Science Case for a UK XFEL

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Contents of talk

- Overview of science drivers for an XFEL
- Survey of the Science Case
- UK X-ray FEL options
- Next steps

- Download case:

https://stfc.ukri.org/news/uk-xfel-draft-science-case-consultation/

Developing a Science Case for a UK XFEL

- Science Team of 25 scientists with ~ 80 additional science and technology expert advisors
- A free format consultation with the UK science and technology community

https://stfc.ukri.org/news/uk-xfel-draft-science-case-consultation/

- Organised 7 community workshops in 2019:

Jul 16th	***Launch Meeting (Royal Society)***	***[72]***
Oct 2nd	***Matter at Extreme Conditions (Edinburgh)***	***[27]***
Nov 5th	***Life Sciences (Crick)***	***[160]***
Nov 13th	***Frontiers in Physical Sciences (Imperial)***	***[102]***
Nov 27th	***Quantum Materials & Nanotechnology (Southampton)***	***[40]***
Dec 4th	***X-ray FEL Applications (Warwick)***	***[29]***
Dec 11th	***Chemical Dynamics & Energy (Newcastle)***	***[50]***

- A science case was drafted through early 2020 with submission 22nd May of a Draft Science Case to STFC which is now available publicly
- From July to mid-September possibilities for continued engagement with the UK community
- **Project Lead:** Jon Marangos, **STFC Project Champion:** John Collier

xfelsciencecase@stfc.ac.uk

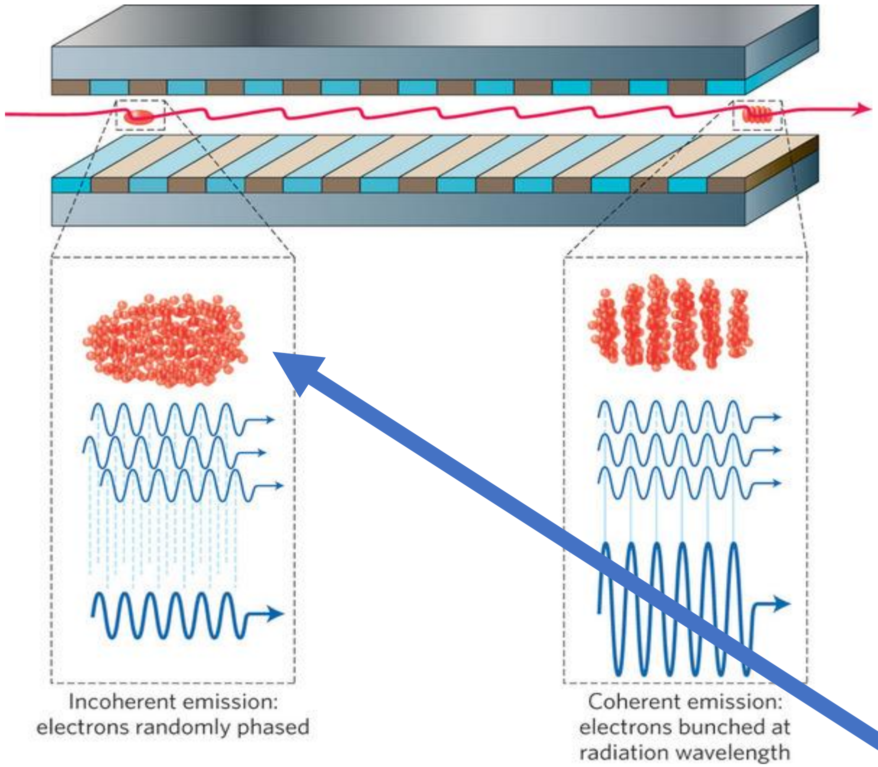
Science Team

- **Matter in extreme conditions**: Andy Higginbotham (York), Andy Comley (AWE), Sam Vinko (Ox), Marco Borghesi (QUB), Malcolm McMahon (Edinburgh), Justin Wark (Ox)
- **Nano/Quantum materials**: Ian Robinson (UCL/Brookhaven), Anna Regoutz (UCL), Marcus Newton (Soton), Mark Dean (Brookhaven), Simon Wall (ICFO)
- **Materials/Applications** : David Rugg (RR), Sven Schroeder (Leeds), David Dye (IC)
- **Life sciences**: Allen Orville (DLS), Jasper van Thor (IC), Xiaodong Zhang (IC)
- **Chemical sciences**: Julia Weinstein (Sheffield), Russell Minns (Soton), Sofia Diaz-Moreno (DLS), Tom Penfold (Newcastle)
- **Physical sciences**: Adam Kirrander (Edinburgh), Amelle Zair (KCL), Jason Greenwood (QUB), Jon Marangos (IC)

X-ray FEL Using Coherent High Brightness X-rays From SASE (Self Amplified Spontaneous Emission)

Undulator

Input
Low emittance,
narrow energy spread,
relativisitic electron
bunch
4 – 15 GeV



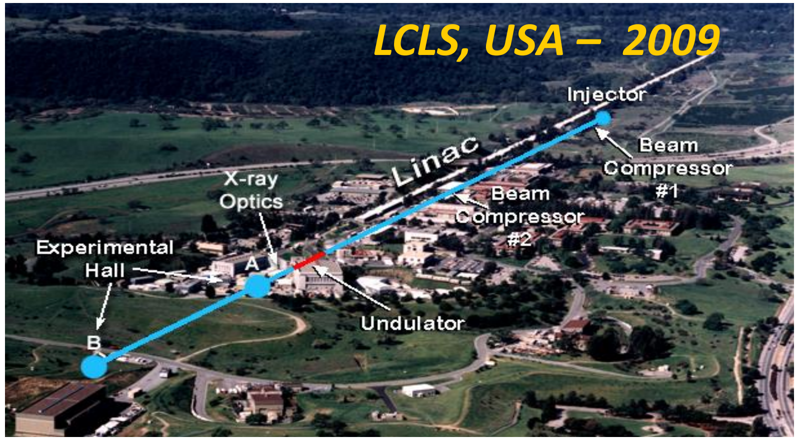
Output
High brightness,
short pulse of coherent
soft to hard X-rays

Further unique opportunities afforded if synchronised to X-rays we have ultrafast sources: XUV to MIR, THz, electron/proton beams, high energy/high power lasers and significant repetition rate

New modes are becoming available that prepare electron bunch properties to increase X-ray coherence and/or shorten pulse – exploiting these will be key to new capabilities of a UK XFEL

- Laser like X-rays
- Pulses < 10 fs
- X-rays for structural dynamics methods (e.g. XAS, IXS, X-ray diffraction)
- Exceptional brightness

Existing X-ray FELs: Developed over the past decade it is anticipated that these will satisfy scientific need for next 5 to 10 years

