UK XFEL: THE UK VISION FOR NEXT-GENERATION XFELS

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Abstract

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. Looking to the future for the UK community, the UK XFEL project has developed a science and technology case and a conceptual design for a next-generation XFEL that can utilise maturing technologies to deliver vast increases in research productivity through enhanced data rates, throughput, and x-ray quality. To achieve this, 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. Such a facility would drive deep and wide-ranging impact across all areas of science and technology and major sectors of the economy. The project has identified and analysed options to realise these capabilities through either hosting a new facility or co-developing upgrades at existing international projects.

INTRODUCTION

Since the late-2000s, X-ray free-electron lasers (XFELs) have proven to be a radical technology breakthrough, delivering X-rays that are many orders of magnitude brighter than other sources. They are now ready to enter a new era, characterised by substantial maturation of the technology, which can be leveraged to deliver world-leading, societally-relevant science at scale.

UK XFEL is a multi-stage project to pursue next-generation XFEL capabilites for the UK science community. The 2020 Science Case [1, 2] was followed by funding from UK Research and Innovation for a three-year conceptual design and options analysis (CDOA), which launched in January 2023. This phase includes developing a conceptual design for a unique new UK facility, alongside examining investment opportunities at existing facilities e.g. [3–12], both with the aim of realising 'next-generation' XFEL capabilities (the features of which are discussed below), alongside developing an updated Science and Technology Case, informed by a series of Town Hall meetings to engage with the user community. The project reports are due for release imminently, via the project website [1].

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THE CASE FOR NEXT-GENERATION XFELS

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, and a peak brightness a billion times higher. Characterised by enhanced data rates, throughput, and x-ray quality as described below, they will provide unprecedented X-ray atomic-level structure determination and nanoscale imaging capabilities that will benefit defence, biotechnology, batteries, fusion energy, 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 and growth, as summarised in Fig. 1. They 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 across fields:

Advancing technology through the boost provided by space- and time-resolved understanding, leading to the development of new energy, data, nuclear and materials technologies.

Improving 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 providing 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.

Expanding 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.

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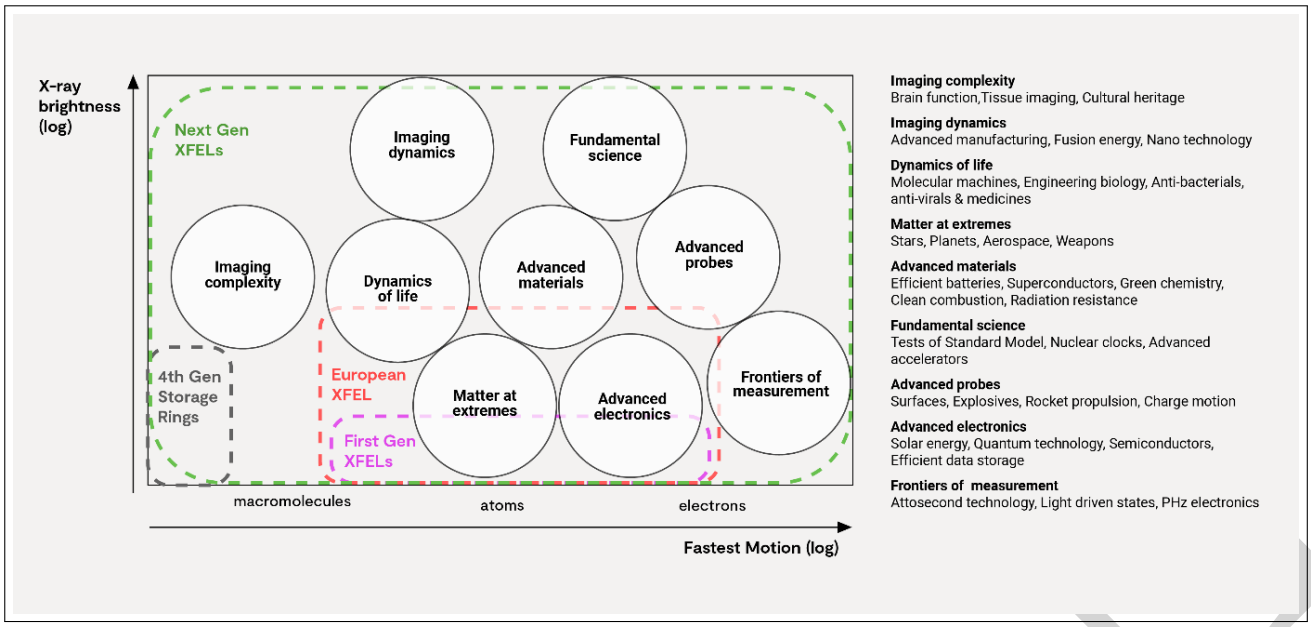

