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CONCLUSIONS FROM THE UK XFEL CONCEPTUAL DESIGN AND OPTIONS ANALYSIS STUDY

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Abstract

UK XFEL is a multi-stage project to pursue 'next-generation' XFEL capabilities, either through developing a new facility in the UK or by investing at existing machines. The project's Science Case envisages a step-change increase in the number of simultaneous experiments, with transform-limited ('laser-like') x-rays across a wide range of pulse durations and photon energies (up to 20 keV) being delivered together with an array of synchronised sources, at high repetition rate to approximately ten FELs (evenly spaced pulses at approximately 100 kHz per experiment, with flexibility). A subset of applications require increased pulse energy and higher photon energies at low repetition rate or in short bursts. The project is now in the final year of its three-year conceptual design and options analysis phase, in which it has produced a conceptual design to efficiently meet these requirements, as well as conducting an analysis of the costs, socio-economic factors, and sustainability of the different investment options.

INTRODUCTION

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 started in October 2022. 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). By the end of the CDOA phase (October 2025), the project will have explored and analysed these options, alongside updating the Science Case, informed by a series of Town Hall meetings to engage with the user community.

Year 1 focused on surveying the science requirements, preliminary engagement with overseas XFEL facilities, planning the Town Hall meetings and initial conceptual design scoping. Year 2 focused on producing a self-consistent design, identifying gaps in key physics and technology areas, working with overseas XFEL facilities, and the majority of the Town Hall meetings. In Year 3, existing R&D activities are continuing, the options analysis is being conducted and roadmaps to address gaps in key areas will be defined. The CDOA report is being written, detailing the preferred options; this will include associated costs, socio-economic analysis, and an update to the Science Case. This paper summarises the conclusions to date.

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NEXT-GENERATION XFEL CAPABILITIES

Next-generation capabilities were defined by distilling the key messages within the Science Case, focusing on transformational future opportunities that can't yet be delivered at existing facilities. These have been refined through a wide-ranging consultation process between the science team, the facility design team, and with external experts. The Science Case and ongoing engagement clearly set 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 concept, we have chosen to assume 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: a 'maximal' layout with up to 12 FELs is shown in Fig. 1, which is under

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comparison against 'minimal' (2 FELs) and 'nominal' (6 FELs) versions. A key element of the conceptual design is that it is 'self-consistent': the numerous technical and physical considerations given to different underpinning systems are built on a set of common assumptions, captured using an internal 'decision log'.

A Stable, Modular, High Repetition Rate, Many-User Accelerator

A next-generation XFEL must be underpinned by a stable, modular, high-repetition rate, many-user accelerator. The key components in this respect are the high-brightness photoinjectors, the linac to accelerate to full energy, and the compression and distribution sections.

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 Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz-Zentrum Berlin, and for the upgrade of Eu-XFEL [14]. Two injector 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 [16]. The studies indicate a clear advantage in terms of beam quality in the former case.

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 the baseline to meet most needs. 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 (likely a NCRF linac) in one line. Emerging technologies, e.g. PWFA [17] 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. The preferred solution is a flexible scheme allowing a bunch-by-bunch choice of arc or chicane compression to allow optimal compression for each individual FEL. For the spreader (switchyard), a modular design approach has been used to assess various combinations of RF-based and pulsed magnetic kickers [18], with the preferred option (assuming magnetic kickers) shown in Fig. 1.

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	EEHG/ HB-SASE	100-20
		Short	XLEAP	2-0.35
FEL-4	1.0-5.0	Long	HB-SASE	40-15
		Short	XLEAP	0.8-0.3
FEL-3	3.0-13	Long	HB-SASE	20-10
		Short	XLEAP	0.4-0.2
FEL-2	5.0-20	Long	HB-SASE	16-12
		Short	XLEAP	0.3-0.2
		Cavity	XFELO	~100
FEL-1 (with	5.0-20	High Power	SASE	~30
booster)	20-45	High Power/ Energy	SASE	~30

Extreme X-Ray Pulse Qualities

Transformational enhancements of the x-ray pulse qualities can be realised by the intersection of the accelerator features described in the previous section and the FEL techniques deployed in the undulators. 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. 2, i.e. FELs 2 - 6. The FEL tuning ranges (see Table 1 and Fig. 2) 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; however significant opportunity remains for development. 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. XLEAP [19]) and narrow bandwidth (e.g. self-seeding [20, 21]) 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 [22, 23] (with potentially TW peak power, few-fs pulses at any FEL wavelength and repetition rate [24]) and XFELO [25] are under experimental development, e.g. [23].

