Science and Technology Facilities Council

The UK XFEL Project: Conceptual Design

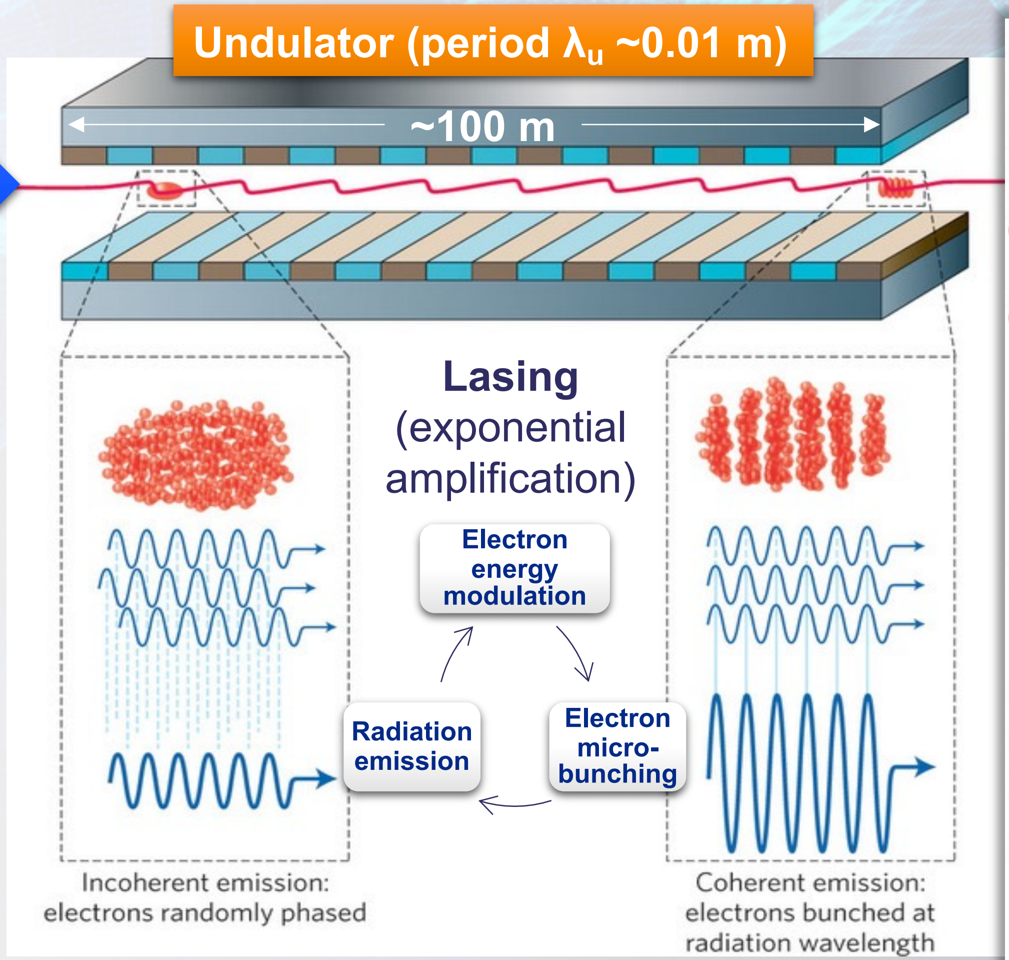
Dave Dunning, STFC Daresbury Laboratory
On behalf of the project team
29th July 2024

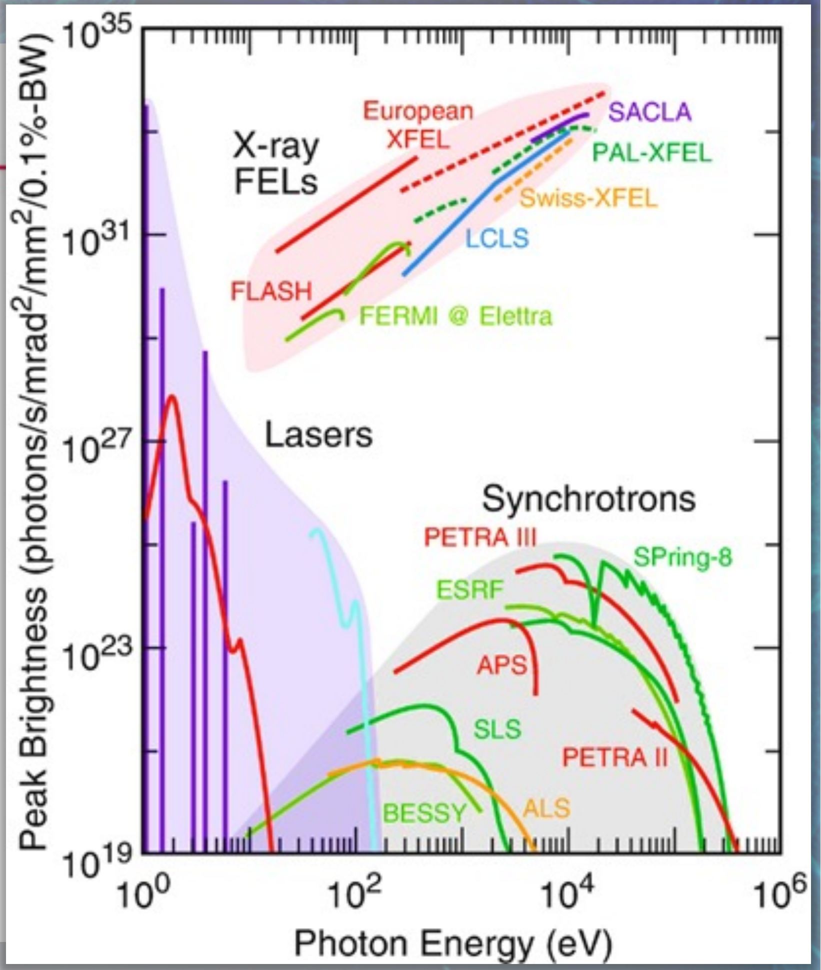
Contents

Introduction to XFELs

- XFEL = X-ray Free-Electron Laser
- ‘free-electron’ means the electrons are not bound in atoms but ‘freely’ propagating in a particle accelerator

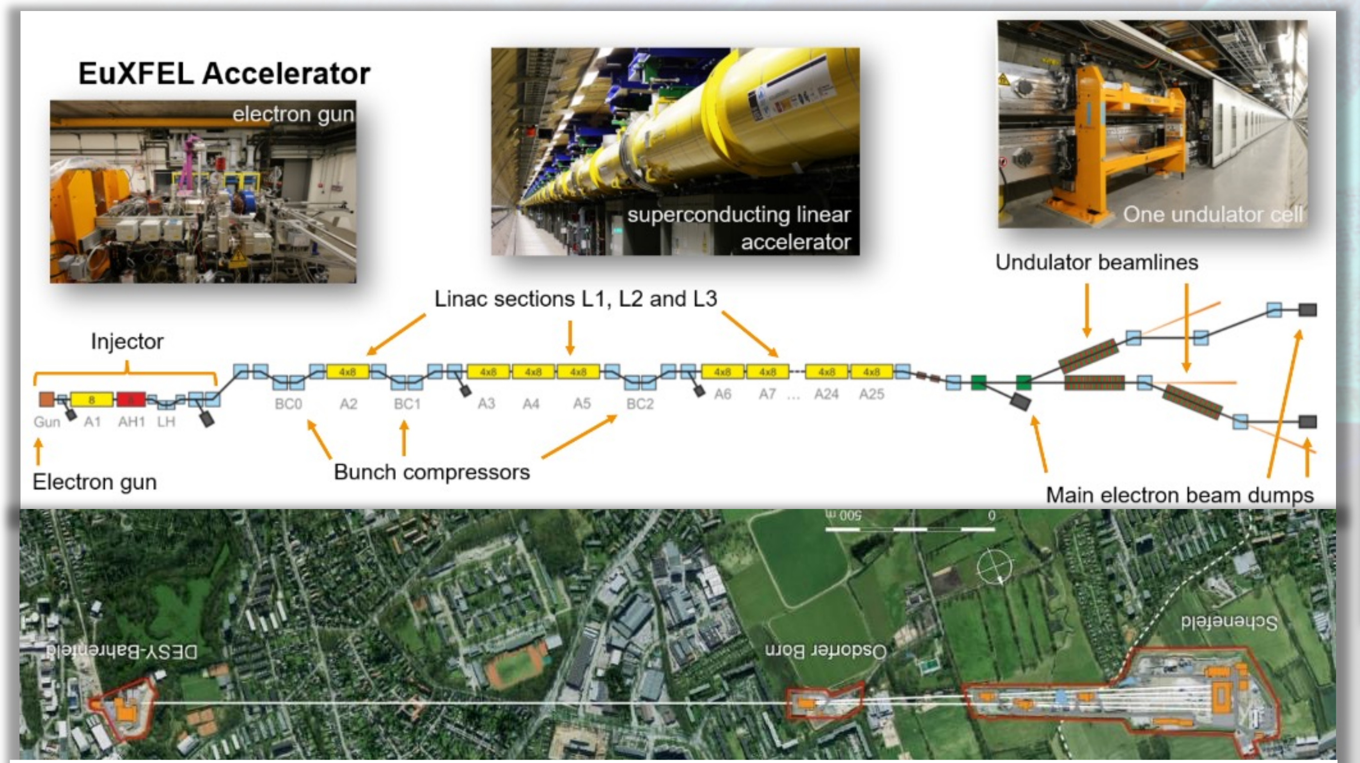
~ 4 – 15 GeV, Lorentz factor ϒ ~ several thousand





XFEL challenges and opportunities

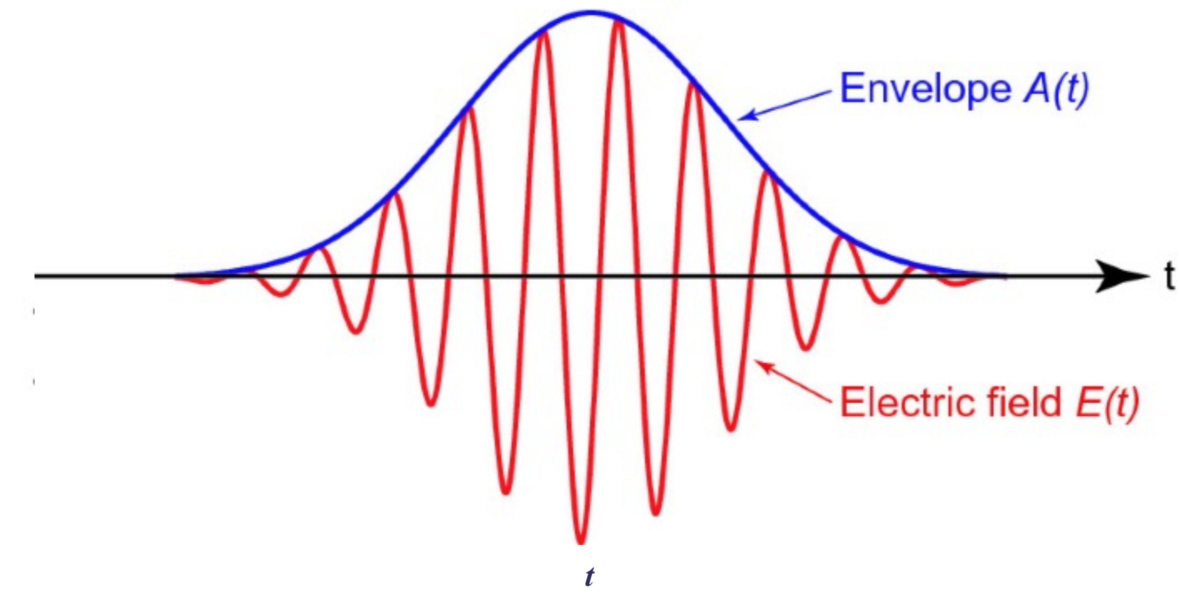
- XFEL lasing spoils the electron bunch quality (bunches can't be re-used). So XFELs are based on *linear* accelerators: **less straightforward to serve many simultaneous experiments**



But bunch repetition rates are increasing by a factor of 10,000 compared to first-gen XFELs (~100 Hz -> ~1 MHz)

Multiplexing to **more simultaneous experiments**, with **much higher average flux** and **much higher data rates**

- **The X-ray pulses are naturally far from transform limited (amplified noise).** In the default SASE mode, there is an intrinsic coherence length of ~hundreds of wavelengths (hundreds of attoseconds at X-ray)



There are many demonstrated or emerging techniques for **near-transform limited pulses (i.e. high quality pulses across a range of pulse durations)**

Increasing capacity and capability go hand in hand

UK XFEL conceptual design process

Understanding/defining the specification

- Capture input from the many user cases, each with different (overlapping) sets of specifications
- Incorporate new ideas developed over time

Informed by the Science Case, survey, Town Halls, Science Team meetings etc.

Specific technical solutions

- Identify and develop technical solutions to best meet each set of user requirements

Informed by research within the design team, facility visits, collaborations etc.