Figure 1: Indicative capabilities of a next-generation XFEL: the high x-ray average brightness coupled to extreme time resolution enable new classes of measurement that will drive discovery in many fields of science and technology.

NEXT-GENERATION XFEL CAPABILITIES

Next-generation capabilities have been defined by distilling the key messages within the Science and Technology Case, focusing on transformational future opportunities that can't yet be delivered at existing facilities. They have been refined through a wide-ranging consultation process between the science team, the facility design team, and with external experts, clearly setting an emphasis on both enhancing XFEL capabilities and on widening access to such capabilities, defined as follows:

A high-efficiency facility with a step-change in the simultaneous operation of multiple end stations.

Near-transform-limited operation across the entire X-ray range (~0.1–20 keV and ~100 as–100 fs). Non-transform-limited pulses from ~20–45 keV.

Evenly-spaced, high repetition rate pulses to match samples and detectors (~100 kHz per FEL, with flexibility).

Synchronisation/timing with external lasers to <1 fs.

Widely separated multiple-colour X-rays to at least one end station.

A full array of synchronised sources: XUV-THz, e-beams, high power and high energy lasers at high repetition rate.

Data and computing systems matched to the demands of high repetition rate acquisition.

Minimal carbon footprint with minimal energy consumption for both operation and build.

NEXT-GENERATION XFEL CONCEPT

To develop a next-generation XFEL conceptual design, we assumed a new-build facility at an international scale, without constraints from location or from upgrading an existing machine. Aspects of this design can be mapped onto and compared against the different options (i.e UK-based and international investments). It also enables consideration of a scaleable set of options for a UK facility that could form the basis of a phased delivery: a 'nominal' layout with 7 independent FELs is shown in Fig. 2, including potential to extend to ~12 FELs. We have developed a self-consistent design based on a set of documented common assumptions, structured around a set of key themes as follows.

Theme 1: High Repetition Rate and High-Efficiency, Many-User Facility

A next-generation XFEL must be a high repetition rate and high-efficiency, many-user facility. At the core of the facility, these capabilities are built upon the accelerator and beam distribution: the photoinjector, linac and spreader must be able to generate and accelerate high-brightness electron bunches at high (~1 MHz) repetition rate and flexibly multiplex them to many more independent FELs (~6-10) compared to present facilities (1-3). This theme propagates through all aspects of the facility design.

To provide low emittance electron bunches to multiple high repetition rate FELs, the most applicable sources are based on either normal-conducting RF (NCRF) or superconducting RF (SRF) technology operating with relatively low frequency (100s MHz, VHF) with a cathode field of 20-30 MV/m, such as those built for LCLS-II [13] and SHINE. It is also attractive to use SRF L-band (1.3 GHz) cavity-based guns like those built for CW FELs and ERLs at HZDR, HZB, and for the upgrade of Eu-XFEL [14]. Two injector