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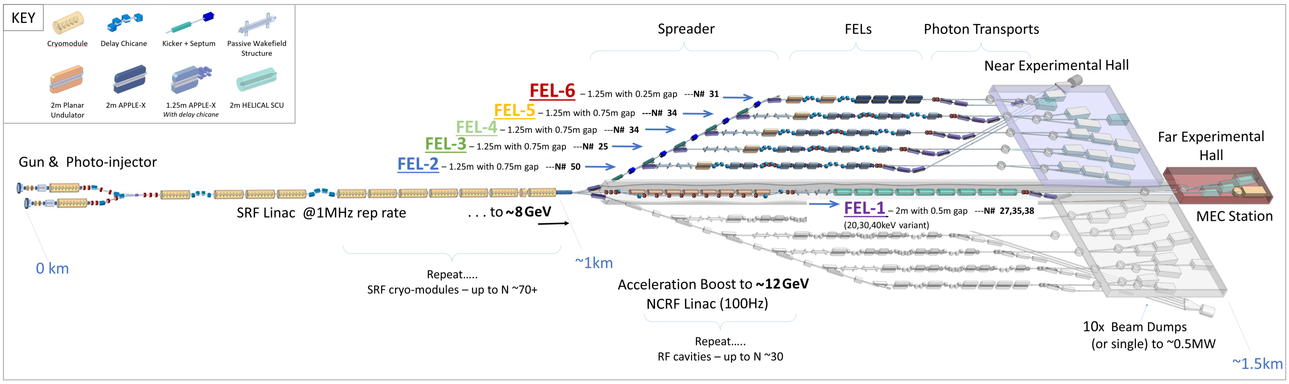

Figure 1: 'Maximal' layout option, showing some of the key features of the concept: two low-emittance, high-repetition-rate VHF injectors; a superconducting RF linac providing acceleration to ~8 GeV; simultaneous distribution to ~6-10 FELs by distributing to both sides of the central axis); and a normal 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.

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 enclosures, allowing experimental setup in one whilst the other in in operation. Period length doubling in a superconducting undulator [26] could also be highly useful to cover the required photon energy range in a single undulator line.

A scheme to deliver FEL pump-probe capability with widely separated wavelengths (SXR + HXR) from two parallel undulators [27] has been included in the FEL-2 line.

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 set of required end stations has been established as shown in Fig. 2, with each one associated with a particular FEL, and a set of required capabilities compiled. This work has fed back to the accelerator design, e.g. the user cases for widely separated two-colour operation have allowed us to focus on combining the FEL-5 and FEL-2 photon energy ranges for SXR-pump/HXR-probe.

The concept presents challenges and opportunities in several other areas. 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 underpinning foundation models. There is a clear trend for data processing at the detector as part of a combined detector-data pipeline. For photon beamlines, challenges include handling high average power and how to combine output from two FELs. Synchronous sources are expected to include high repetition rate lasers over a wide range of spectral/temporal regimes using Yb-

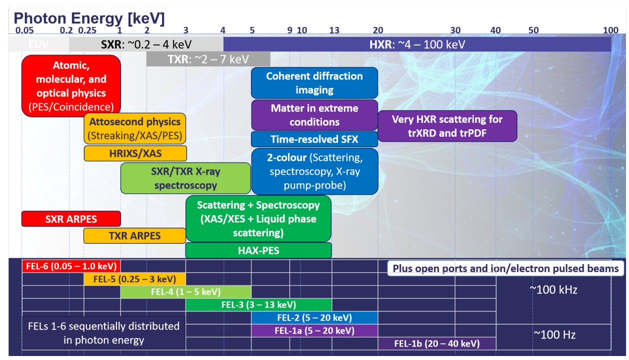

Figure 2: Preliminary version of the anticipated end stations, mapped to the FEL photon energy ranges. It is expected to continue to develop over the course of the project.

based technology and a high pulse energy laser for MEC, e.g. DiPOLE technology [28]. Various laser or accelerator-based options for THz sources are also being considered.

SUMMARY AND NEXT STEPS

The project has developed a self-consistent conceptual design for an ambitious, internationally competitive facility that is also robust and technically feasible. It enables consideration of a scaleable set of options for a UK facility, which are now being assessed alongside international investment options in terms of the UK's strategic interests, socioeconomic impact and environmental sustainability.

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