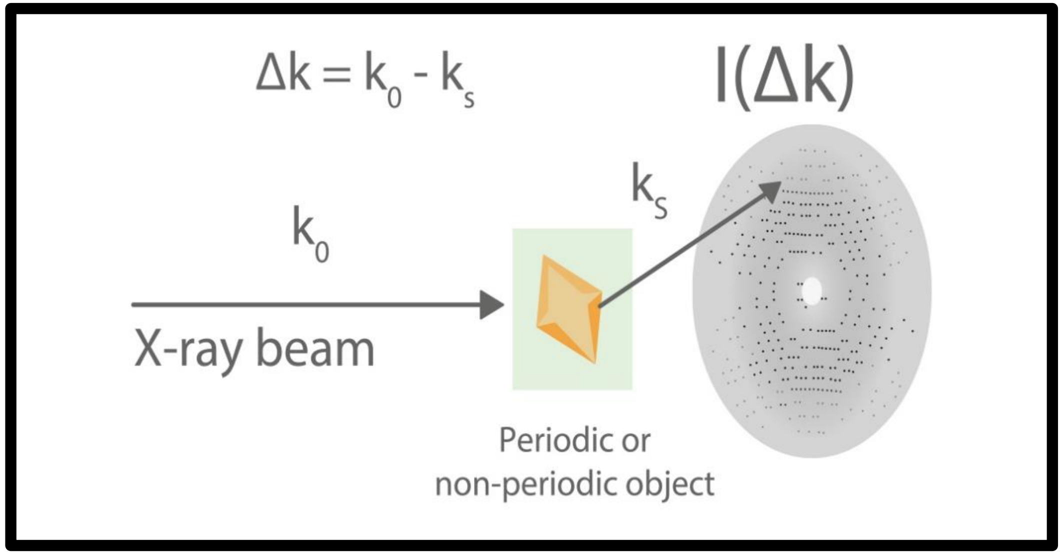


Facility Summary

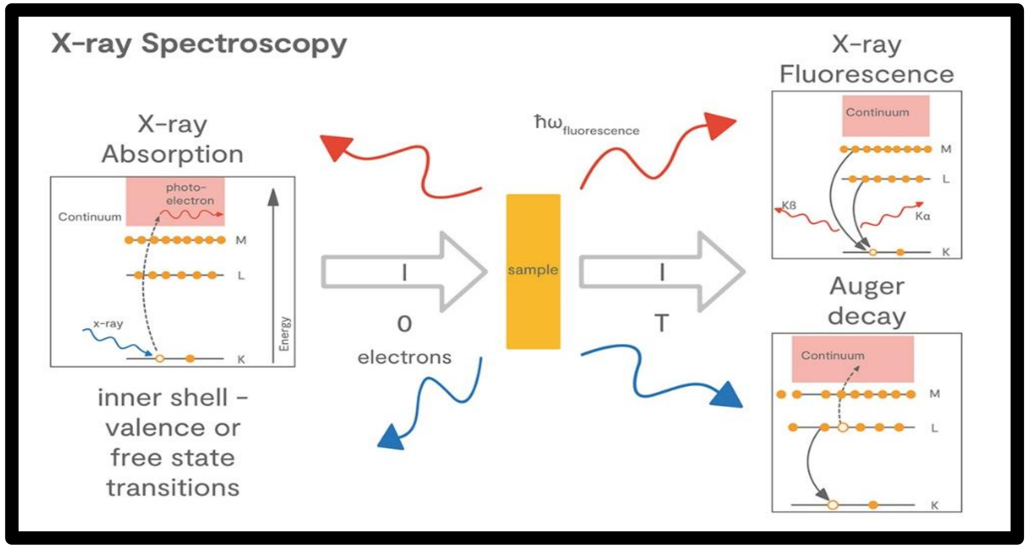
LCLS (USA)
LCLS II & LCLS II HE (USA)
SACLA (Japan)
European XFEL (Germany)
Flash I & II (Germany)
Fermi@Elettra (Italy)
Swiss FEL (Switzerland)
PAL XFEL (Korea)
Dalian Light Source (China)
Shanghai Light Source (China)

Other projects under consideration

X-ray time resolved probing of the nanoscale



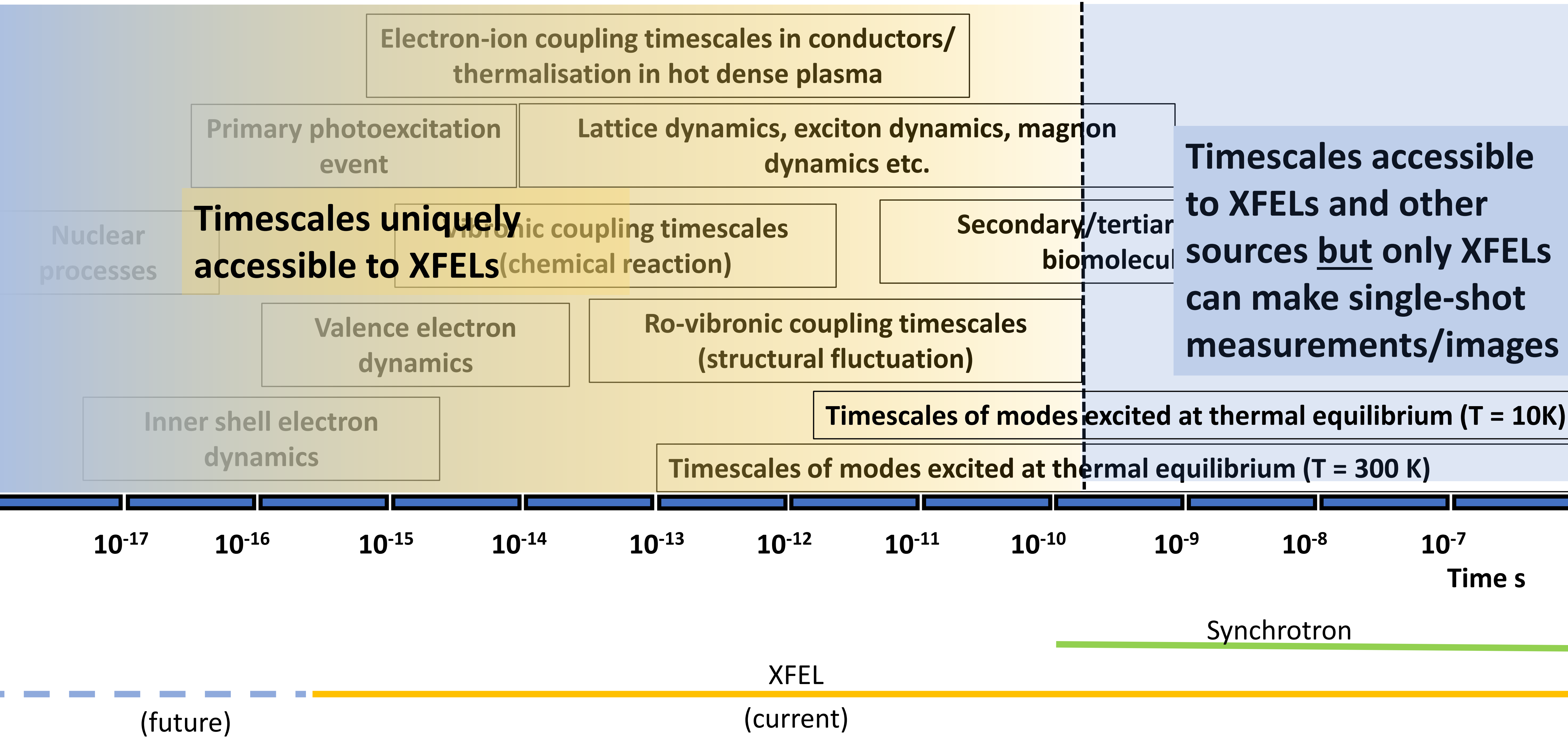
X-ray Scattering for
Structure & Structural Dynamics



X-ray Spectroscopy
Electronic States and Occupations

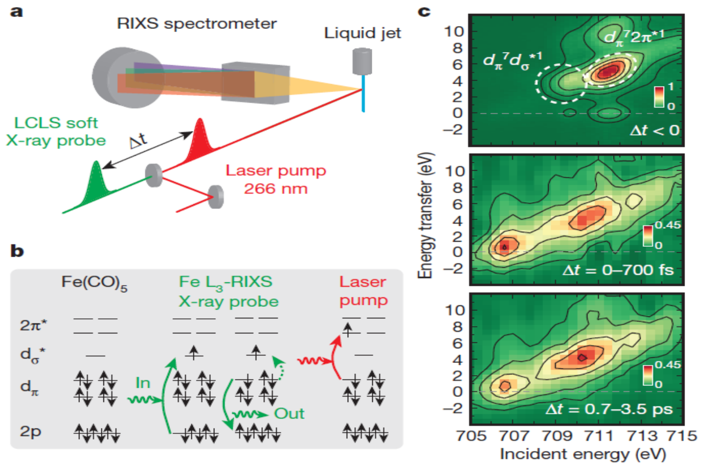
New Methods Enabled by High Brigthness e.g.
X-ray Thompson Scattering
Coherent Diffraction Imaging
Resonant Inelastic Scattering
Non-linear X-ray Spectroscopy