Compelling facility proposals

Integrate technical solutions into self-consistent facility proposals:

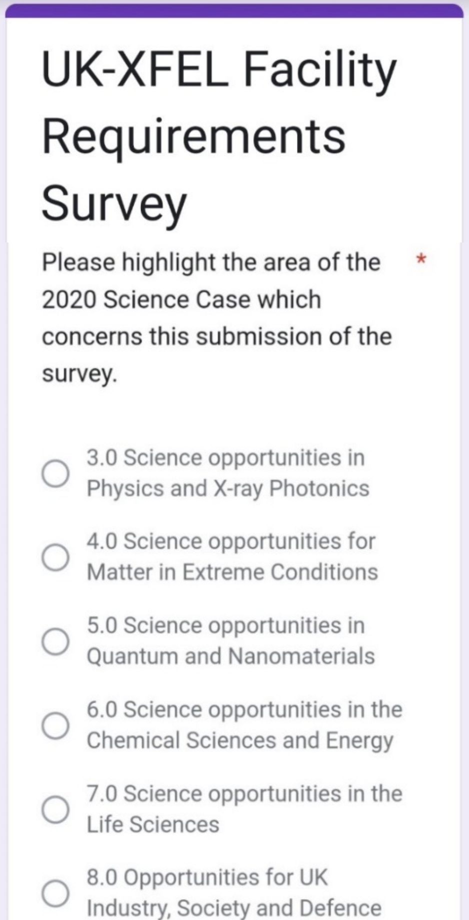
- Ensure compatibility of features
- Consider scope, international context, sustainability, socioeconomic factors

To develop a next-generation XFEL concept, we initially **assume a new-build facility at an international scale**, without constraints from location or from upgrading an existing machine.

Defining the specification: User survey

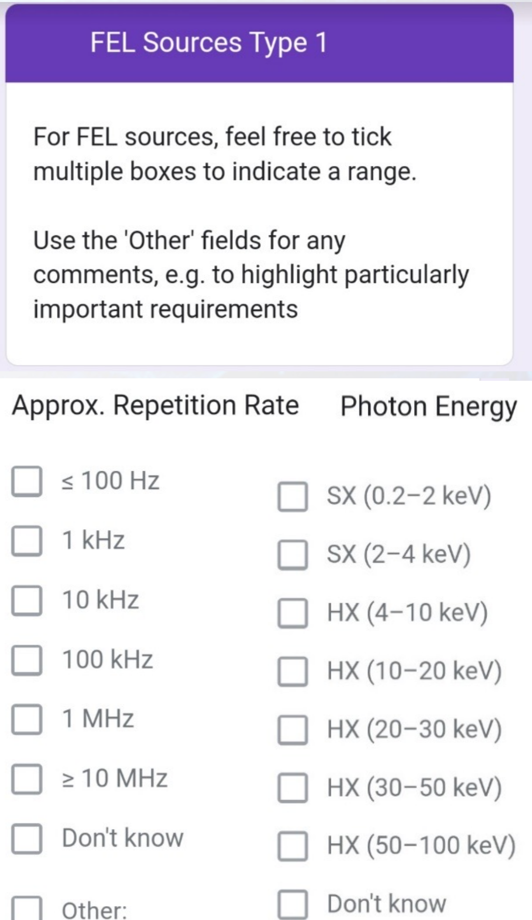
One of the first major activities towards the CDOA phase was a detailed survey to capture requirements

- Structured around the Science Case and recorded more granular specifications
- Captured ~70 case studies: each includes several ‘tick box’ parameters and text entries
- Very useful for defining high-level accelerator and FEL choices, and as a starting point for more detailed areas


UK-XFEL Facility Requirements Survey

Please highlight the area of the 2020 Science Case which concerns this submission of the survey. *

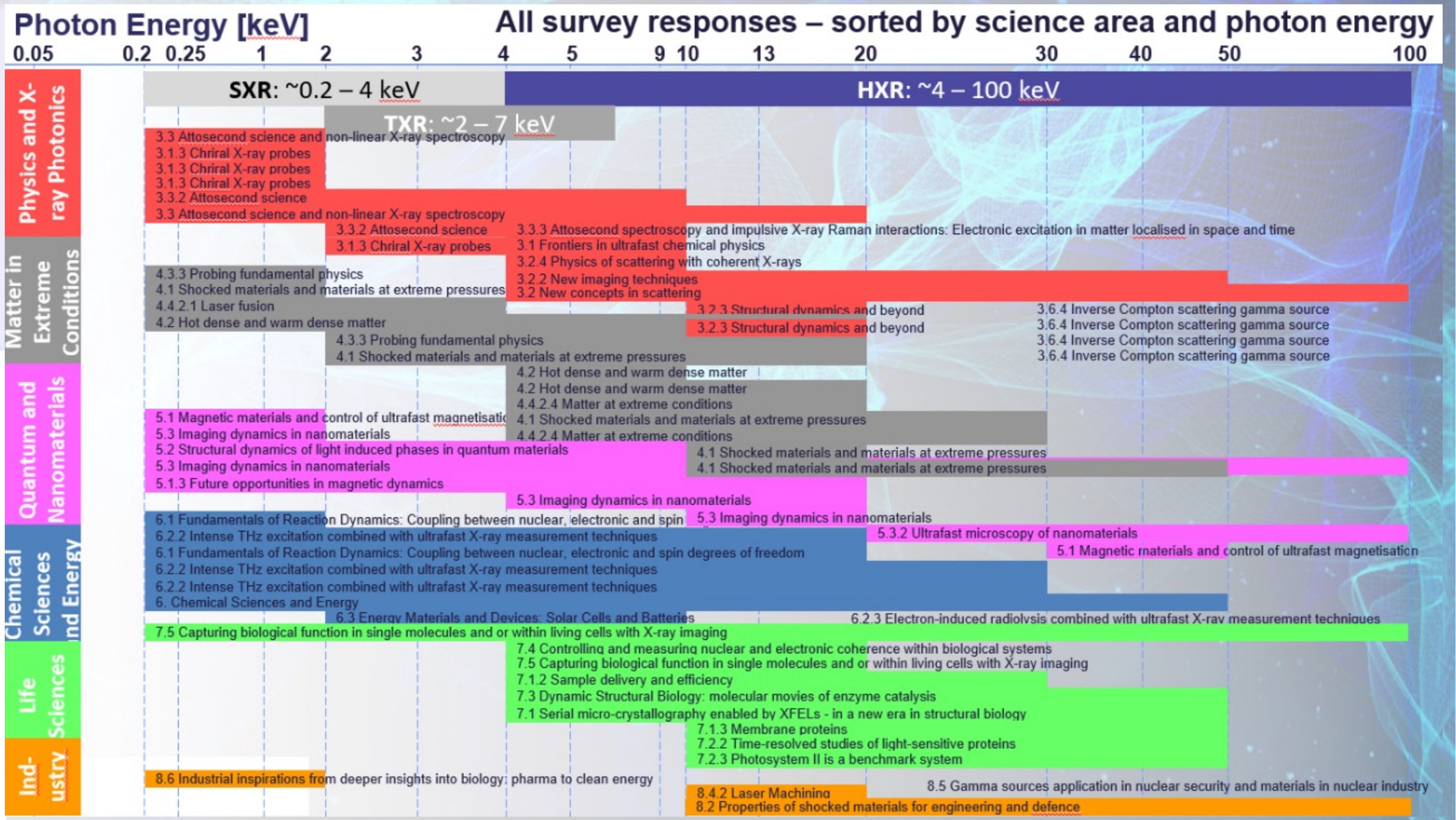
- 3.0 Science opportunities in Physics and X-ray Photonics
- 4.0 Science opportunities for Matter in Extreme Conditions
- 5.0 Science opportunities in Quantum and Nanomaterials
- 6.0 Science opportunities in the Chemical Sciences and Energy
- 7.0 Science opportunities in the Life Sciences
- 8.0 Opportunities for UK Industry, Society and Defence


FEL Sources Type 1

For FEL sources, feel free to tick multiple boxes to indicate a range.

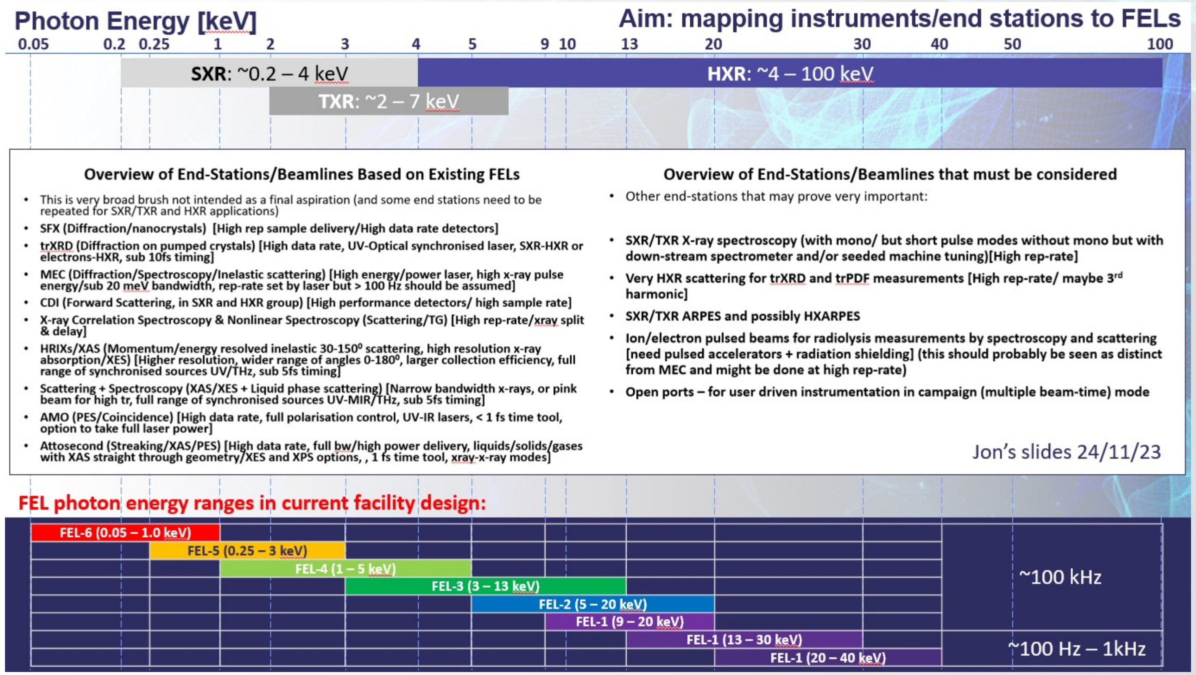
Use the 'Other' fields for any comments, e.g. to highlight particularly important requirements

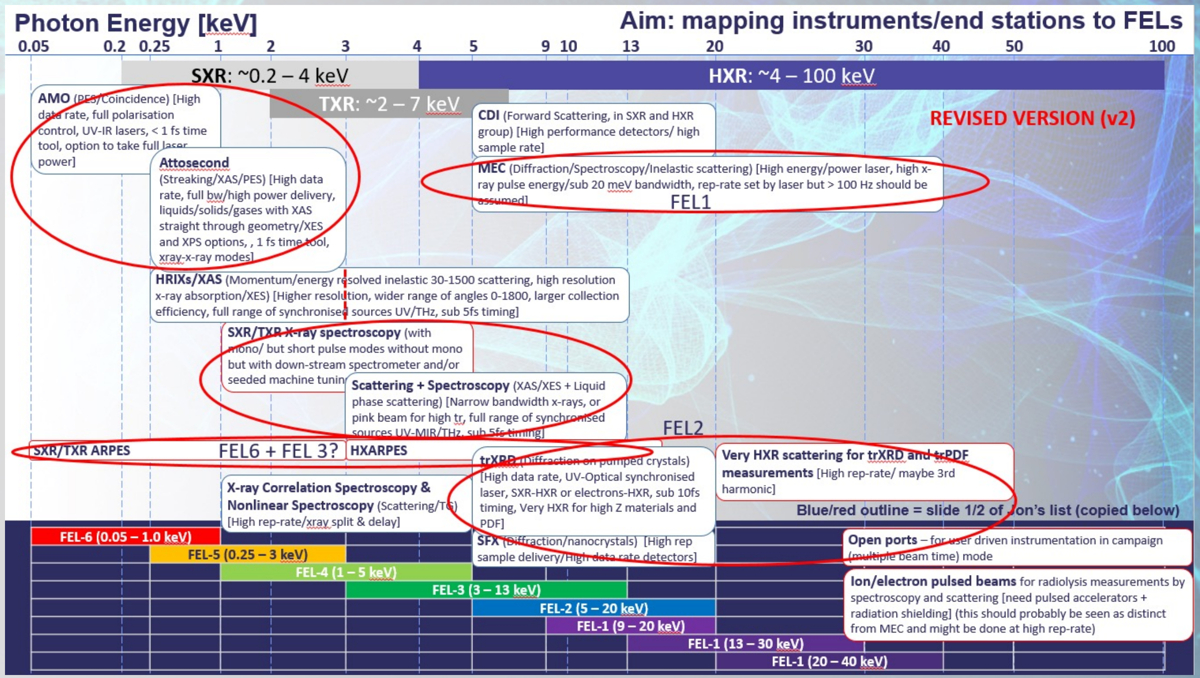
Approx. Repetition Rate	Photon Energy
≤ 100 Hz	SX (0.2–2 keV)
1 kHz	SX (2–4 keV)
10 kHz	HX (4–10 keV)
100 kHz	HX (10–20 keV)
1 MHz	HX (20–30 keV)
≥ 10 MHz	HX (30–50 keV)
Don't know	HX (50–100 keV)
Other:	Don't know