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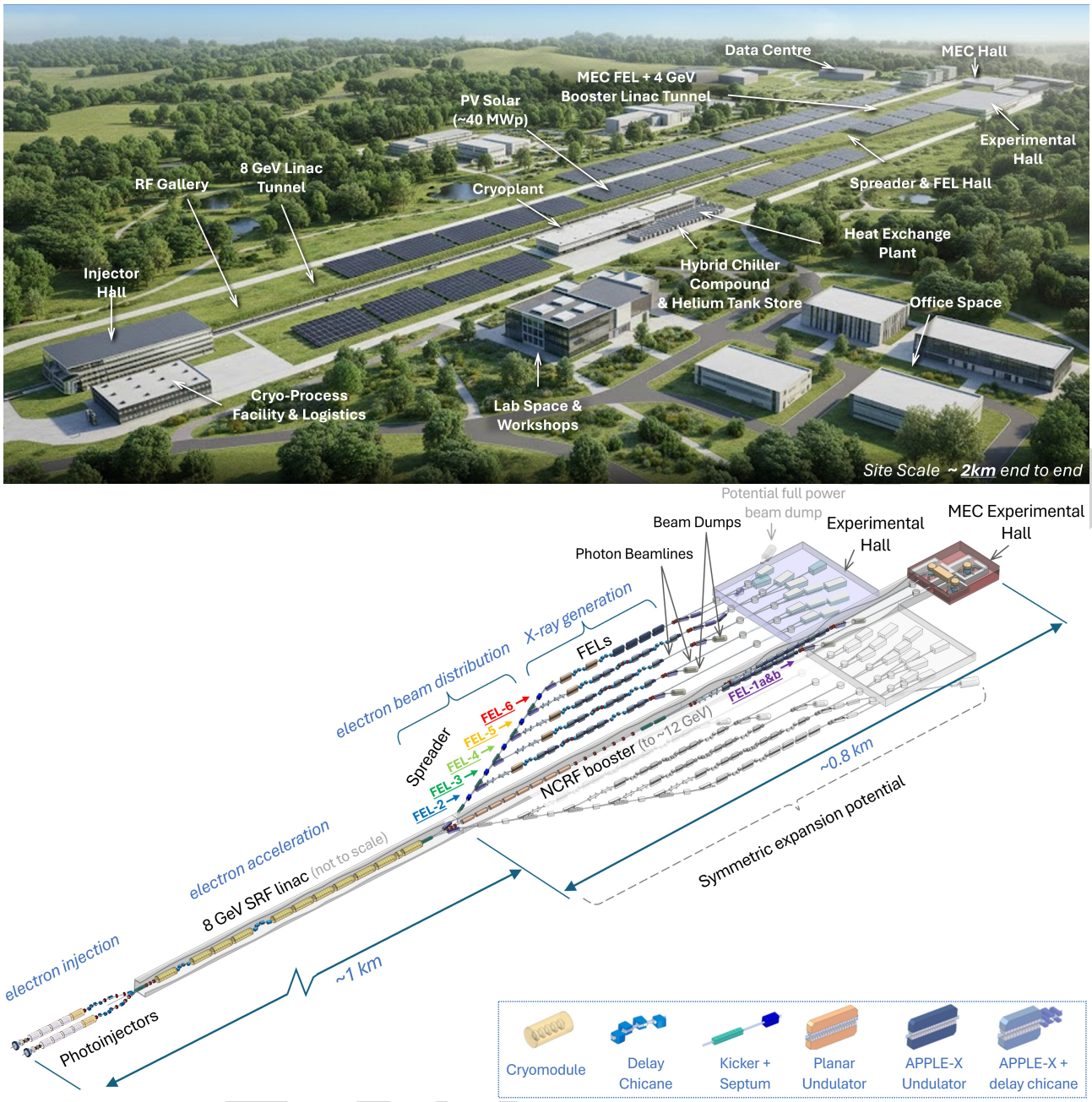

Figure 2: Site visualisation (above) and layout (below) of the next-generation XFEL design to meet the Science and Technology Case. Two low-emittance, high-repetition-rate VHF injectors feed into an SRF linac providing acceleration to ~8 GeV, followed by distribution to five high-repetition rate FELs (with potential to mirror this about the central axis), and a normal conducting booster to ≳12 GeV in the central line to support higher power/higher photon energy FEL output at lower repetition rate. The FEL parameters match those in Table 1. A repeating section of the SRF linac is omitted for clarity.

designs have been developed, based on a VHF gun operated in the 'cigar' photoemission mode [15] with a bunch length of 10°of RF phase: 1) RF and magnetic compression, and 2) two-stage RF compression. The former option (shown in Fig. 3) is set as the baseline for its higher beam quality through better control of the longitudinal phase space [16, 17].