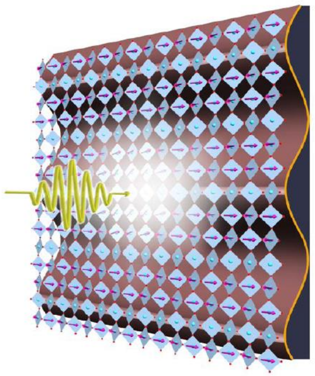
Primary science driver is real-time access to the characteristic processes and fluctuations in matter at the quantum scale



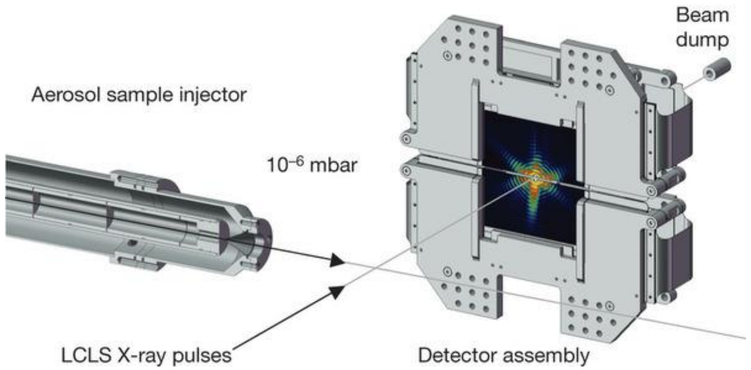
Demonstrated science opportunities with an XFEL

Access to structural dynamics: *electronic dynamics, lattice dynamics and chemical bonds breaking/forming*. Important to e.g**. catalysis, biochemistry, fast data storage, energy storage, solar energy, solar fuels & carbon capture**

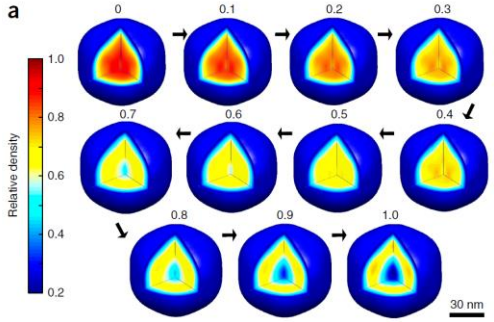




Access to transient states: *extreme pressure, high E & B fields, laser dressing and high energy density.* Important to e.g. **planetary science, astrophysics, quantum materials, engineering & defence**



New modes of crystallography & nanoscopic imaging: *nanomaterials, bioimaging and protein structures.* Important to e.g. **drug discovery, functional materials and aerosols/particulates**



Capturing rare events/Mapping conformational pathways : In *physical, chemical and biological systems.* Important to e.g. understanding **fundamentals in biology, chemistry in aerosols/particulates, solvation, crystallization, stress development and drug activity**

Development of Science Case

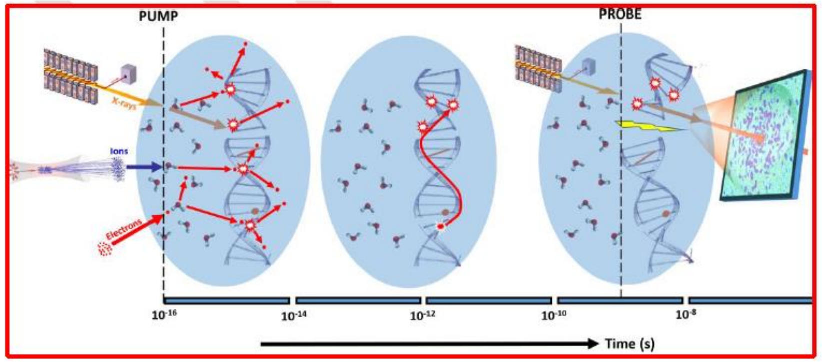
Taking a long view we looked at what kind of science we will do with an advanced XFEL operating from 2030. Extrapolating current technology advances to frame what will be possible…….

Draft UK XFEL Science Case

Released beginning of July 2020 following further revision and input from external reviewers

Here we will overview this (275 page) Science Case……..

Ultrafast X-rays probe attosecond electron dynamics, radiation damage of materials & biomolecules & elementary processes in chemical reactions



3. Science Opportunities in Physics and X-ray Photonics

3.1. Frontiers in ultrafast chemical physics

3.2. New concepts in scattering

3.3. Attosecond science and non-linear X-ray spectroscopy

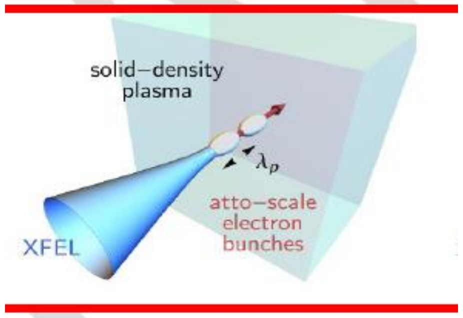
3.4. Capturing conformational dynamics and rare thermodynamic states

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

3.6. High brightness relativistic electron beam science

3.7. References for Section 3

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



4. Science Opportunities for Matter in Extreme Conditions

4.1. Shocked materials and matter at extremes

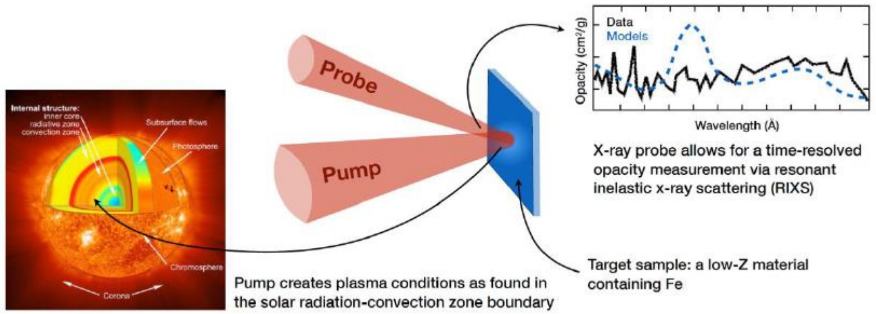
4.2. Quantum plasmas: warm and hot dense matter

4.3. X-ray interactions with laser accelerated electrons

4.4. Coupling an XFEL to a laser-driven spherical compression facility

4.5. References for Section 4

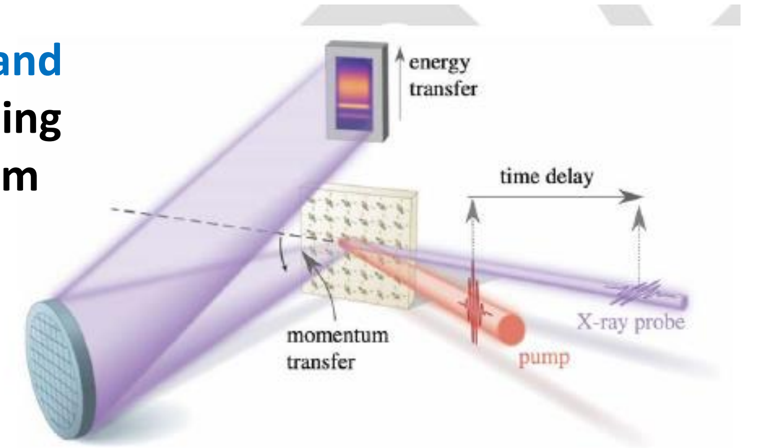
High energy/power optical lasers and bright X-rays access the conditions inside planets, stars and shocked materials in engineering, defence & fusion energy



