nothing' or a 'do little' strategy is now the riskiest (as we discuss in **Section 9**) and could severely damage national competitiveness, technology and sovereign capability, and scientific standing. The more ambitious the machine, the lower the future risks to UK science and technology.

In this Science Case, we discuss the main scientific opportunities as currently foreseen and identify the capabilities required to realise these opportunities. We recommend that the most effective way to proceed, that maximises national benefit, is to develop an ambitious, advanced UK XFEL that is world-leading in key respects. We map out how this might be done and further recommend that the UK now embarks on the next stages towards building this infrastructure. There is a **timely opportunity** to develop a **world-leading scientific infrastructure with unique capability**, that enhances the portfolio of international XFELs and provides a **huge boost to UK science and innovation**.

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

stfc.ukri.org