To meet the requirements of the FEL schemes, the facility will need to deliver multiple beam modes (e.g. ~0.2 mm·mrad at 75 pC, ~0.35 mm·mrad at 150 pC etc.). It has been established that the various beam modes can be achieved with the same hardware, but with different tuning required for each. In order to provide both flexibility and redundancy, while focusing on a single technology, it has been decided that two injectors should be included, which will be identical in terms of hardware, based on VHF guns, with multiple photoinjector lasers per gun to provide flexibility.

To operate at ~1 MHz requires an SRF linac, and to operate multiple beamlines efficiently, it is advantageous to set a fixed electron beam energy, with ~8 GeV selected as

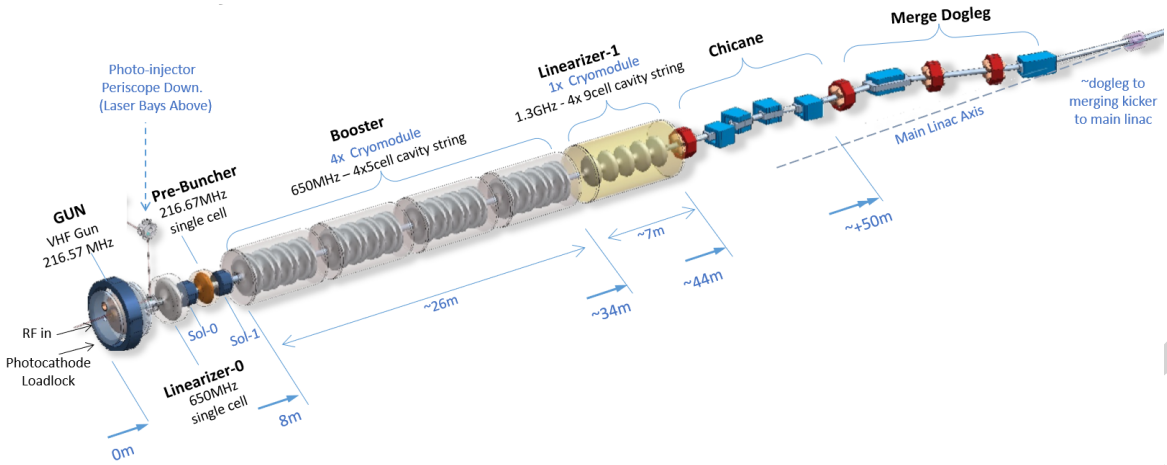

Figure 3: Novel injector concept for the Low Energy Beamlines, featuring RF compression (the pre-buncher) and magnetic compression (in the chicane), with a progressive increase in RF frequency for optimal beam quality. The length of the section is ~50 m. Two identical injectors are envisaged to run in parallel before merging into a single linac.

the baseline to meet most needs. Studies have been carried out to assess dipole mode wakefield [18] and mode mixing [19] effects. For a subset of science areas, e.g. matter in extreme conditions (MEC), that require higher photon energy or higher pulse energy (at a lower repetition rate of ≤200 Hz), a booster to higher energy is included (NCRF linac) to feed two FELs (1a and 1b). Emerging technologies, e.g. PWFA [20] are integrated from the outset, with an R&D line alongside the FELs envisaged to provide a continuous source of enhancements beyond the initial design.