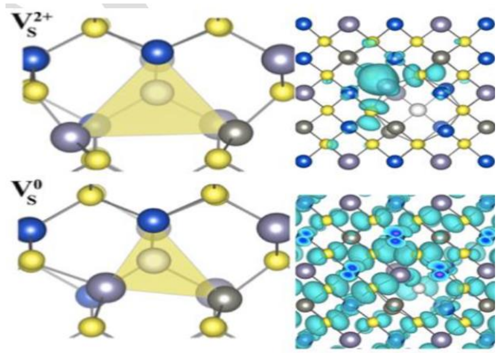
5. Science Opportunities in Quantum and Nanomaterials
5.1. Magnetic materials and control of ultrafast magnetisation
5.2. Structural dynamics and light induced phases in quantum materials
5.3. Imaging dynamics in nanomaterials
5.4. Electronic dynamics in quantum materials
5.5. Time resolved pair distribution functions
5.6. Concluding remarks
5.7. References for Section 5

6. Science Opportunities in the Chemical Sciences and Energy
6.1. Fundamentals of reaction dynamics: Coupling between nuclear, electronic and spin degrees of freedom
6.2. Exploring complex energy landscapes through chemical activation
6.3. Energy materials and devices: Solar cells and batteries
6.4. Understanding catalysis
6.5. Chemistry and the environment: Aerosol, atmospheric, space chemistry, combustion, corrosion
6.6. Conclusions and vision: XFEL and chemical sciences
6.7. References for Section 6

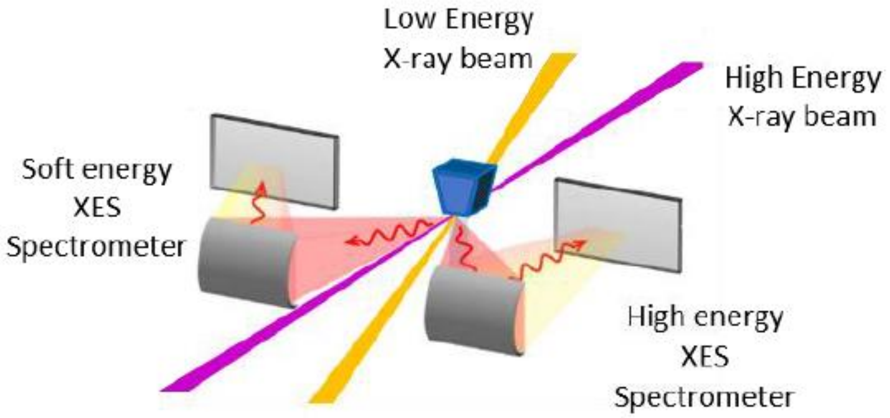
High spectral purity X-rays and high data rates enable probing and optimisation of quantum materials, ultrafast magnetisation & functional materials



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



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



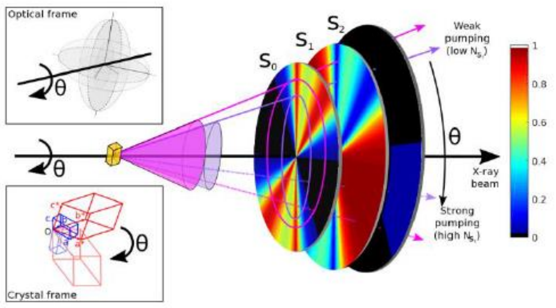
7. Science Opportunities in the Life Sciences

7.1. Serial femtosecond crystallography enabled by XFELs - a new era in structural biology
7.2. Dynamic structural biology: Photosensitive systems
7.3. Dynamic structural biology: Molecular movies of enzyme catalysis
7.4. Controlling and measuring nuclear and electronic coherence within biological systems
7.5. Capturing biological function in single molecules
7.6. Conclusion and summary
7.7. References for Section 7

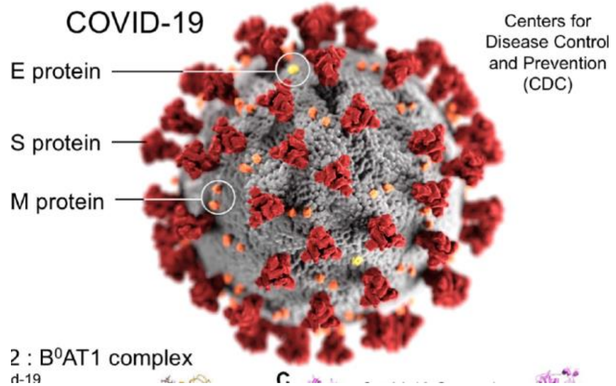
8. Opportunities for UK Industry, Society and Defence

8.1. Addressing national strategic priorities
8.2. Properties of shocked materials for engineering and defence
8.3. Nucleation, solidification and crystallisation in soft-matter
8.4. Dynamic processes in additive manufacturing, combustion, laser machining and photolithography
8.5. Gamma sources application in nuclear security and materials in nuclear industry
8.6. Industrial inspirations from deeper insights into biology: Pharma to clean energy
8.7. Overall economic context
8.8. References for Section 8

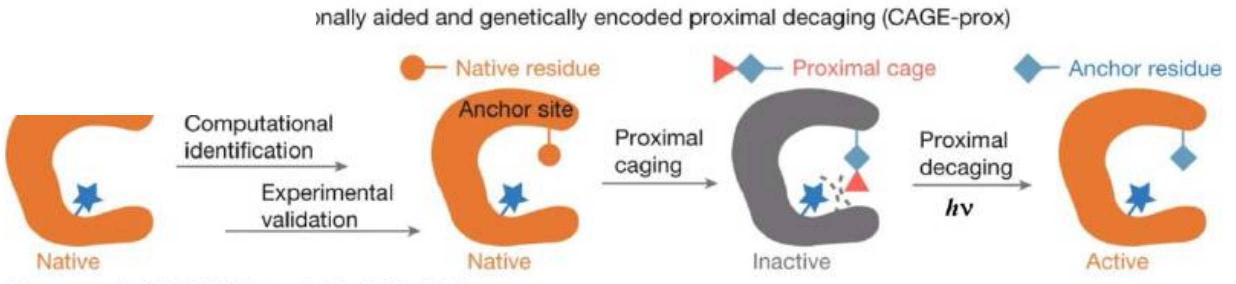
Controlled X-rays and samples will extends the power of serial femtosecond nanocrystallography for advancing knowledge and drug discovery



High data rate will advance the understanding of structural biology and biochemistry under the conditions of life



Multi time-scale X-ray approaches from fs to ns will unravel the complex dynamics of biochemistry: photosynthesis, vision and enzymology



Wang et al (2019) *Nature* 569, 509–513

9. Facility Requirements and Options Analysis

9.1. Facility X-ray requirements

9.2. Facility general requirements

9.3. Synergies with other national facilities and capability: Synergistic technology transfer among XFELs, synchrotrons and electron microscopy / diffraction

9.4. Options analysis:

A. Build a unique UK XFEL optimised for new capability

B. Build a UK XFEL providing capacity well beyond 10 years

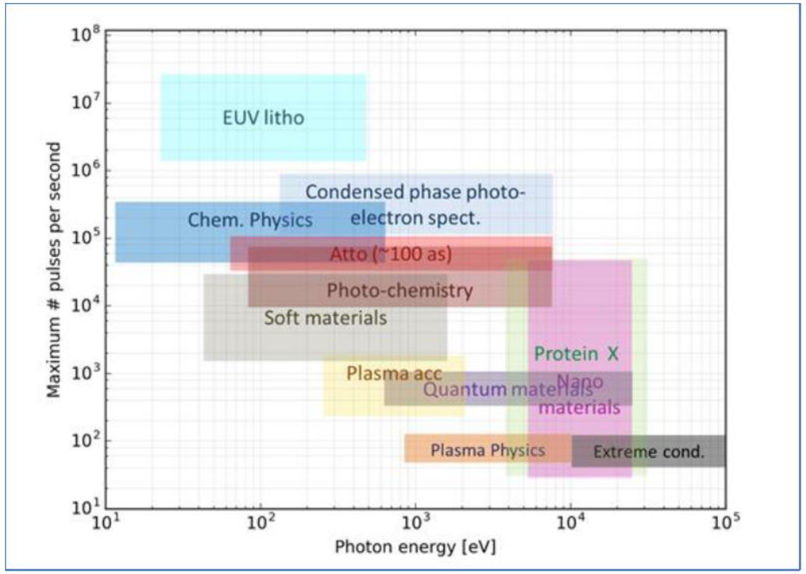
C. Invest more in dedicated UK facilities at existing XFELs