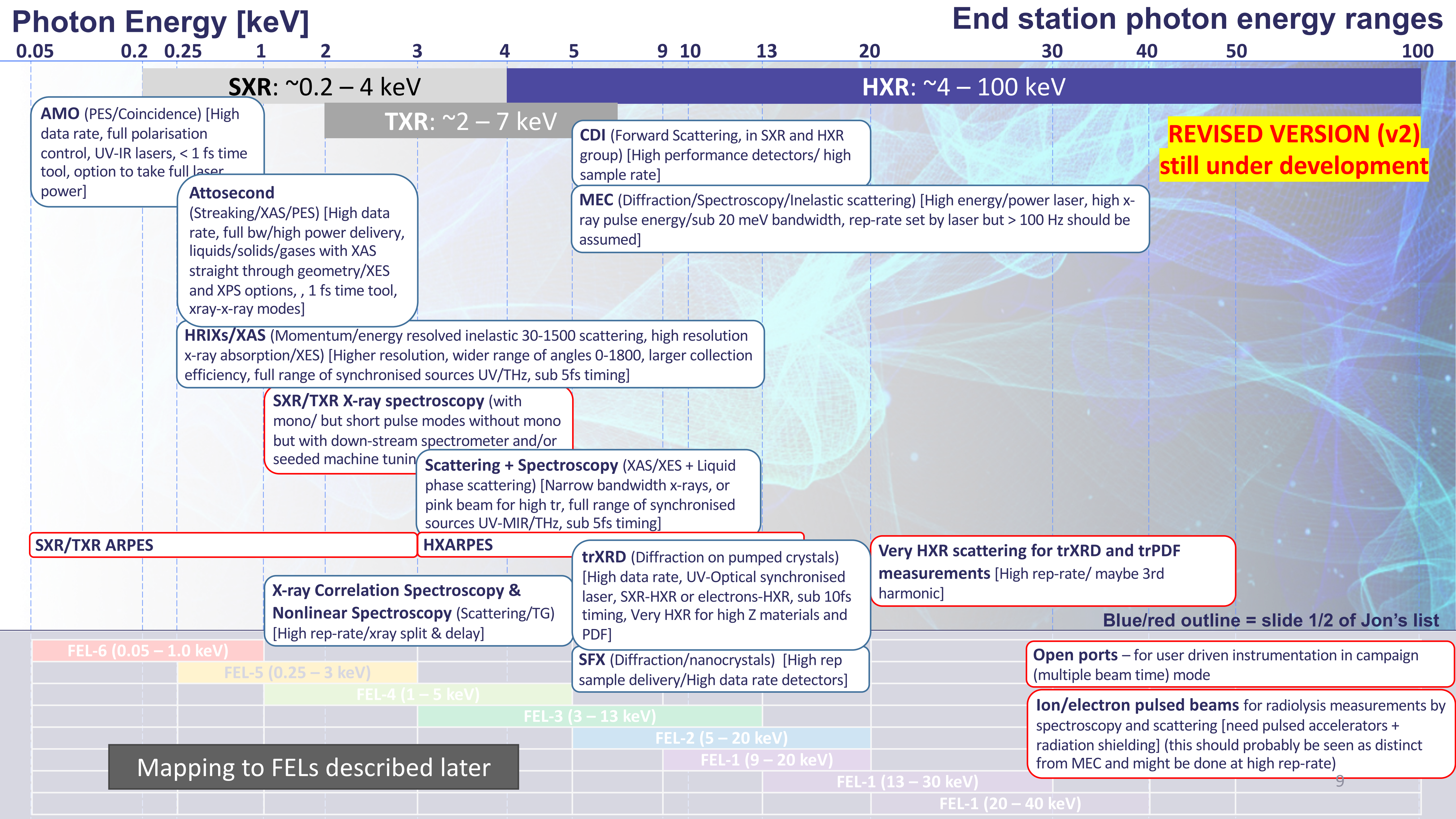


End Station Away Day (28th Feb 2024)

- Identified key end stations and relevant team members.
- Associated end stations with specific FELs and completed specification spreadsheet for each
- Follow-up meetings with each group are underway






Photon Energy [keV]
End station photon energy ranges
0.05 0.2 0.25 1 2 3 4 5 9 10 13 20 30 40 50 100
SXR: ~0.2 – 4 keV
HXR: ~4 – 100 keV
TXR: ~2 – 7 keV
REVISED VERSION (v2) still under development
AMO (PES/Coincidence) [High data rate, full polarisation control, UV-IR lasers, < 1 fs time tool, option to take full laser power]
Attosecond (Streaking/XAS/PES) [High data rate, full bw/high power delivery, liquids/solids/gases with XAS straight through geometry/XES and XPS options, , 1 fs time tool, xray-x-ray modes]
CDI (Forward Scattering, in SXR and HXR group) [High performance detectors/ high sample rate]
MEC (Diffraction/Spectroscopy/Inelastic scattering) [High energy/power laser, high x-ray pulse energy/sub 20 meV bandwidth, rep-rate set by laser but > 100 Hz should be assumed]
HRIXs/XAS (Momentum/energy resolved inelastic 30-1500 scattering, high resolution x-ray absorption/XES) [Higher resolution, wider range of angles 0-1800, larger collection efficiency, full range of synchronised sources UV/THz, sub 5fs timing]
SXR/TXR X-ray spectroscopy (with mono/ but short pulse modes without mono but with down-stream spectrometer and/or seeded machine tunin
Scattering + Spectroscopy (XAS/XES + Liquid phase scattering) [Narrow bandwidth x-rays, or pink beam for high tr, full range of synchronised sources UV-MIR/THz, sub 5fs timing]
SXR/TXR ARPES
HXARPES
trXRD (Diffraction on pumped crystals) [High data rate, UV-Optical synchronised laser, SXR-HXR or electrons-HXR, sub 10fs timing, Very HXR for high Z materials and PDF]
Very HXR scattering for trXRD and trPDF measurements [High rep-rate/ maybe 3rd harmonic]
X-ray Correlation Spectroscopy & Nonlinear Spectroscopy (Scattering/TG) [High rep-rate/xray split & delay]
SFX (Diffraction/nanocrystals) [High rep sample delivery/High data rate detectors]
Blue/red outline = slide 1/2 of Jon's list
Open ports – for user driven instrumentation in campaign (multiple beam time) mode
Ion/electron pulsed beams for radiolysis measurements by spectroscopy and scattering [need pulsed accelerators + radiation shielding] (this should probably be seen as distinct from MEC and might be done at high rep-rate)
FEL-6 (0.05 – 1.0 keV)
FEL-5 (0.25 – 3 keV)
FEL-4 (1 – 5 keV)
FEL-3 (3 – 13 keV)
FEL-2 (5 – 20 keV)
FEL-1 (9 – 20 keV)
FEL-1 (13 – 30 keV)
FEL-1 (20 – 40 keV)
Mapping to FELs described later

UK XFEL Next Generation Definition

- **Evenly spaced, high repetition rate pulses to match samples, lasers, and detectors**
  - 100 kHz per FEL, with flexibility of repetition rate

- **High efficiency facility, with a step-change in the simultaneous operation of multiple end stations**
  - Minimum of six FELs, with upwards of ten end stations to be simultaneously operated

- **Near transform-limited operation across the x-ray range**
  - Photon energies from 0.05-20 keV
  - Pulse durations from 100 as to 100 fs
  - Non-transform-limited operation at 20-50 keV

- **Widely separated, multiple colour x-rays to at least one end station**

- **Full array of synchronized sources**
  - XUV-THz, e-beams, ion beams, high power & high energy lasers at high repetition rate

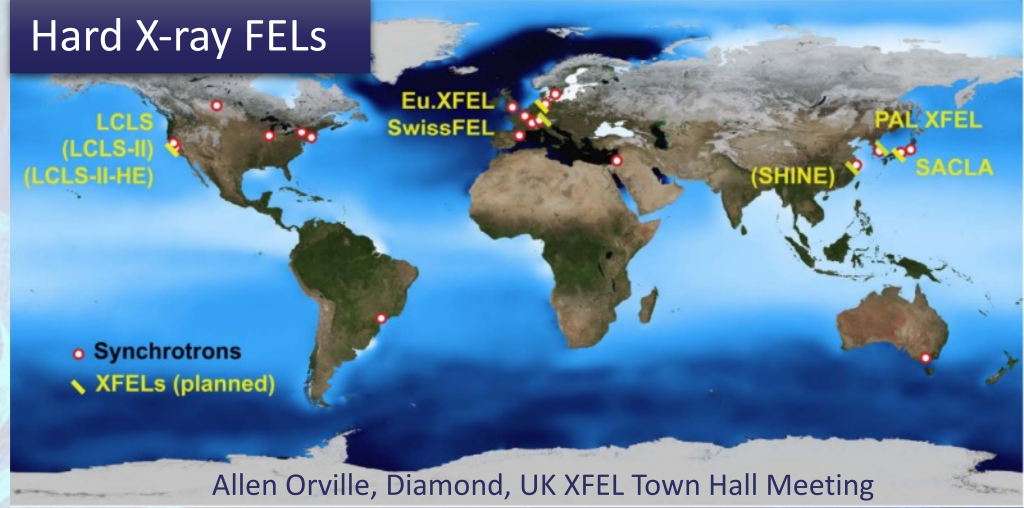
- **Improved synchronization/timing data with external lasers to <1 fs**

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

-> contents for remainder of the talk:

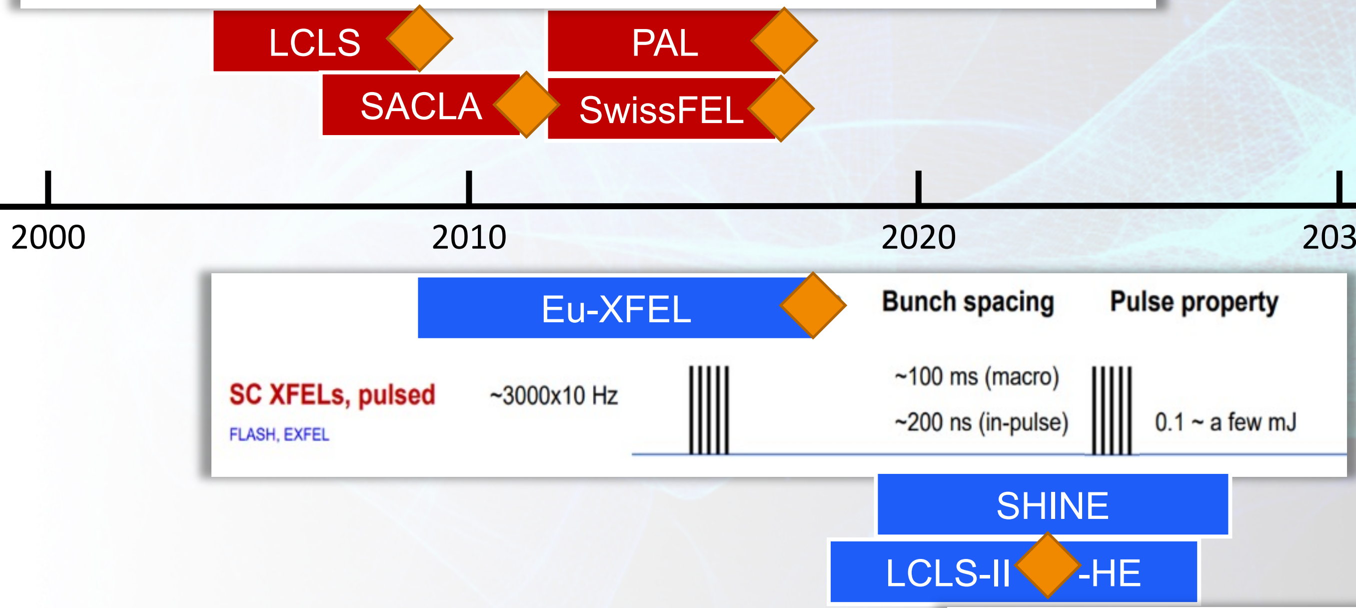
- Multiplexing to ~6-10 FELs
- High peak and average brightness
- Near-transform-limited pulses
- High pulse energy/high photon energy
- Two-colour, synchronous sources, high data rates/AI
- Sustainability

Evenly spaced, high rep. rate pulses



Allen Orville, Diamond, UK XFEL Town Hall Meeting
https://www.clf.stfc.ac.uk/Pages/final_AMOrville_RS-TownMeeting_16July2019-b2.pdf

	Rep-rate	Pulse structures	Bunch spacing	Pulse property
Warm XFELs LCLS, SACLA, Fermi, PAL, SwissFEL, SXFEL	~100 Hz		~10 ms	0.1 ~ a few mJ



	Rep-rate	Pulse structures	Bunch spacing	Pulse property
SC XFELs, pulsed FLASH, EXFEL	~3000x10 Hz		~100 ms (macro) ~200 ns (in-pulse)	0.1 ~ a few mJ