Owing to the stringent requirements on the FEL quality, alternative designs to the symmetric C-type magnetic chicane are proposed, namely an asymmetric 5-dipole chicane and an arc compressor [21, 22]. The proposed lattice contains both compressor types in parallel for maximum flexibility, which will be assessed further in future phases. For the spreader (switchyard), a modular design approach has been used to assess various combinations of RF-based and pulsed magnetic kickers [23], with the preferred option (assuming magnetic kickers) shown in Fig. 4.

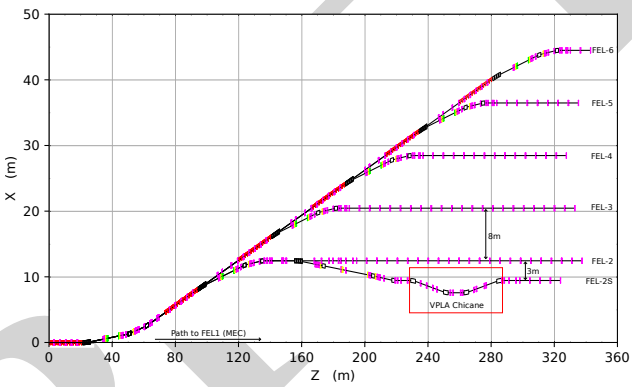

Figure 4: Spreader layout for the nominal case. In the full version, this layout is reflected about the z-axis. The FEL-2 line includes an RF deflector to an adjacent undulator line for two-colour operation.

Theme 2: Exceptional X-ray Pulse Qualities Including 'Laser-Like' X-rays

Transformational enhancements of the X-ray pulse qualities can be realised through the interplay between the accelerator features and the FEL techniques deployed in the undulators, while bespoke photon beamlines will optimise the properties for experiments.

The primary feature is that of full 3D-coherence, so called 'laser-like' or near-transform-limited pulses across a wide range of photon energies and pulse durations. With the energy of the high repetition rate electron beam fixed at ~8 GeV, the photon energy range can be covered by 5 FELs (with some overlap) as shown in Fig. 5, i.e. FELs 2 - 6. The FEL tuning ranges (see Table 1 and Fig. 5) have been developed through iteration with the Science Team, and appropriate methods to achieve near-transform-limited pulses have been identified, as shown in Table 1.

Many such schemes are well-established at international XFELs but significant development opportunities remain. For example, to utilise advances in conventional lasers to drive external seeding as used at e.g. FERMI [5] to much higher repetition rate (~100 kHz) and to higher photon energy. Techniques for attosecond (e.g. ESASE/XLEAP [24]) and narrow bandwidth (e.g. self-seeding [25, 26]) pulses are well-established and so present opportunities to pursue high repetition rate operation, increased tunability and other advanced features. Techniques such as HB-SASE [27] and cavity-based XFEL operation [28] have recently been demonstrated [29, 30] and will be important to include.

The MEC requirements encompass very high pulse energy (10s of mJ) at 5-10 keV, as well as lasing at ≥40 keV, with both at relatively low repetition rate (e.g. ≤200 Hz) or a short (≤10-pulse) burst mode. Studies indicate that boosting the energy to ≳12 GeV in the FEL-1 line will be needed to meet these requirements. FEL-1 is divided into two very slightly diverging lines, leading to two high-power laser user

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Table 1: Proposed FEL Tuning Ranges and Modes

FEL	Photon Energy [keV]	Mode	FEL Scheme	Pulse Duration [fs]
FEL-6	0.1-1.0	Seeded	EEHG	5-100
FEL-5	0.25-3.0	Long Short	HB-SASE ESASE	75-30 2-0.35
FEL-4	1.0-5.0	Long Short	HB-SASE ESASE	30-10 0.8-0.3
FEL-3	3.0-13	Long Short	HB-SASE ESASE	12-7 0.4-0.2
FEL-2	5.0-20	Long Short Cavity	HB-SASE ESASE XFELO	10-7 0.3-0.2 ~100
FEL-1a (with booster)	5.0-20	High Power	SASE	~30
FEL-1b (with booster)	20-45	High Power/ Energy	SASE	~30

enclosures, allowing experimental setup in one whilst the other is in operation.