D. Increase investment to support users in exploiting existing opportunities (e.g. long term grant funding schemes, CDTs, "UK XFEL Institute")

E. Dedicated R & D effort towards a future XFEL ("test facility")

F. Extend activities of existing Life and Physical Sciences Hubs

9.5. Next steps



Appendices

Appendix 1: An outline of a technical solution

A1.1 Introduction

A1.2 Key parameters for facility design

A1.3 Other key features

A1.4 Concept outline 1: Superconducting accelerator

A1.5 Concept outline 2: Hybrid accelerator

A1.6 Concept outline 3: Normal conducting accelerator

Appendix 2: Complementarity of techniques

A2.1 Cryo-Electron Microscopy (Cryo-EM), Tomography (cryo-ET), and Diffraction (cryo-ED)

A2.2 Next generation synchrotron light sources

A2.3 Ultrafast electron diffraction (UED)

A2.4 Life Sciences Hub and Roadmap

A2.5 References for Appendix 2

Appendix 3: Complementary Technologies

A3.1 Complementary pulsed X-ray technologies

A3.2 Plasma and laser wakefield acceleration

A3.3 High harmonic sources

A3.4 References for Appendix 3

Appendix 4: Community Engagement, Case Authorship and Development of User Community

A4.1 Workshops and community engagement events

A4.2 Science team

A4.3 Full authorship team of draft Science Case

A4.4 Development of user community

Key science & technology questions that an advanced XFEL can answer

- How can we control states in quantum materials (e.g. superconductivity) with light?
- What are the time scales of electron-, spin- and orbital- coupling in a material?
- What is the x-ray opacity in a stellar interior?
- How do materials behave at the high pressures of planetary cores?
- What are the properties of the quantum vacuum for high intensity X-rays?
- Can we detect dark matter candidates (e.g. axions) using intense X-ray beams?
- How can we understand systems beyond the Born-Oppenheimer approximation?
- What role does quantum coherence play in photochemistry and photophysics?
- How do enzyme catalysed reactions occur in a living cell?
- How do molecular machines efficiently cross energy barriers to drive biological processes?
- What are the fluctuation dynamics of solvation networks in liquids?
- What are the mechanisms of catalysis and how to design better catalysts?
- How can laser processing be made more specific and efficient?
- Can intense X-ray pulses be used for advanced and efficient photolithography?

Amongst many others…….

Impact of space-time resolved X-ray studies

- **New energy materials (e.g. PV's)** can be created based on our emerging understanding of nanoscopic mechanism and quantum scale dynamics
- **Optimised function of catalytic processes** higher efficiency and better use of rare materials, acceleration of recycling of materials through full mechanistic understanding

- **Deeper understanding of biomolecular processes in living cells** will lead to new concepts in healthcare & therapy, advanced therapy and diagnostics
- **Protein structure** (e.g. from serial nano-crystallography) of hard to crystallize molecules leading to drug discovery

- Basic research to **improve batteries and other energy storage materials** from the atomistic level up with full mechanistic understanding
- **More efficient use of energy & distribution** e.g. via new classes of quantum materials with optimized performance

- **New materials and processes for energy efficient data storage** with new insights on nanoscopic and ultrafast mechanisms
- **New ultrafast electronic/optoelectronic devices for advanced information processing (both classical and quantum)** will emerge from research into the nanoscopic dynamics in nanomaterials & quantum materials

Grand challenges

Clean Growth

We will maximise the advantages for UK industry from the global shift to clean growth – through leading the world in the development, manufacture and use of low carbon technologies, systems and services that cost less than high carbon alternatives.

Ageing Society

We will harness the power of innovation to help meet the needs of an ageing society.

The Future of Mobility

We will become a world leader in shaping the future of mobility.

Growing the AI & Data-Driven Economy

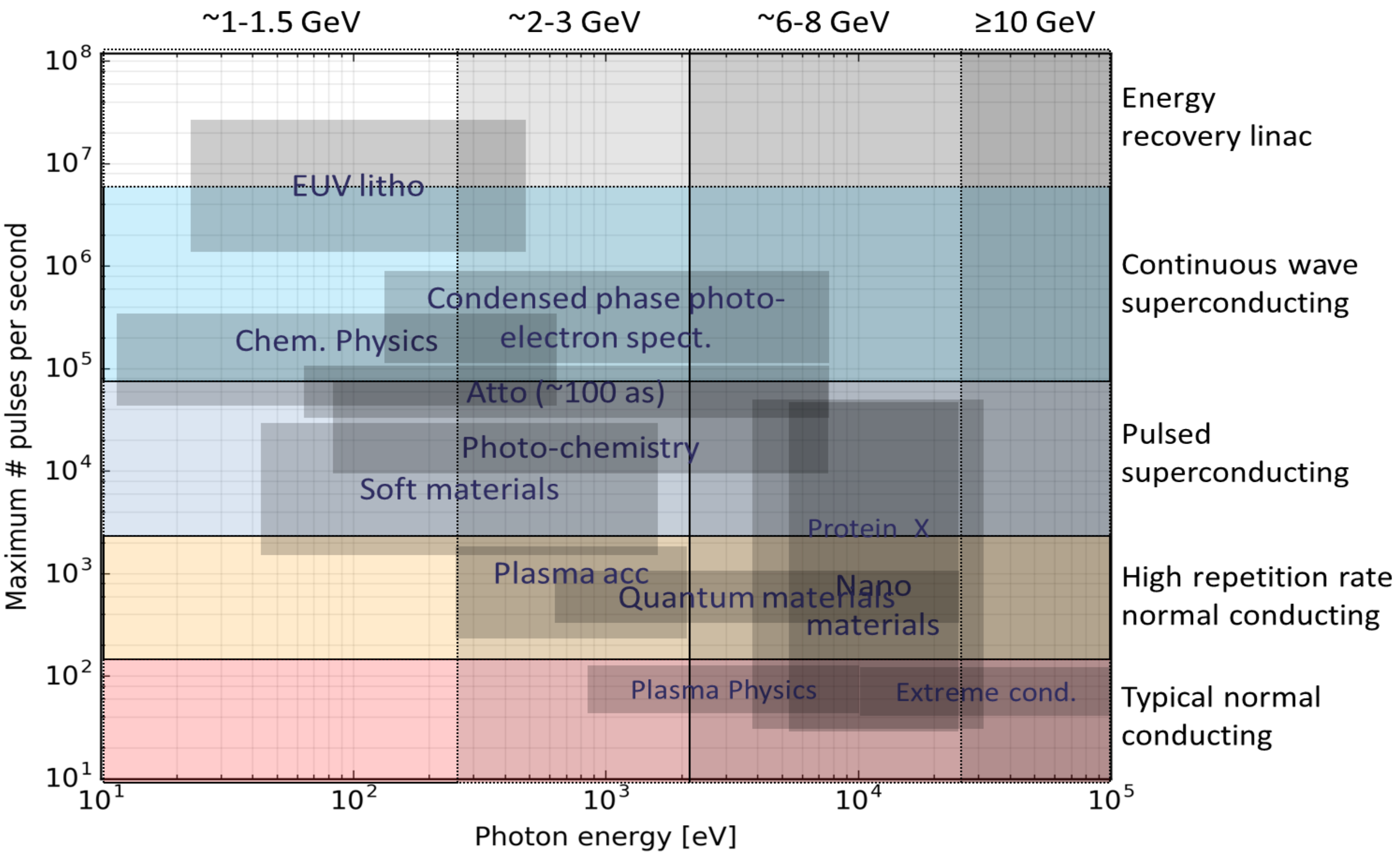
We will put the UK at the forefront of the AI and data revolution.