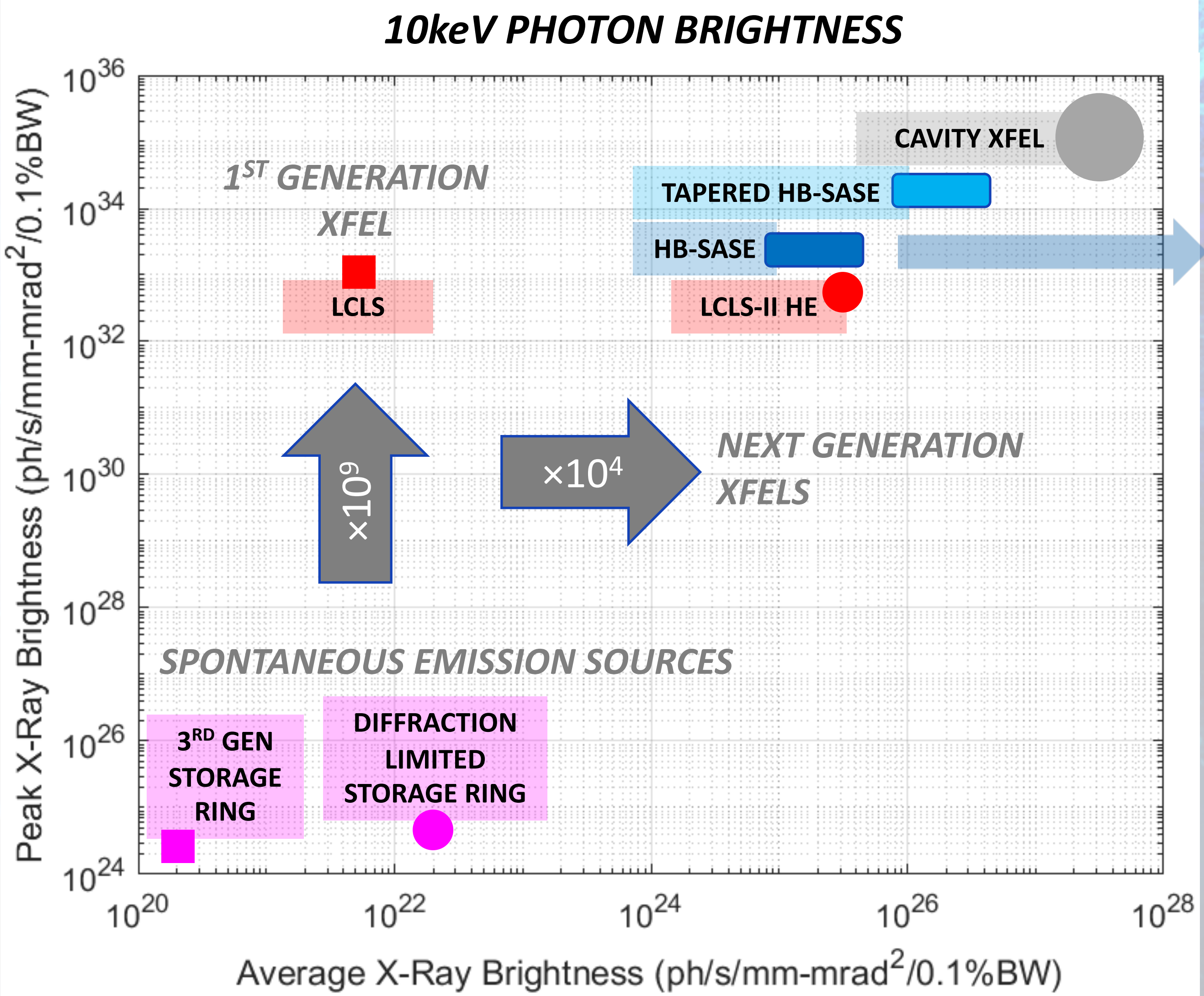
	Rep-rate	Pulse structures	Bunch spacing	Pulse property
SC XFELs, cw LCLS-II, SHINE	~1 MHz		~ 1 us	0.1 ~ mJ

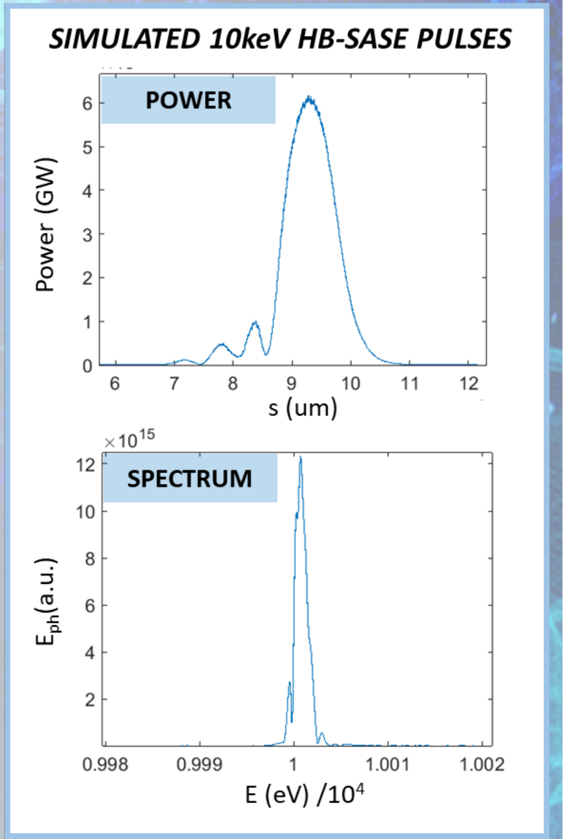
	Rep-rate	Pulse structures	Bunch spacing	Pulse property
Future XFELs Upgrades and new projects	MHz+kHz+X		~1 us + 1 ms + …	0.1 ~ mJ ~ a few mJ customized

Adapted from: Outlook to Future XFELs, Dong Wang Shanghai Advanced Research Institute, Chinese Academy of Sciences and SHINE IPAC23, Venice, May 12, 2023
https://accelconf.web.cern.ch/ipac2023/pdf/FRXD2_talk.pdf

Evolution of peak and average brightness

- Superconducting accelerator technology enables a significant increase in *average* brightness, as well as peak brightness
- Advanced FEL modes provide further advantages



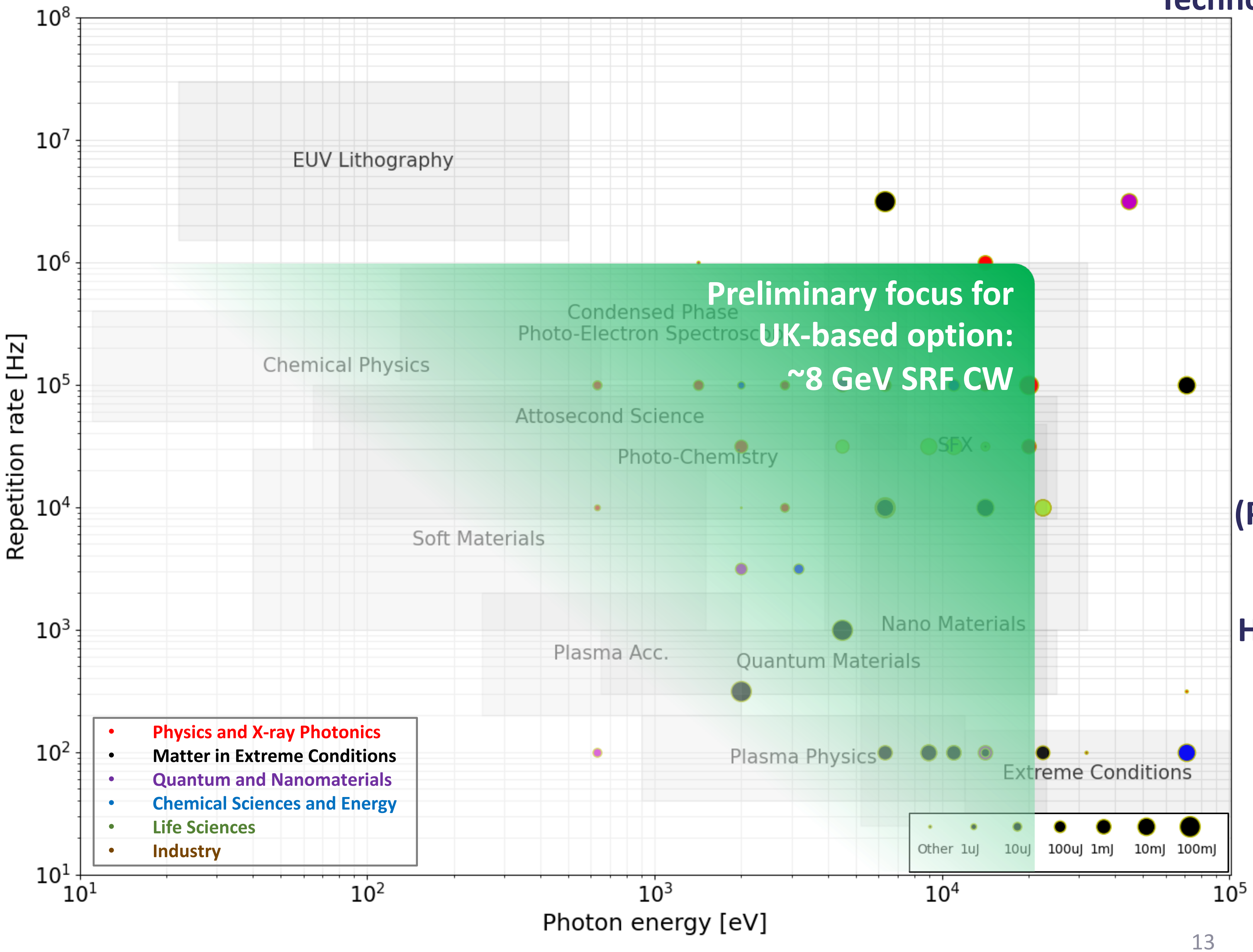


Adapted from LCLS figure: Mike Dunne, SLAC, Future Developments at LCLS, UK XFEL Launch Event 2023 https://youtu.be/sxipwNyXMhg

Top-level facility design choices

- Max. **photon energy** strongly influences the required **electron beam energy**
- **Repetition rate** largely dictates the **type of acceleration technology**
- Requirements suggest ~8 GeV superconducting RF linac

User Requirements from the Science Case & Survey



Acceleration Technology:

ERLs

SRF (CW)

SRF (Pulsed)

HRR NC

NC

Electron Beam Energy: ~1-1.5 GeV ~2-3 GeV ~6-8 GeV ≥10 GeV

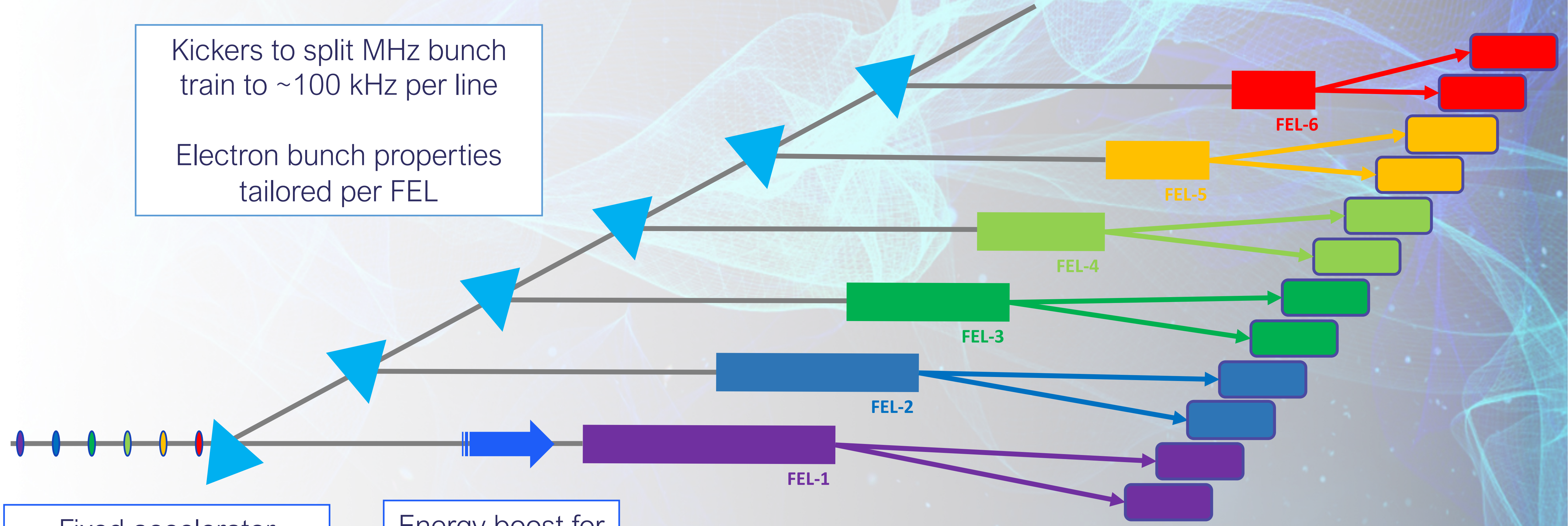
Science and Technology Facilities Council

Facility concept: a step change in the simultaneous operation of multiple end stations

~6-10 FELs independently tuneable in terms of photon energy, pulse duration etc.
+ potential direct uses of electron beam

Kickers to split MHz bunch train to ~100 kHz per line

Electron bunch properties tailored per FEL



Fixed accelerator energy ~8 GeV, electron bunches at ~1 MHz

Energy boost for higher pulse energy/high photon energy

100 kHz Kicker

Mapping instruments/end stations to FELs

Photon Energy [keV]

0.05 | 0.2 | 0.25 | 1 | 2 | 3 | 4 | 5 | 9 | 10 | 13 | 20 | 30 | 40 | 50 | 100

SXR: ~0.2 – 4 keV

HXR: ~4 – 100 keV

TXR: ~2 – 7 keV

REVISED VERSION (v2) still under development

AMO (PES/Coincidence) [High data rate, full polarisation control, UV-IR lasers, < 1 fs time tool, option to take full laser power]

Attosecond (Streaking/XAS/PES) [High data rate, full bw/high power delivery, liquids/solids/gases with XAS straight through geometry/XES and XPS options, , 1 fs time tool, xray-x-ray modes]

CDI (Forward Scattering, in SXR and HXR group) [High performance detectors/ high sample rate]