A scheme to deliver FEL pump-probe capability with widely separated wavelengths (SXR + HXR) from two parallel undulators [31] has been included in the FEL-2 line. Combining output from these is one of the challenges for photon beamline design, together with general challenges due to the high repetition-rate CW operation, the near-transform-limited pulses, and the fully flexible polarisation.

Theme 3: World-Class Instruments, Synchronous Sources, Data and AI

Defining the end station capabilities has served as a focus for many of the project's activities, including two dedicated away days on this topic. A comprehensive initial provision of end stations has been established to exploit the cutting-edge capabilities of the facility, as shown in Fig. 5, with each one associated with a particular FEL, and a set of required capabilities compiled, which has fed into the facility design.

A next-generation XFEL must leverage the transformative impacts of AI and digital twinning. MHz XFELs will bring unprecedented data rates (towards TB/s) and scales (PB per data set) that will require exascale computing and AI, as well as presenting synergistic opportunities with these fields e.g, real-time experiment steering and developing new foundation models across fields. State-of-the-art detectors will be key to manage the extreme brightness and high repetition rates, requiring a range of sensor materials to cover the photon energy range, with data processing at the detector as part of a combined detector-data pipeline.

A next-generation XFEL will be considered as a laser facility as well as a particle accelerator facility, with exceptional synchronisation across both aspects. Synchronous sources are expected to include high repetition rate lasers over a wide range of spectral/temporal regimes using Yb-based technology and a high pulse energy laser for MEC, e.g. DiPOLE technology [32]. THz sources will also be important, with laser-based methods showing rapid progress and the option to include an accelerator-based source.

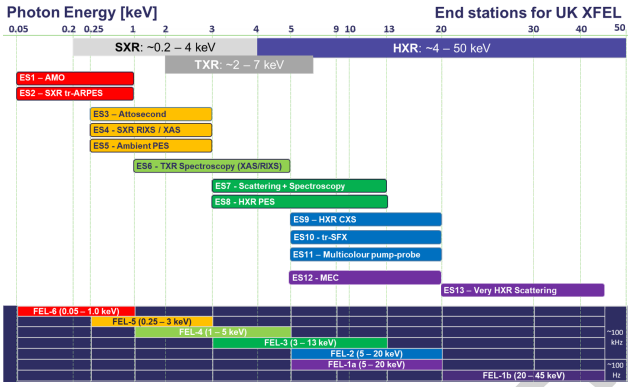

Figure 5: Map of proposed end stations across all of the FELs covering the soft X-ray (SXR), tender X-ray (TXR) and hard X-ray (HXR) range.

Project Delivery and Environmental Sustainability

The engineering design drivers for a new facility are to achieve a high-throughput, user-centric facility with high uptime, while being cost-efficient and relatively compact, and allowing for phased delivery and flexible upgrades. This is enabled by being based around established technologies and by a ground-level design, which uses modular building and shielding techniques to give generous experimental space and expandability. A new facility must utilise low-carbon construction methods, efficient cooling, and renewable energy options to meet environmental sustainability aims.

SUMMARY AND NEXT STEPS

UK XFEL's Science and Technology Case and Conceptual Design Report lay out a roadmap to an ambitious future generation of XFEL capabilities that is robust and technically feasible. An Options Analysis, to be published in tandem, analyses the potential routes to UK access either by hosting a new facility or co-developing an international project, and these will be reviewed by UK funding agencies. Access to such facilities would be transformational for the existing international light source user community, and would attract a new generations of researchers across industry, medicine, academia and defence to solve emerging challenges.

ACKNOWLEDGEMENTS

While the authorship of this paper is limited to the facility design leads and our Science Lead, we would like to recognise the innovative contributions and advice of all our team and international collaborators. The project is greatly aided by collaboration with international XFEL facilities and the feedback of our international advisory board.

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