Science Case Requirements

- 200 eV - > 20 keV in XFEL fundamental (up to 100 keV in harmonics)
- 100 kHz to MHz repetition rate in SXR, > 5 kHz in HXR
- External seeded to ~1 keV, self-seeded SXR-HXR
- Attosecond pulses and multi-colour operation across a wide photon energy range
- Femtosecond laser based sources 10,000 nm to < 10 nm
- Synchronization to < 10 fs, time-stamping to sub-fs
- High energy (kJ class)/ high power (multi-PW) rep-rated laser system/s
- Bright synchronized ultrafast THz sources
- Synchronized electron/proton beams
- Gamma source by laser scattering from primary e-beam (also at high rep-rate)

Science Case Requirements

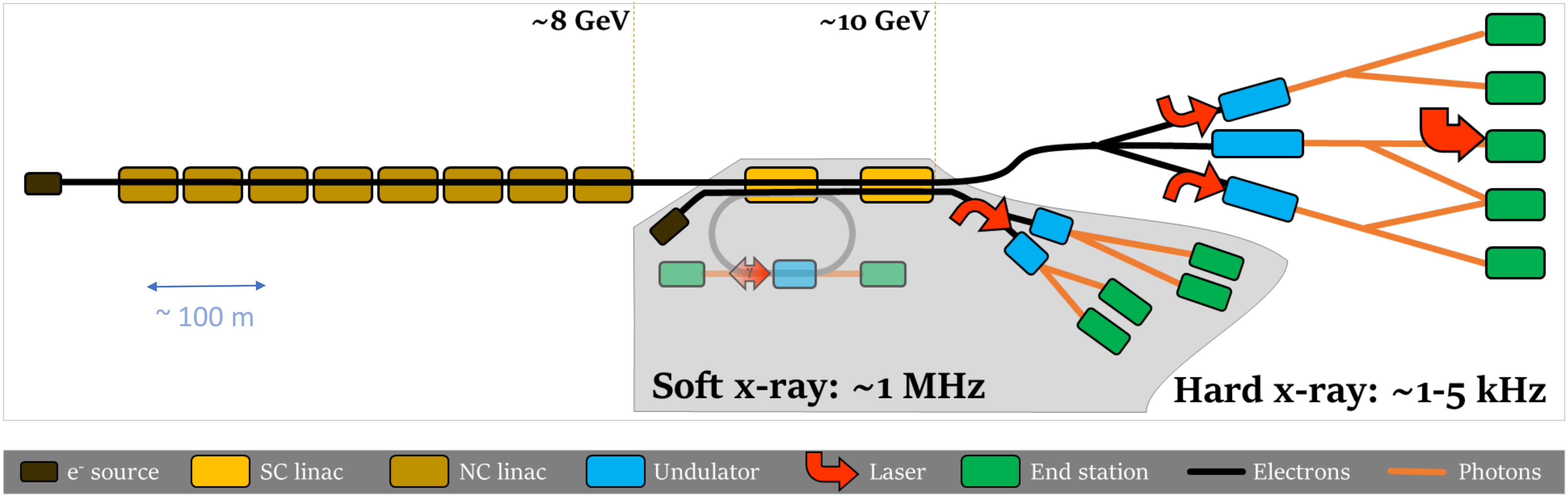
Repetition rate and photon energy are a key pair of parameters that determine facility cost and scale



Analysis & Design: Jim Clarke, David Dunning, Peter Williams, Neil Thompson, Louise Cowie, Brian McNeil, et al

UK XFEL conceptual layout options

- We have looked at 3 options, for example NC/SC and SC linacs in hybrid facility (below) – all would provide multiple beamlines and an extensive range of capability
- High brightness γ source, a plasma wakefield facility and an X-ray lithography facility can be readily incorporated along with the X-ray beamlines
- Compatible with high energy/intensity lasers and a wide range of other excitations including THz & e^-
- Upgrade path to: fully SC at 10 GeV, options for oscillator FEL in SXR and for seeding of HXR



Concept outline 1: Superconducting accelerator

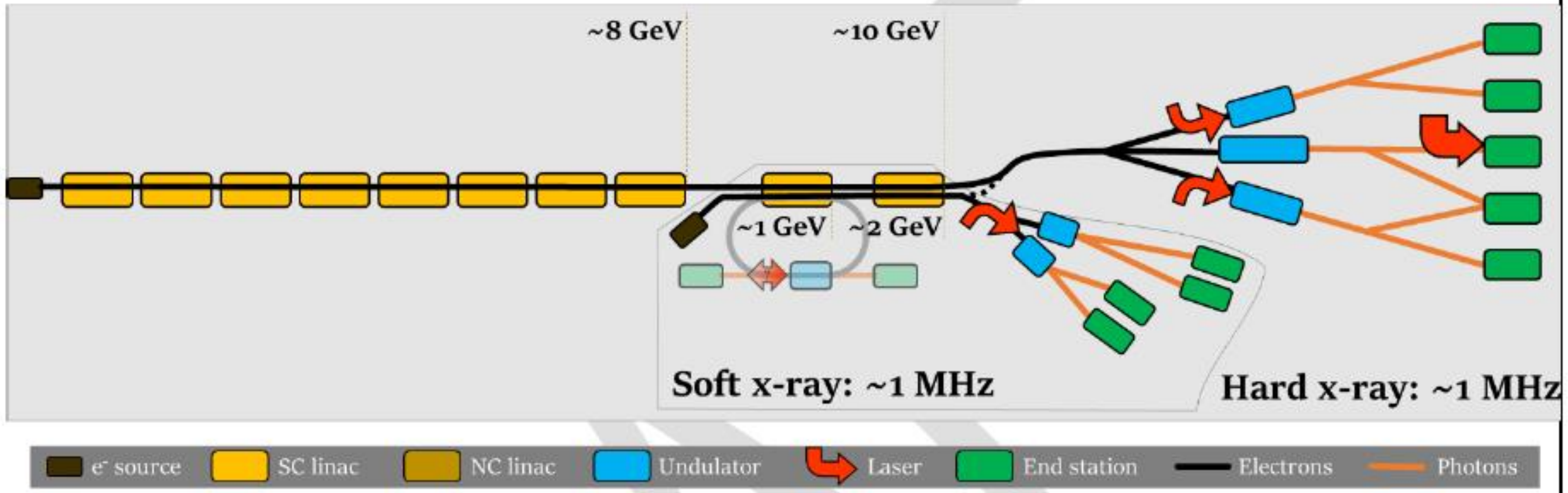
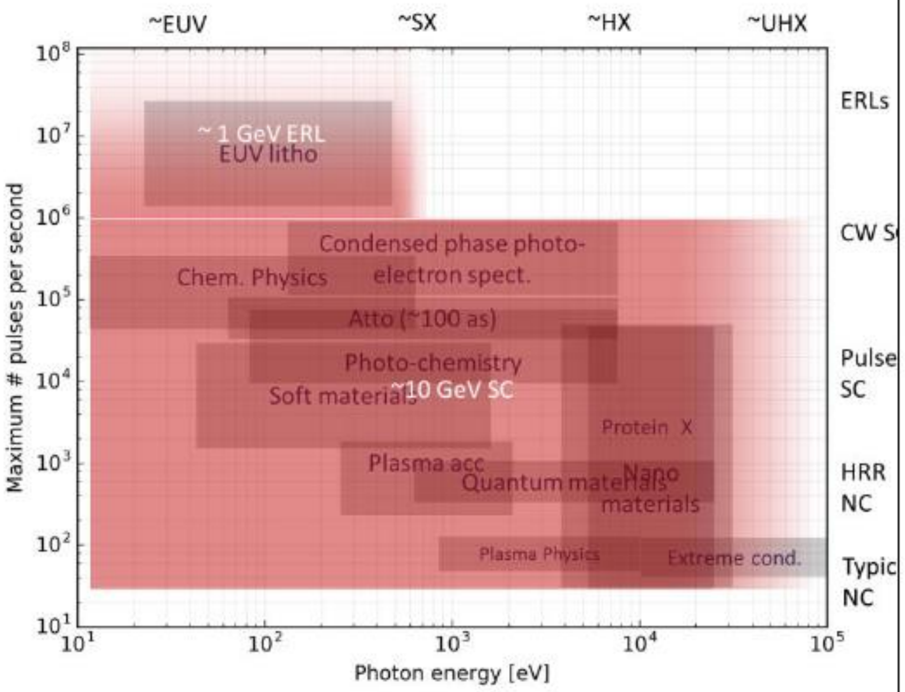