MEC (Diffraction/Spectroscopy/Inelastic scattering) [High energy/power laser, high x-ray pulse energy/sub 20 meV bandwidth, rep-rate set by laser but > 100 Hz should be assumed]

HRIXs/XAS (Momentum/energy resolved inelastic 30-1500 scattering, high resolution x-ray absorption/XES) [Higher resolution, wider range of angles 0-1800, larger collection efficiency, full range of synchronised sources UV/THz, sub 5fs timing]

SXR/TXR X-ray spectroscopy (with mono/ but short pulse modes without mono but with down-stream spectrometer and/or seeded machine tunin

Scattering + Spectroscopy (XAS/XES + Liquid phase scattering) [Narrow bandwidth x-rays, or pink beam for high tr, full range of synchronised sources UV-MIR/THz, sub 5fs timing]

SXR/TXR ARPES

HXARPES

trXRD (Diffraction on pumped crystals) [High data rate, UV-Optical synchronised laser, SXR-HXR or electrons-HXR, sub 10fs timing, Very HXR for high Z materials and PDF]

Very HXR scattering for trXRD and trPDF measurements [High rep-rate/ maybe 3rd harmonic]

FELs sequentially dis

X-ray Correlation Spectroscopy & Nonlinear Spectroscopy (Scattering/TG) [High rep-rate/xray split & delay]

Blue/red outline = slide 1/2 of Jon's list

SFX (Diffraction/nanocrystals) [High rep sample delivery/High data rate detectors]

Open ports – for user driven instrumentation in campaign (multiple beam time) mode

Ion/electron pulsed beams for radiolysis measurements by spectroscopy and scattering [need pulsed accelerators + radiation shielding] (this should probably be seen as distinct from MEC and might be done at high rep-rate)

FEL-6 (0.05 – 1.0 keV)

FEL-5 (0.25 – 3 keV)

FEL-4 (1 – 5 keV)

FEL-3 (3 – 13 keV)

FEL-2 (5 – 20 keV)

FEL-1 (9 – 20 keV)

FEL-1 (13 – 30 keV)

FEL-1 (20 – 40 keV)

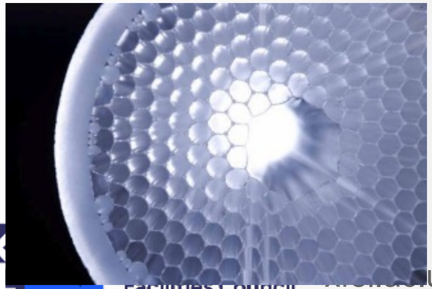
~100 Hz

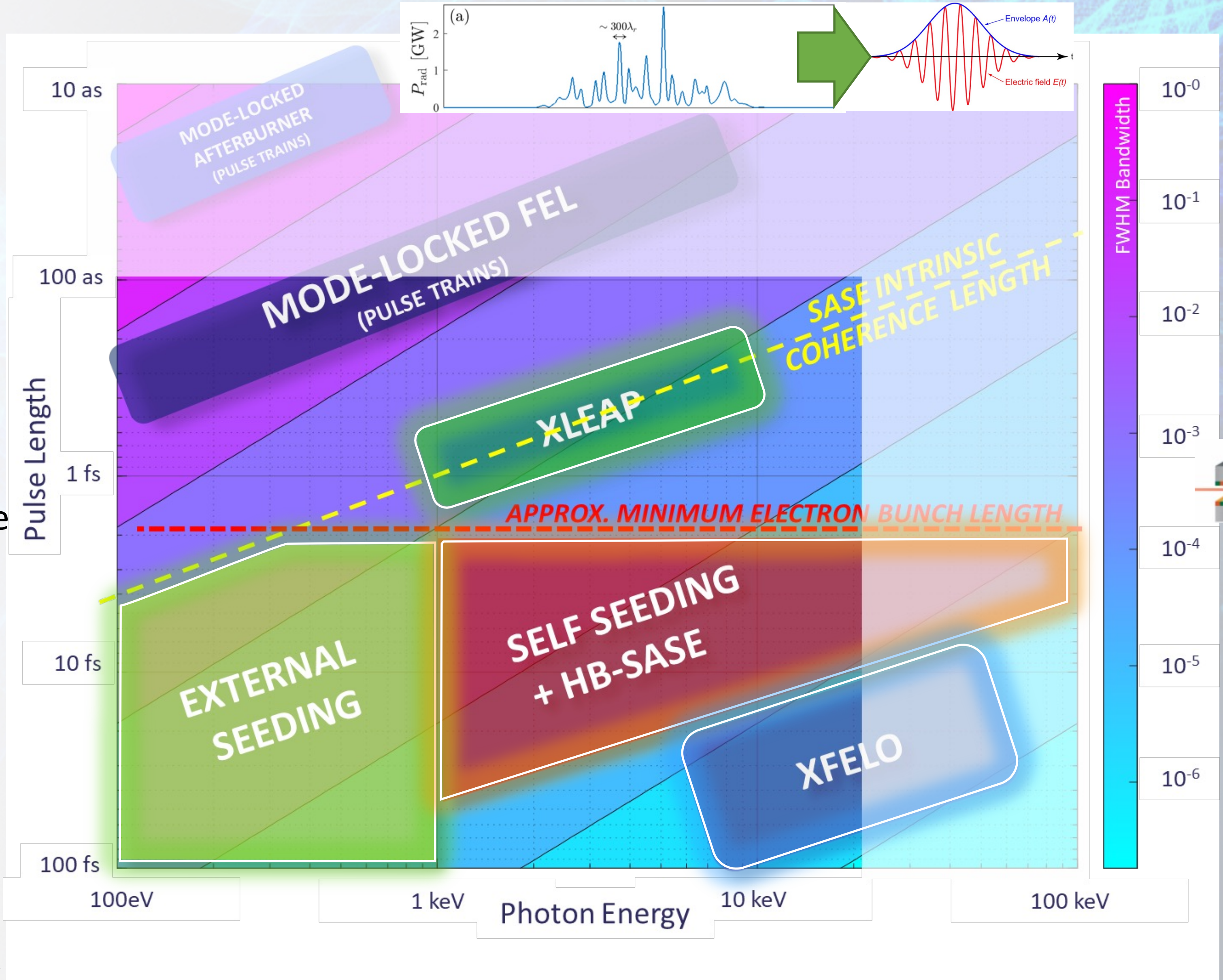
Near-transform-limited pulses

Generating near-transform-limited pulses across a wide range of energies and pulse lengths requires a variety of techniques

- Attosecond pulses tightly synchronised to external sources (e.g. **XLEAP**)

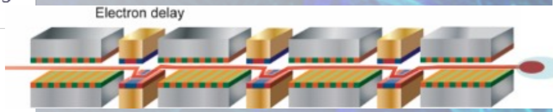
- Advances in high rep-rate lasers (e.g. Kagome fibres) for ≤ 1MHz UV **seeding** + harmonic FEL conversion to ≤ 2 keV





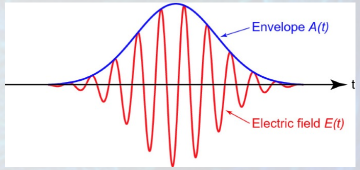
- **HB-SASE** for 25keV, 2.5 fs duration, TW peak power, >mJ pulse energy, 8 × 10^{-5} FWHM BW, at any e-beam repetition rate

HB-SASE schematic



- Enhanced **self-seeding** for few-GW 30 fs stable coherent SXR pulses
- Cavity XFELs: RAFEL, **XFELO** for narrowest bandwidth

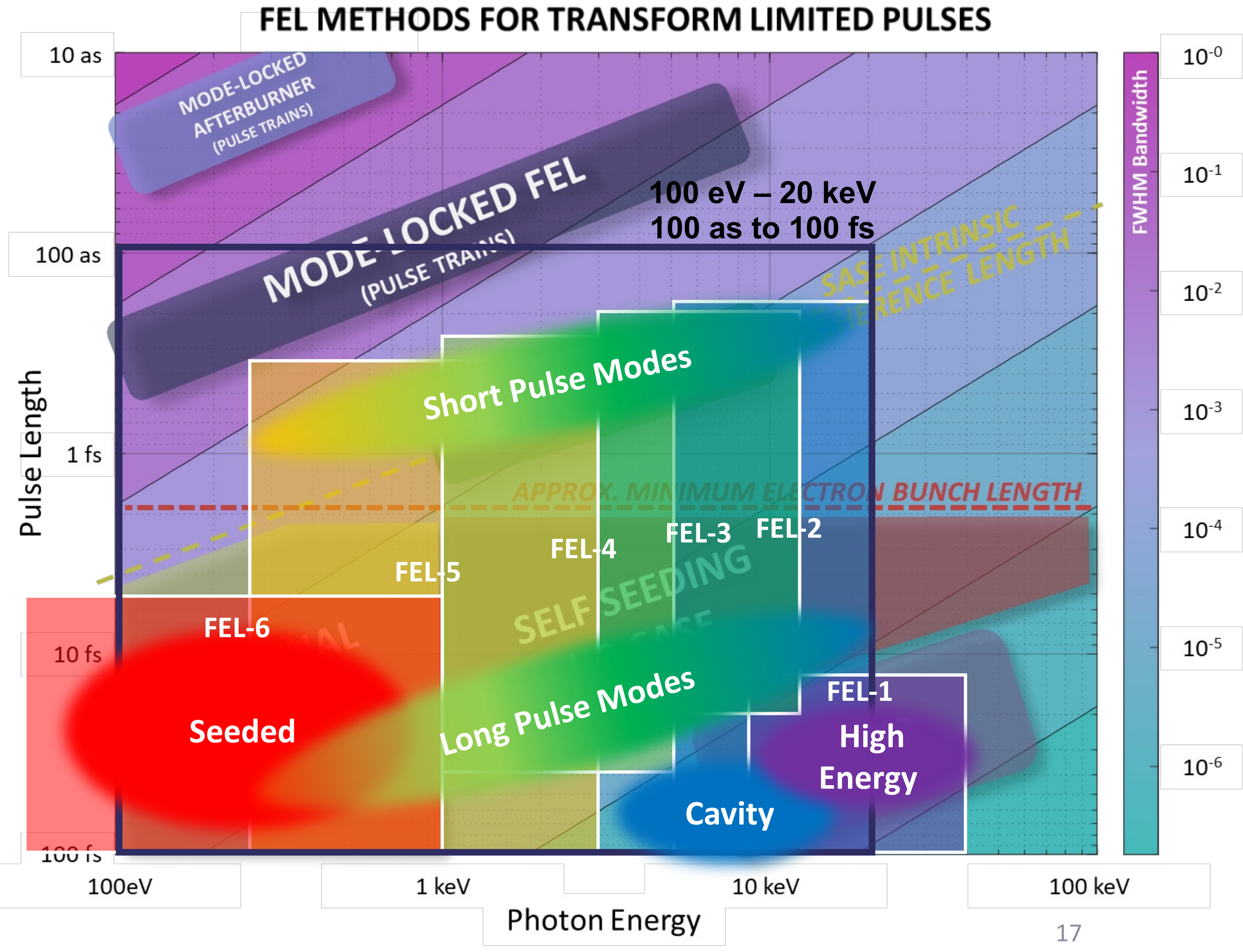
Proposed FEL modes



Each FEL has 1-3 primary operating modes, covering both short-pulse and long-pulse options