Figure 2: UK XFEL Concept outline 1: superconducting accelerator. The above schematic shows the layout for a ~10 GeV superconducting accelerator facility proposed to meet the science requirements.

The plot to the right shows how such a technical solution would cover the repetition rate-photon energy requirements of the science case.



Concept outline 2: Hybrid accelerator

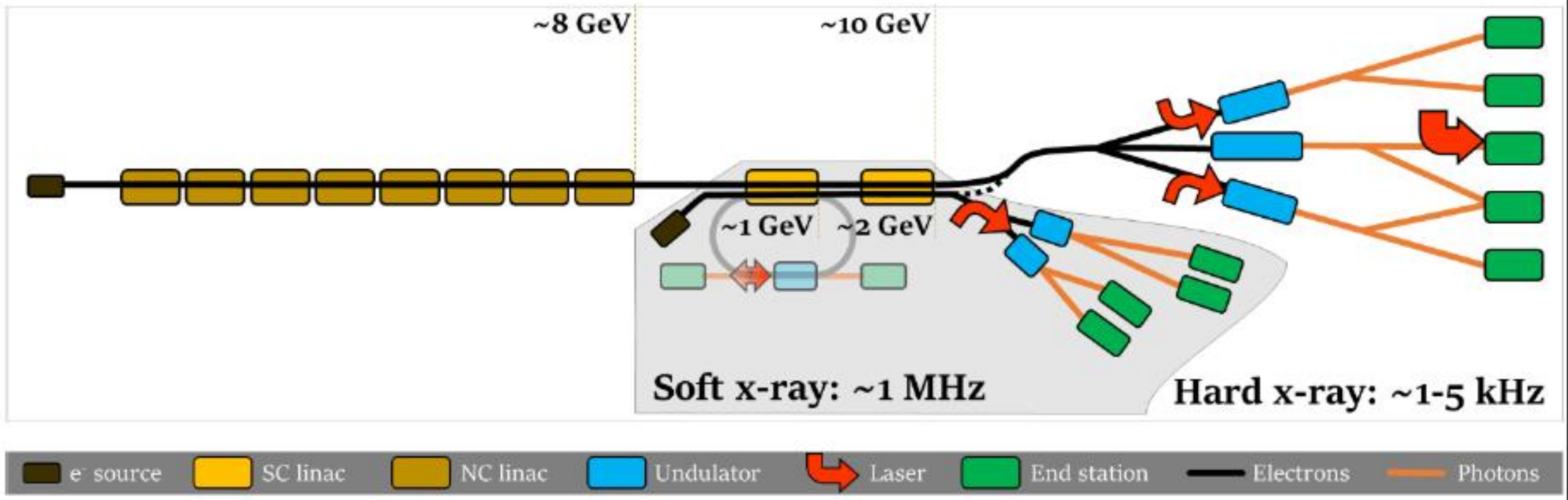
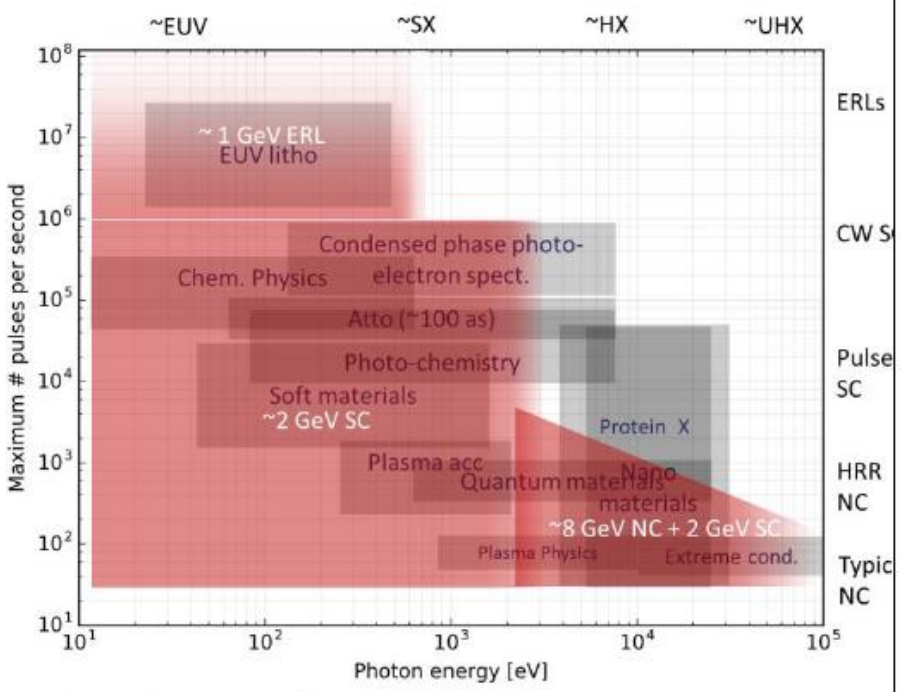


Figure 3: Concept outline 2: hybrid accelerator. The above schematic shows the layout for a ~10 GeV hybrid accelerator facility proposed to meet the science requirements. The plot to the right shows how such a technical solution would cover the repetition rate-photon energy requirements of the science case. The plots below show the trade-off between repetition rate and gradient (left) and corresponding linac length for an 8 GeV NC linac (right), with estimated peak field limits imposed at lower repetition rates.



Concept outline 3: Normal conducting accelerator

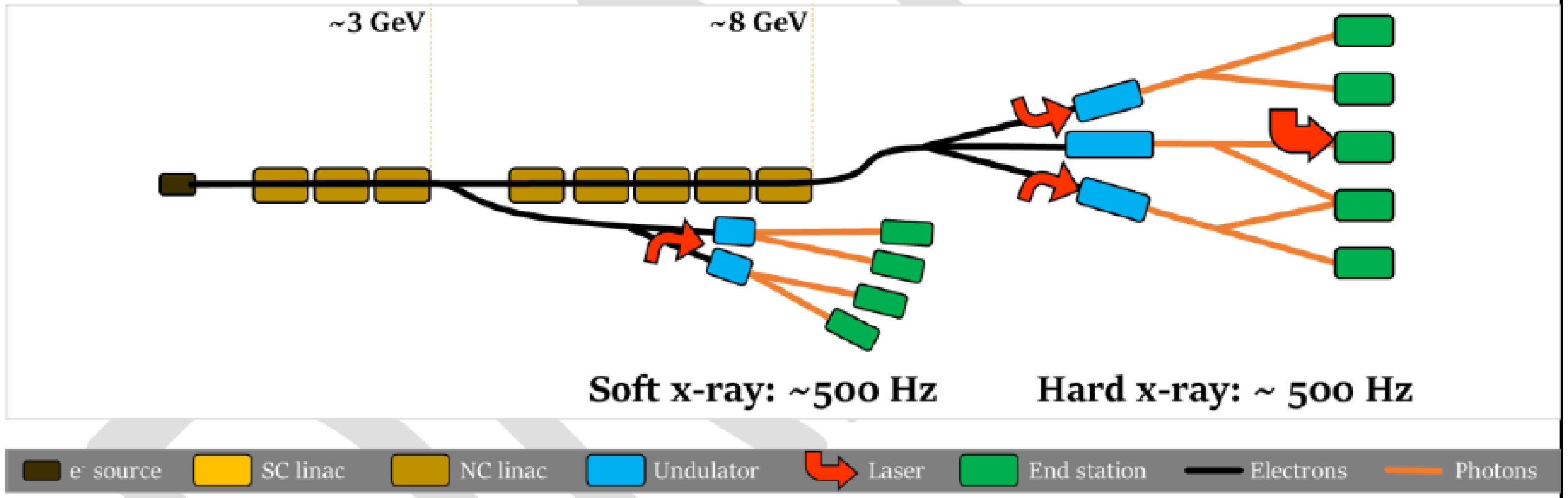
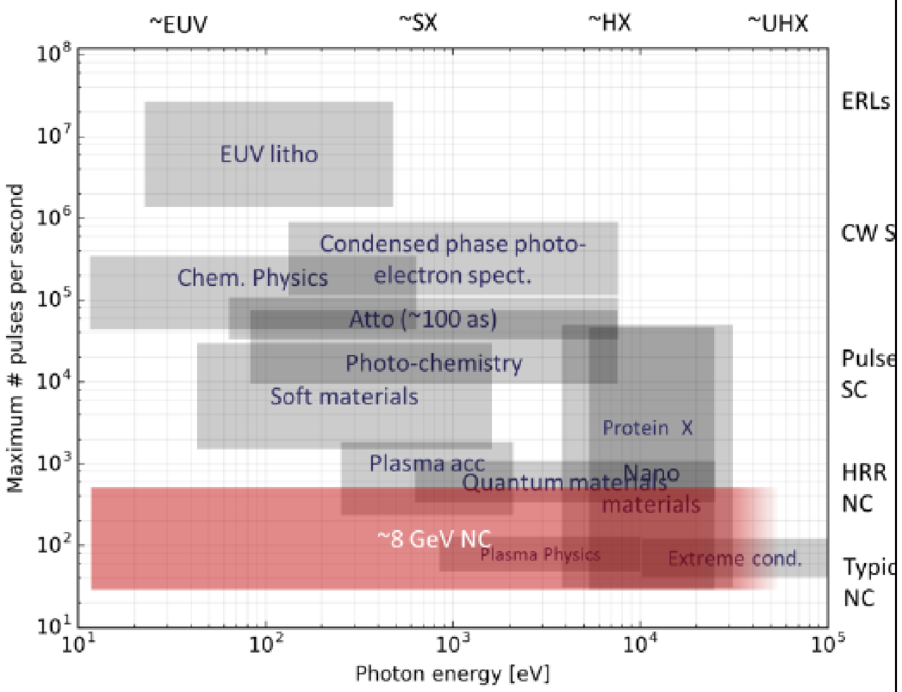


Figure 4: Concept outline 3: normal conducting accelerator.

The above schematic shows the layout for an ~8 GeV normal conducting accelerator facility proposed to provide world competitive national capacity

The plot to the right shows how such a technical solution would cover the repetition rate-photon energy requirements of the science case.

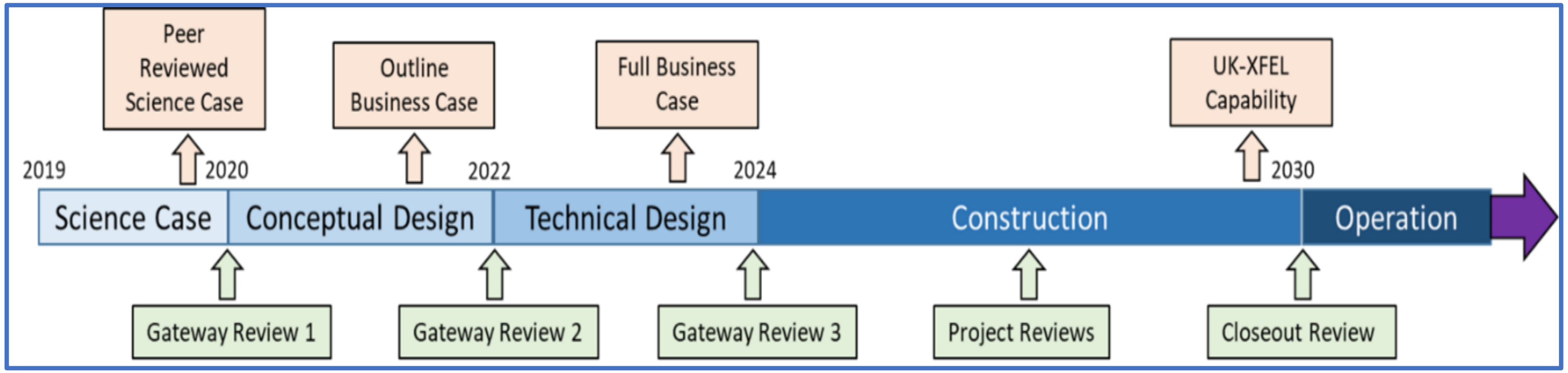


Construction and Operation will Provide Major Opportunities for UK Industry, Business & Employment

- Large scale civil construction and service infrastructure
- Multiple accelerator modules, undulator magnets, cryoplant, ebeam kickers etc.
- Extensive vacuum systems (e.g. for ebeam and X-ray distribution, end-stations)
- Control systems and sensors
- X-ray optics and precision positioning and steering systems
- Data & control infrastructure
- Multiple ultrafast lasers and optics (Diode pumped & fibre technology, OPA, OPCPA)
- High energy (kJ class)/high power (PW class) laser system
- THz sources, optics and detectors
- Advanced Detectors (e.g. X-ray & particles, beam diagnostics, spectrometers)
- Sample environments (e.g. cryostats, free space delivery systems, targets)
- High performance computing infrastructure
- Accommodation, catering, education and recreation
- Transportation
- Creation of many jobs in Construction, Technical, Engineering, Administrative, Safety & Security, Support Services, Outreach & Scientific roles

Next steps

- STFC are reviewing the science case to determine the extent to which it demonstrates "Mission Need"
- If positive the funding for the next stage (Conceptual Design, Business Case) will be sought from Infrastructure fund
- We are expanding engagement to share the case with the wider UK scientific and technology community and to consult with industry, other funders, large research institutes and learned societies
- Looking at other actions that will strengthen UK science in the many areas impacted by XFELs



Why build an XFEL in the UK ?

- Unique emerging x-ray capabilities can be optimised for new science
- Creates also opportunities in e-beam science, THz sources, high power lasers and γ sources
- We retain full control over the science and technology programme
- Direct benefits to UK economy from construction, procurement and operation
- Puts the UK at the centre of the most advanced science and innovation
- Safeguards future capabilities for industry and defence
- Golden opportunity to use as a catalyst for regional development
- Will build, and help retain, a wide range of skills in UK workforce
- Will attract the best scientists from around the world to the UK
- A national flagship for attracting young people to STEM subjects & increasing public appreciation of science

Subject	Date	Time	Live Webinar Link / Recording
Science Case Overview	23 July	2 pm	https://ukri.zoom.us/j/94235044032
Life Sciences	28 July	2 pm	https://ukri.zoom.us/j/96812137959
Chemical and Material Sciences	30 July	2 pm	https://ukri.zoom.us/j/92124133599
Physical and Extreme Conditions	5 August	2 pm	https://ukri.zoom.us/j/93469399137

Thank you for your attention