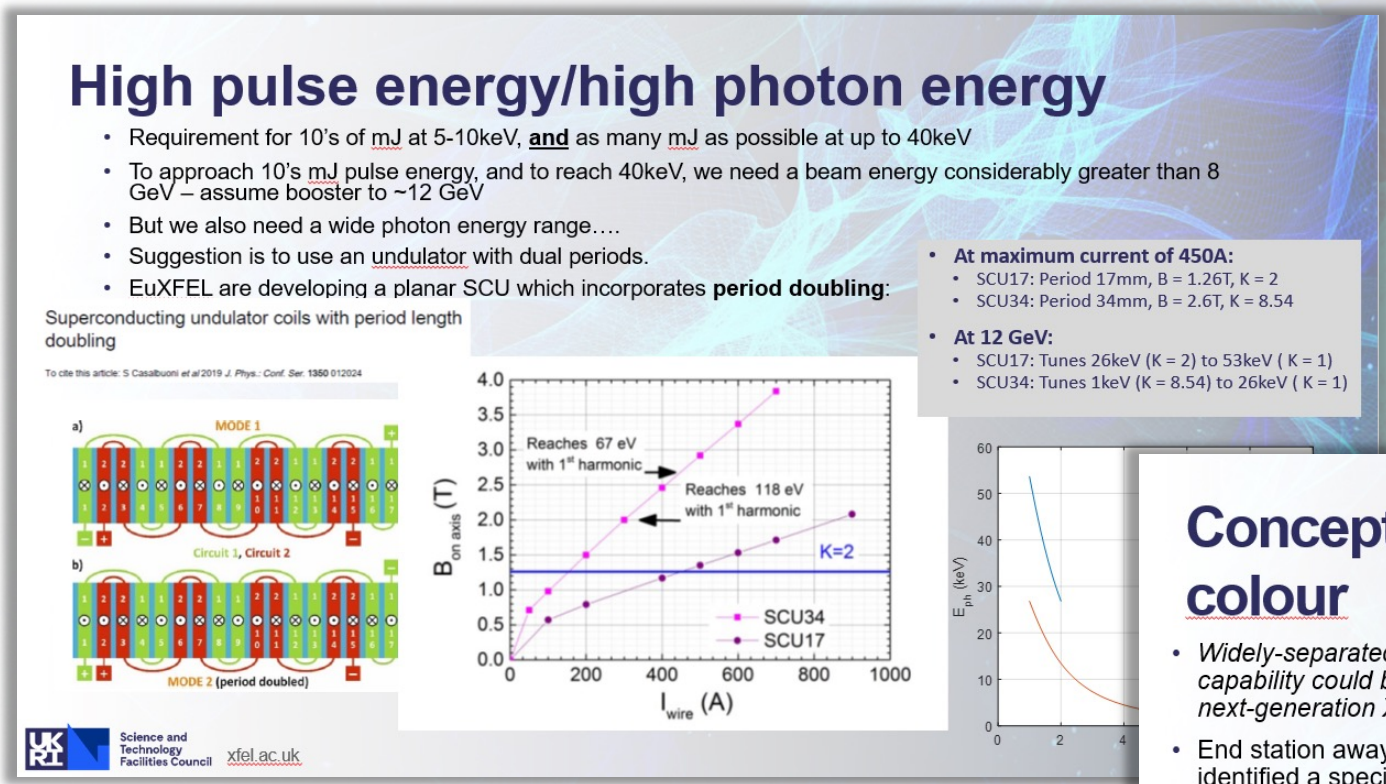
FEL	Tuning	Mode	Technique	Transform Limited Pulse Duration
FEL-6	0.05 – 1.0 keV	Seeded	EEHG	5 – 100 fs
FEL-5	0.25 – 3.0 keV	Long pulse	EEHG/HB	100 fs – 20 fs
		Short Pulse	XLEAP	2 fs – 350 as
FEL-4	1.0 – 5.0 keV	Long Pulse	HB-SASE	40 fs – 15 fs
		Short Pulse	XLEAP	800 as – 275 as
FEL-3	3.0 – 13.0 keV	Long Pulse	HB-SASE	20 fs – 10 fs
		Short Pulse	XLEAP	400 as – 200 as
FEL-2	5.0 – 20.0 keV	Long Pulse	HB-SASE	16 fs - 12 fs
		Short Pulse	XLEAP	300 as – 200 as
		Cavity	XFELO	~ 100 fs
FEL-1	9 – 20 keV	High Power	SASE	~ 30 fs (not TL)
	13 – 30keV*	High Energy		
	20 – 40keV*	High Energy		

*via booster, possibly at lower rep. rate

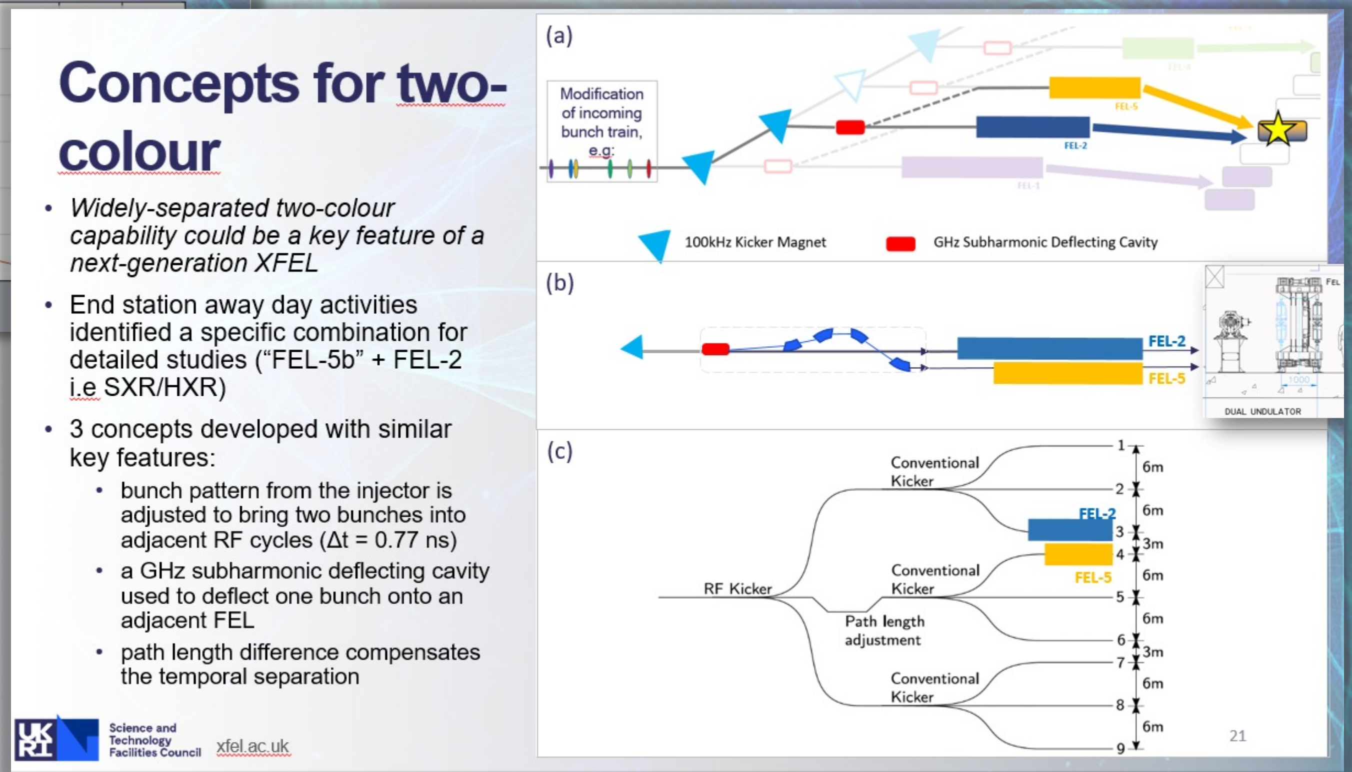


Pulse durations estimated from simulations/scaling, intermediates between short and long pulse modes also accessible.

Other FEL capabilities



- **Demand for 10's mJ pulse energy at 5-10 keV, and to reach 40 keV**
- We need a beam energy considerably greater than 8 GeV – assume booster to ~12 GeV
- Potential to use dual-period undulators



- **Widely-separated two-colour capability could be a key feature of a next-generation XFEL**
- Various concepts to generate SXR + HXR combinations

Other key facility features

Synchronous sources

A laser facility as well as an XFEL facility:

- High rep. rate femtosecond pumping from 10 nm - 10 μm, as per UK Artemis and Ultra facilities
- A high power (multi-PW, $>10^{22}$ Wcm^{-2}) and high energy (kJ-class) laser facility as large as budget allows
  - Scalable and tunable diode-pumped laser technology (e.g. CLF DiPOLE)
  - High repetition-rate (>10 Hz)

Central Laser Facility's Gemini facility

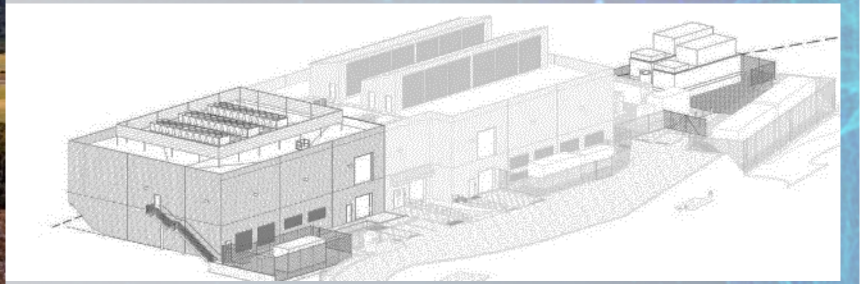
Next-gen XFELs are expected to be some of the biggest data machines on the planet

Unprecedented requirements in both data rates (towards TB/s) and scale (PB per data set). AI potential for real-time feedback for experiment steering. Trend for data processing at the detector as part of combined detector-data pipeline

Focus is on the following areas:

- Data handling
- Applications of Machine Learning at an XFEL
- Conceptual designs and frameworks to enable Machine Learning
- Developing connections with relevant AI and Exascale expertise within the UK

Data Centres



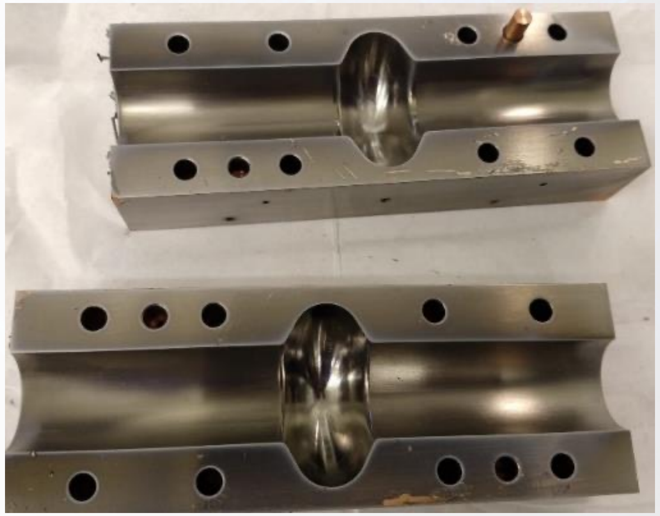
Footprint ~ 80x30m
Power ~ 6MW

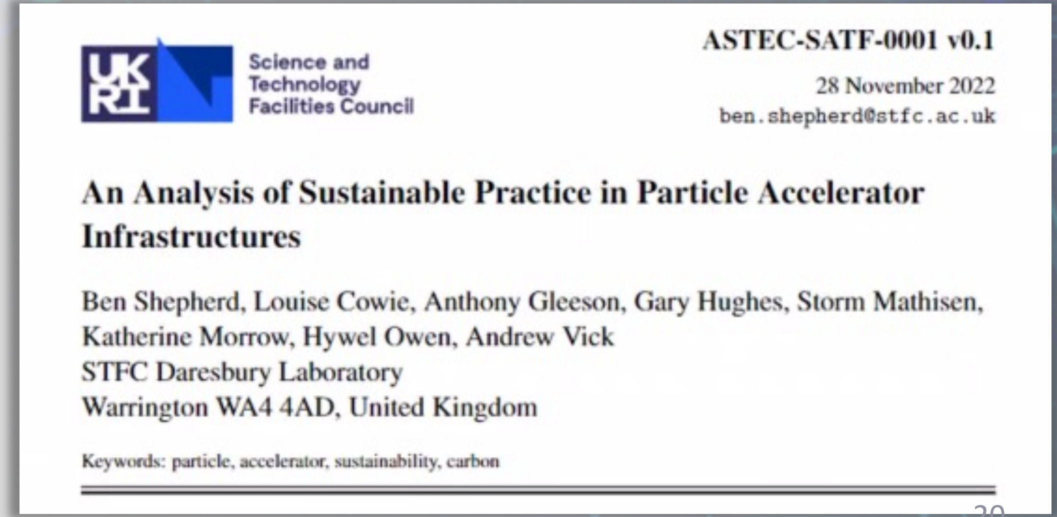
Sustainability

The UK accelerator community is already very active in developing more sustainable technologies:

- Using permanent magnets instead of electromagnets
- Making use of different superconducting materials and coatings for RF cavities so that they can operate at 4K instead of 2K
- Developing more efficient RF power sources and much faster RF cavity tuners

In addition we are assessing accelerators more broadly in terms of carbon footprint throughout the full project life cycles (many other factors besides accelerator technology: buildings, travel, data centres etc.). This analysis will continue and feed directly into the CDOA project.





Science and Technology Facilities Council

ASTEC-SATF-0001 v0.1

28 November 2022

ben.shepherd@stfc.ac.uk

An Analysis of Sustainable Practice in Particle Accelerator Infrastructures

Ben Shepherd, Louise Cowie, Anthony Gleeson, Gary Hughes, Storm Mathisen, Katherine Morrow, Hywel Owen, Andrew Vick
STFC Daresbury Laboratory
Warrington WA4 4AD, United Kingdom

Keywords: particle, accelerator, sustainability, carbon

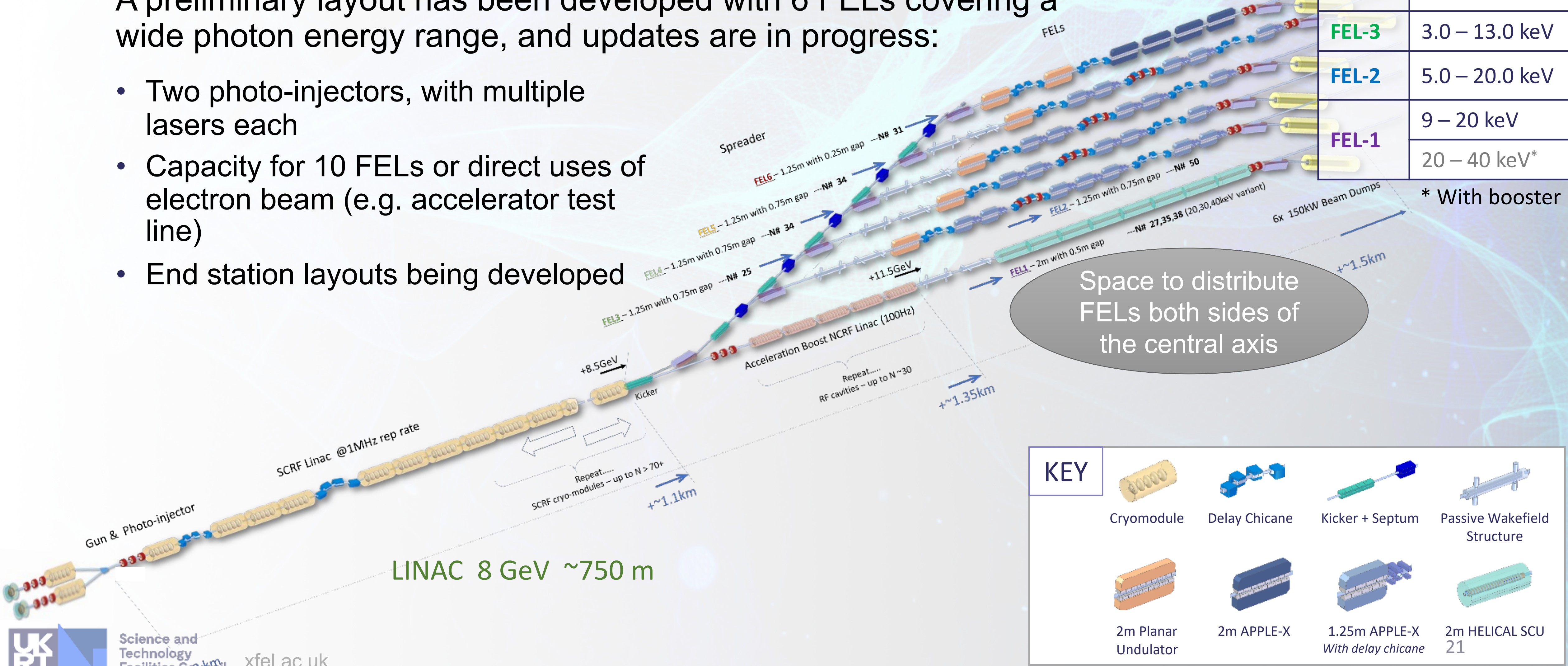
Preliminary layout (1)

A preliminary layout has been developed with 6 FELs covering a wide photon energy range, and updates are in progress:

- Two photo-injectors, with multiple lasers each
- Capacity for 10 FELs or direct uses of electron beam (e.g. accelerator test line)
- End station layouts being developed

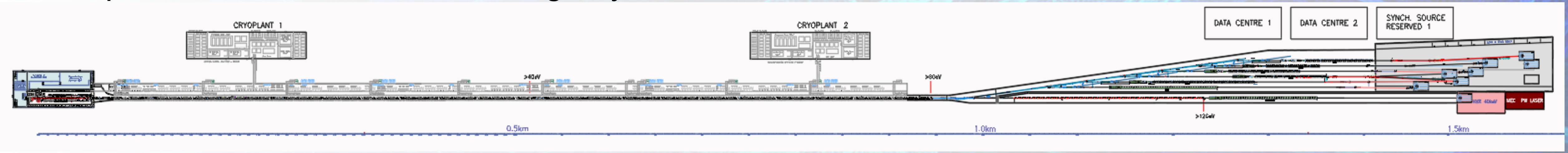
FEL	Tuning
FEL-6	0.05 – 1.0 keV
FEL-5	0.25 – 3.0 keV
FEL-4	1.0 – 5.0 keV
FEL-3	3.0 – 13.0 keV
FEL-2	5.0 – 20.0 keV
FEL-1	9 – 20 keV
	20 – 40 keV*

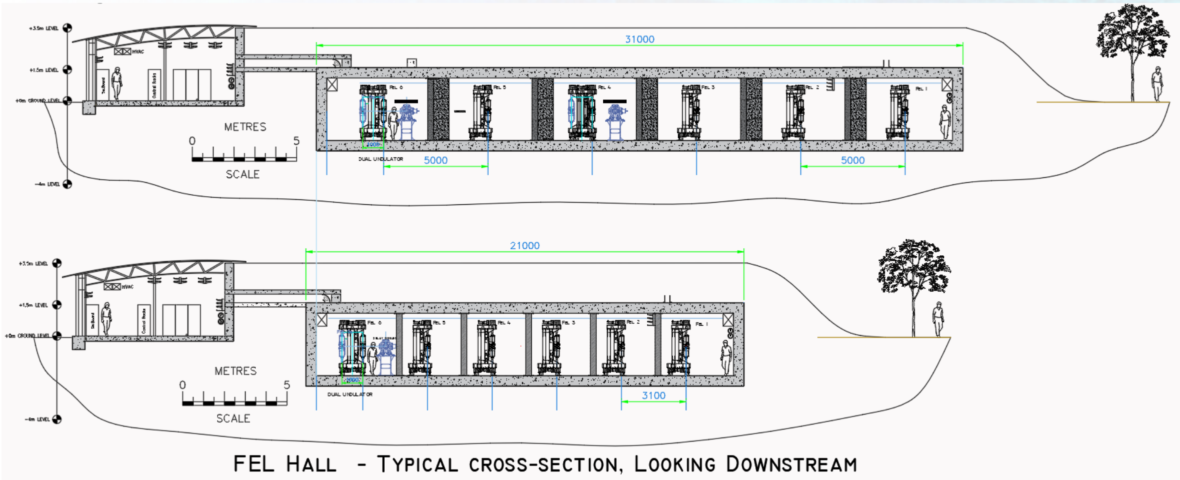
* With booster



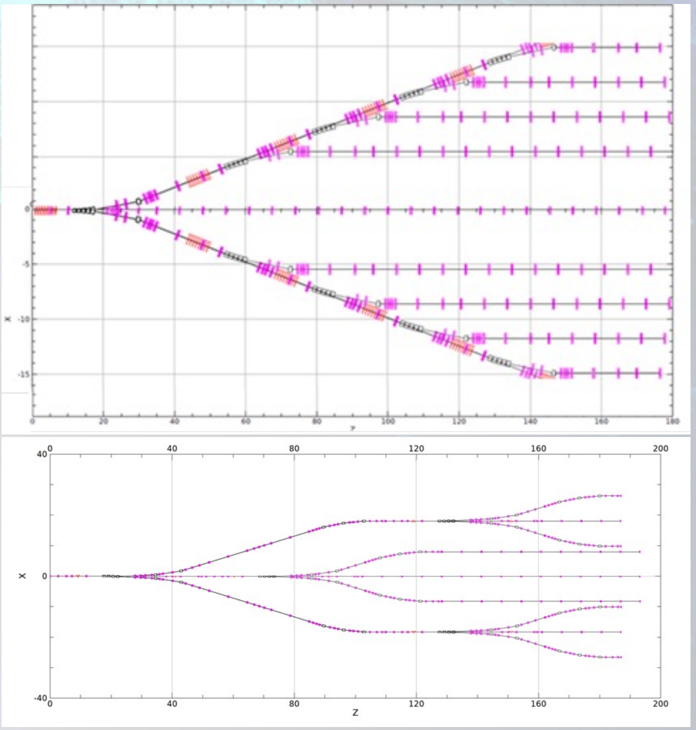
Preliminary layout (2)

Various options are still being considered for different aspects of the design, aiming to produce a self-consistent design by October 2024

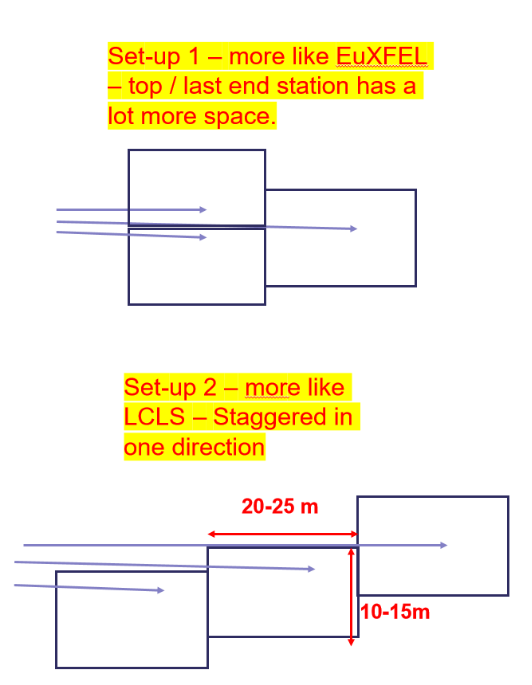




Undulator enclosures



Spreader layouts



End-station layouts

Summary and next steps

- XFELs are a revolutionary technology, which are set to develop substantially in capability and capacity in coming years
- We've formed strong links with existing XFELs, working towards similar aims
- We've made significant progress in developing a concept to meet the key requirements: self-consistent design by October 2024
- Next, we will compare UK vs international investment options + identify key R&D areas for future phases
- Continuing Town Hall meeting series to extend the community and inform the design
  https://xfel.ac.uk/events/

- **North-West England Townhall (hosted by Royce Institute, 8th and 9th August 2024)**
  Focus discussion topic: Electronics, photonics and quantum technologies
- **Wales Townhall (hosted Cardiff 17th and 18th September 2024)**
  Focus discussion topic: Advanced materials and manufacturing

Contact: ukxfel@stfc.ac.uk

UK XFEL

UKRI Science and Technology Facilities Council

Science Team

- Imperial College London
- Brookhaven National Laboratory
- Newcastle University
- University of Plymouth
- The University of Edinburgh
- University of Oxford
- King's College London
- University of Southampton
- ICFO
- University of Leeds
- AWE
- The Cockcroft Institute of Accelerator Science and Technology
- UCL
- diamond
- University of York
- Rolls-Royce
- University of Strathclyde Glasgow
- Queen's University Belfast
- University of Sheffield

UK Research Councils & Government

- UKRI UK Research and Innovation
- Biotechnology and Biological Sciences Research Council
- Economic and Social Research Council
- Research England
- Engineering and Physical Sciences Research Council
- Natural Environment Research Council
- Innovate UK
- Medical Research Council
- Arts and Humanities Research Council
- Department for Science, Innovation & Technology

Other XFELs

- European XFEL
- Paul Scherrer Institut PSI
- LCLS
- 中国科学院上海高等研究院 SHANGHAI ADVANCED RESEARCH INSTITUTE, CHINESE ACADEMY OF SCIENCES
- SACLA

Science and Technology Facilities Council

Thank You

- North-West England Townhall (hosted by Royce Institute, 8th and 9th August 2024)
  Focus discussion topic: Electronics, photonics and quantum technologies
- Wales Townhall (hosted Cardiff 17th and 18th September 2024)
  Focus discussion topic: Advanced materials and manufacturing

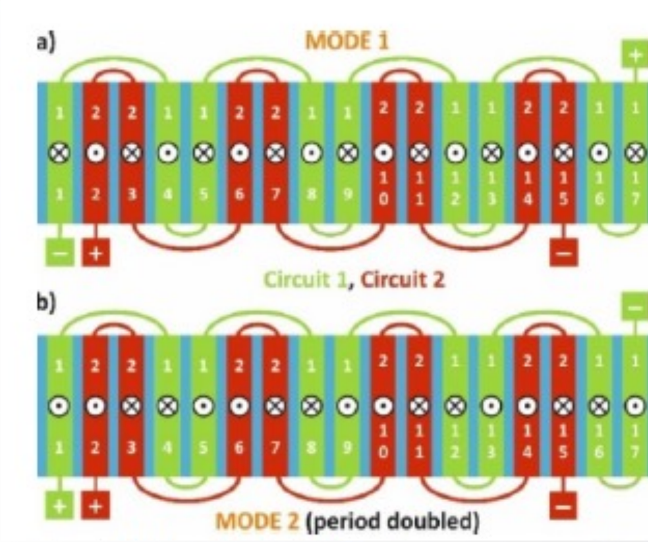
Contact: ukxfel@stfc.ac.uk

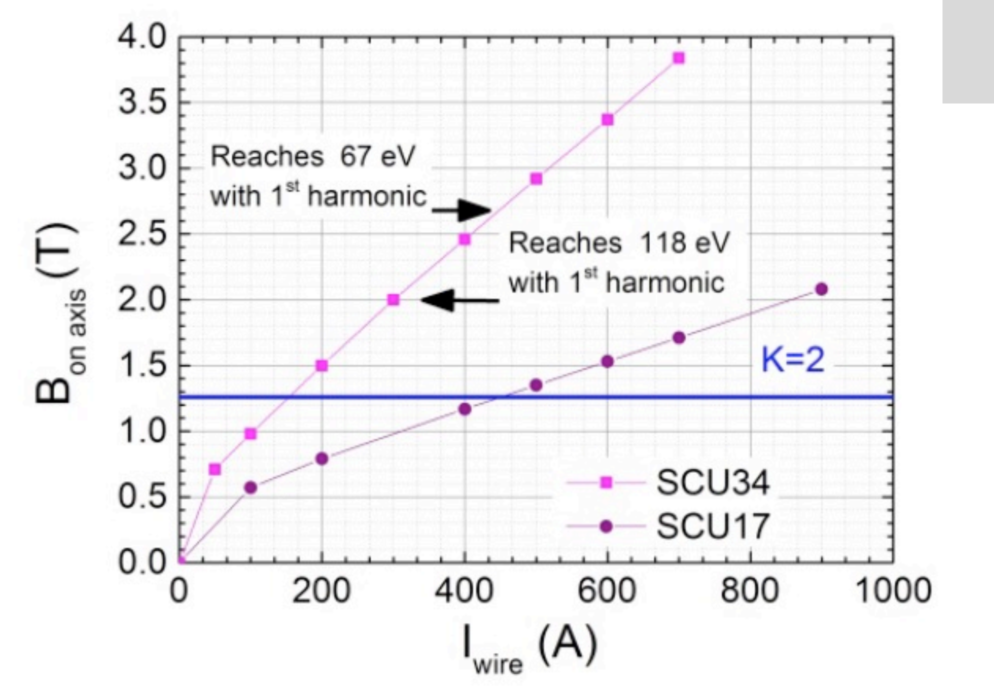
High pulse energy/high photon energy

- Requirement for 10's of mJ at 5-10keV, **and** as many mJ as possible at up to 40keV
- To approach 10's mJ pulse energy, and to reach 40keV, we need a beam energy considerably greater than 8 GeV – assume booster to ~12 GeV
- But we also need a wide photon energy range….
- Suggestion is to use an undulator with dual periods.
- EuXFEL are developing a planar SCU which incorporates **period doubling**:

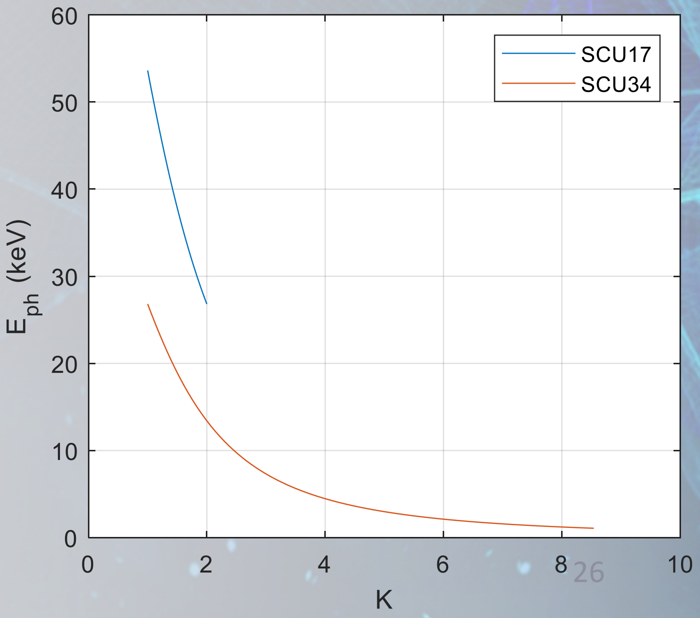
Superconducting undulator coils with period length doubling

To cite this article: S Casalbuoni *et al* 2019 *J. Phys.: Conf. Ser.* **1350** 012024





- **At maximum current of 450A:**
  - SCU17: Period 17mm, B = 1.26T, K = 2
  - SCU34: Period 34mm, B = 2.6T, K = 8.54
- **At 12 GeV:**
  - SCU17: Tunes 26keV (K = 2) to 53keV (K = 1)
  - SCU34: Tunes 1keV (K = 8.54) to 26keV (K = 1)

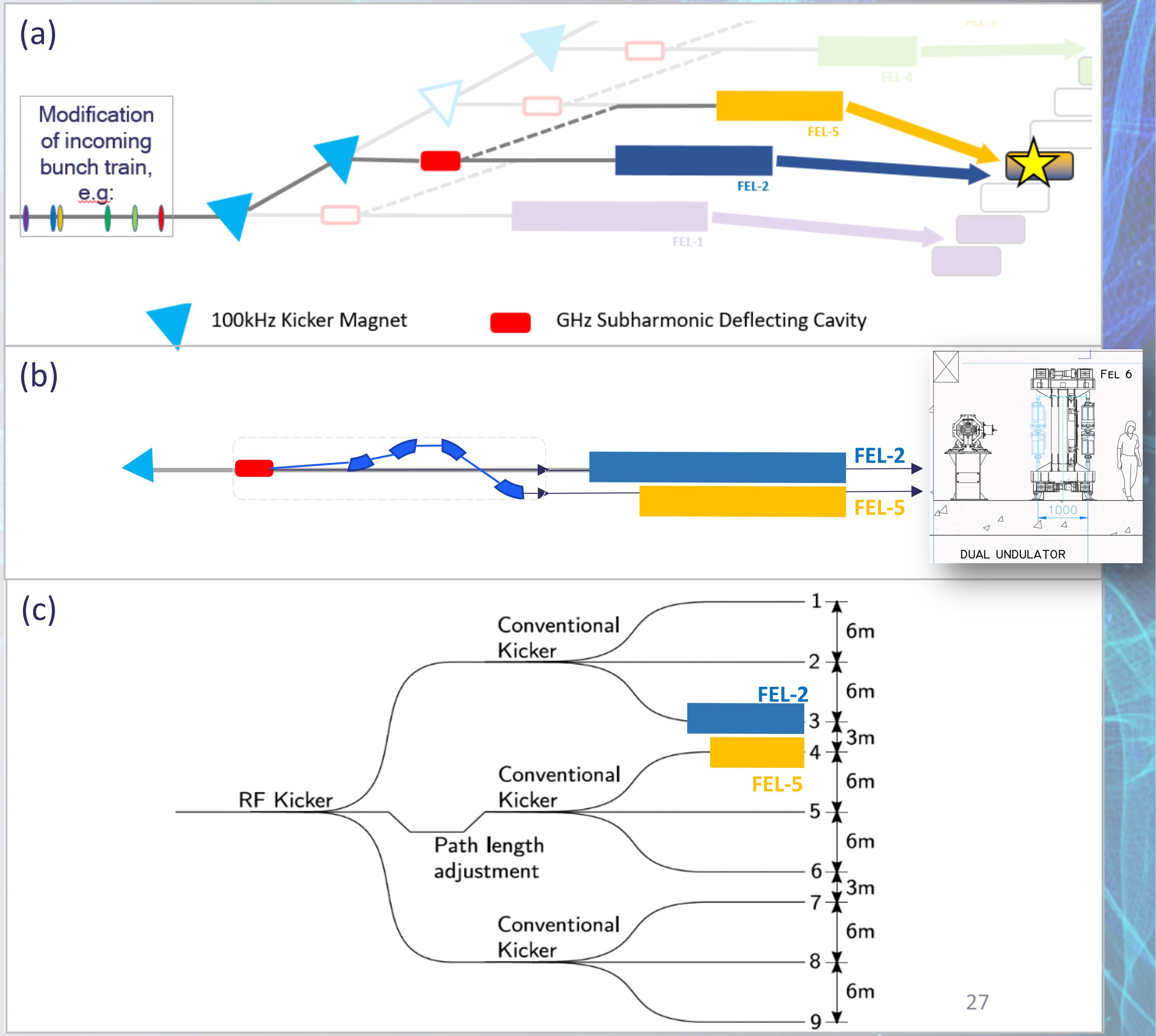


Science and Technology Facilities Council

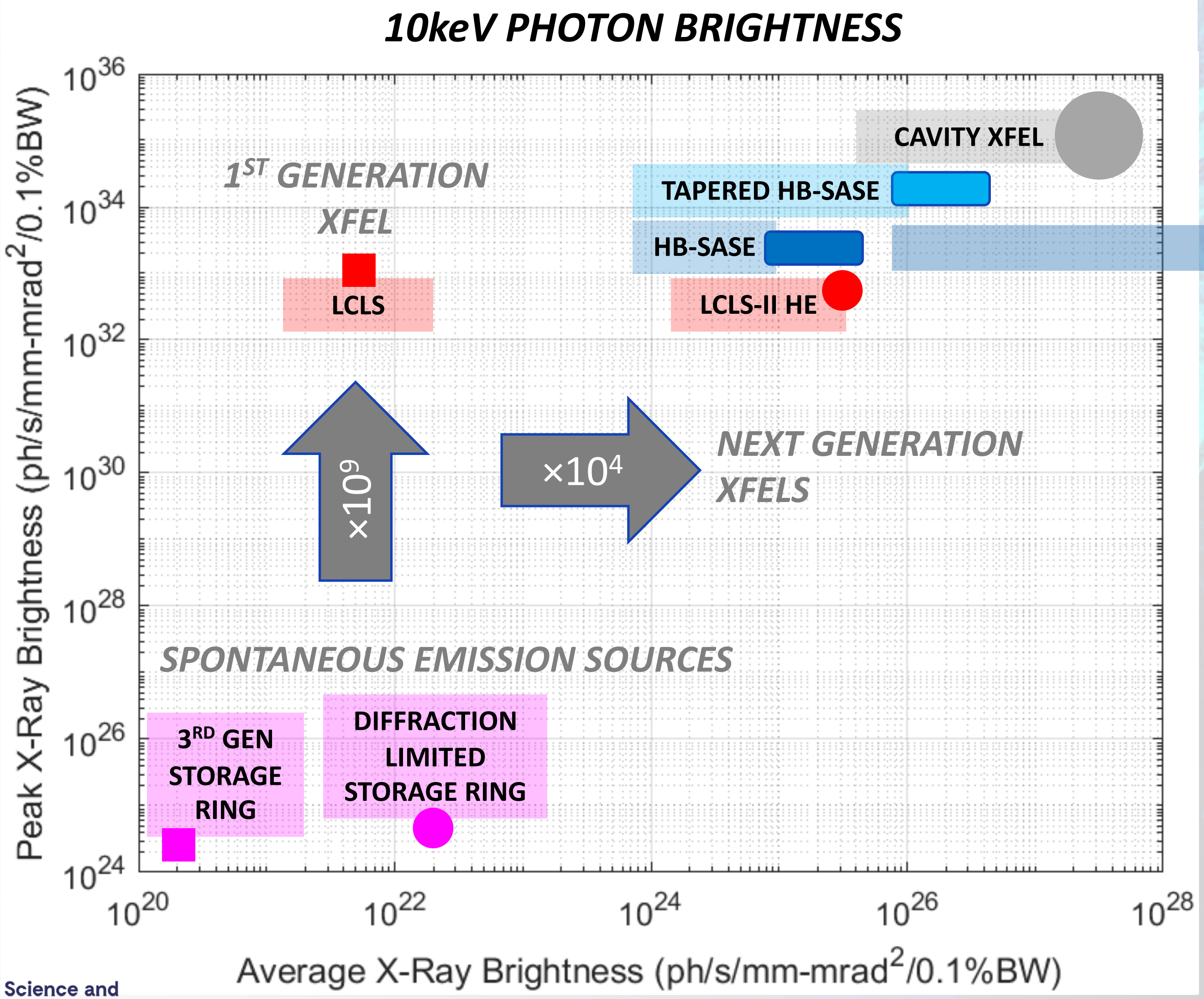
xfel.ac.uk

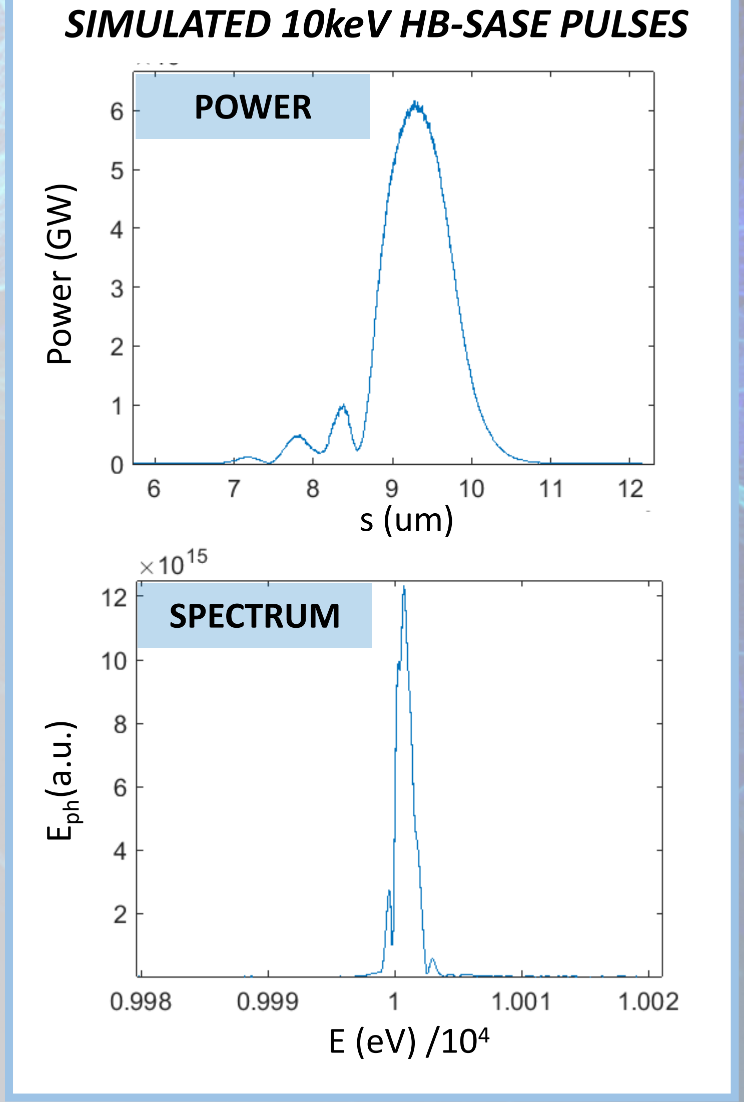
Concepts for two-colour

- *Widely-separated two-colour capability could be a key feature of a next-generation XFEL*
- End station away day activities identified a specific combination for detailed studies (“FEL-5b” + FEL-2 i.e SXR/HXR)
- 3 concepts developed with similar key features:
  - bunch pattern from the injector is adjusted to bring two bunches into adjacent RF cycles (Δt = 0.77 ns)
  - a GHz subharmonic deflecting cavity used to deflect one bunch onto an adjacent FEL
  - path length difference compensates the temporal separation



Evolution of peak and average brightness





Adapted from LCLS figure: Mike Dunne, SLAC, Future Developments at LCLS, UK XFEL Launch Event 2023 https://youtu.be/sxipwNyXMhg