Science Case Update for a UK X-ray Free Electron Laser (UK XFEL)

- Commissioned by STFC on behalf of UKRI to be completed by May 2020 to support in consideration of “Mission Need” (CD0)
- We are seeking to identify scientific opportunities for an X-ray FEL with capabilities at, and beyond, the current state-of-the-art
- We need to consider the current science landscape, and the future opportunities that may emerge over the coming decades
- We are seeking engagement with Academia, UK Government (AWE, Facilities, Research Councils, DSTL), Industry, Learned Societies & Research Charities etc.

You can find more project information at:
https://www.clf.stfc.ac.uk/Pages/UK-XFEL-Scientific-Case-Consultations.aspx
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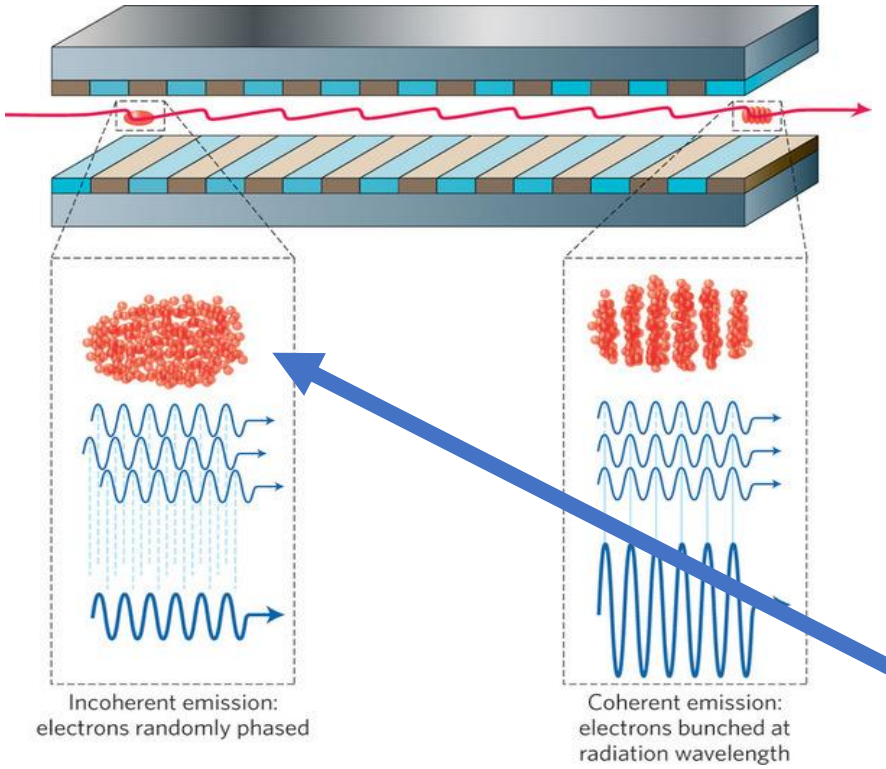
Science Team

- **Chemical sciences**: Julia Weinstein (Sheffield), Russell Minns (Soton), Sofia Diaz-Moreno (DLS), Tom Penfold (Newcastle)
- **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 (IC), Marcus Newton (Soton), 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)
- **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

New modes are becoming available that prepare electron bunch to increase coherence or shorten pulse

- Pulses < 10 fs
- Two colour/two pulse modes possible (x-ray/x-ray & x-ray/laser/THz)
- Narrow spectral bandwidth
- Wide tuning range e.g. 0.1 – 10 keV photons for structural methods (e.g. XAS, IXS, X-ray diffraction)
- Exceptional available brightness (focused peak intensity up to ~ 10^{20} Wcm^{-2} or greater)
- Repetition rate ~100 Hz increasing to 10 – 1000 kHz with superconducting machines

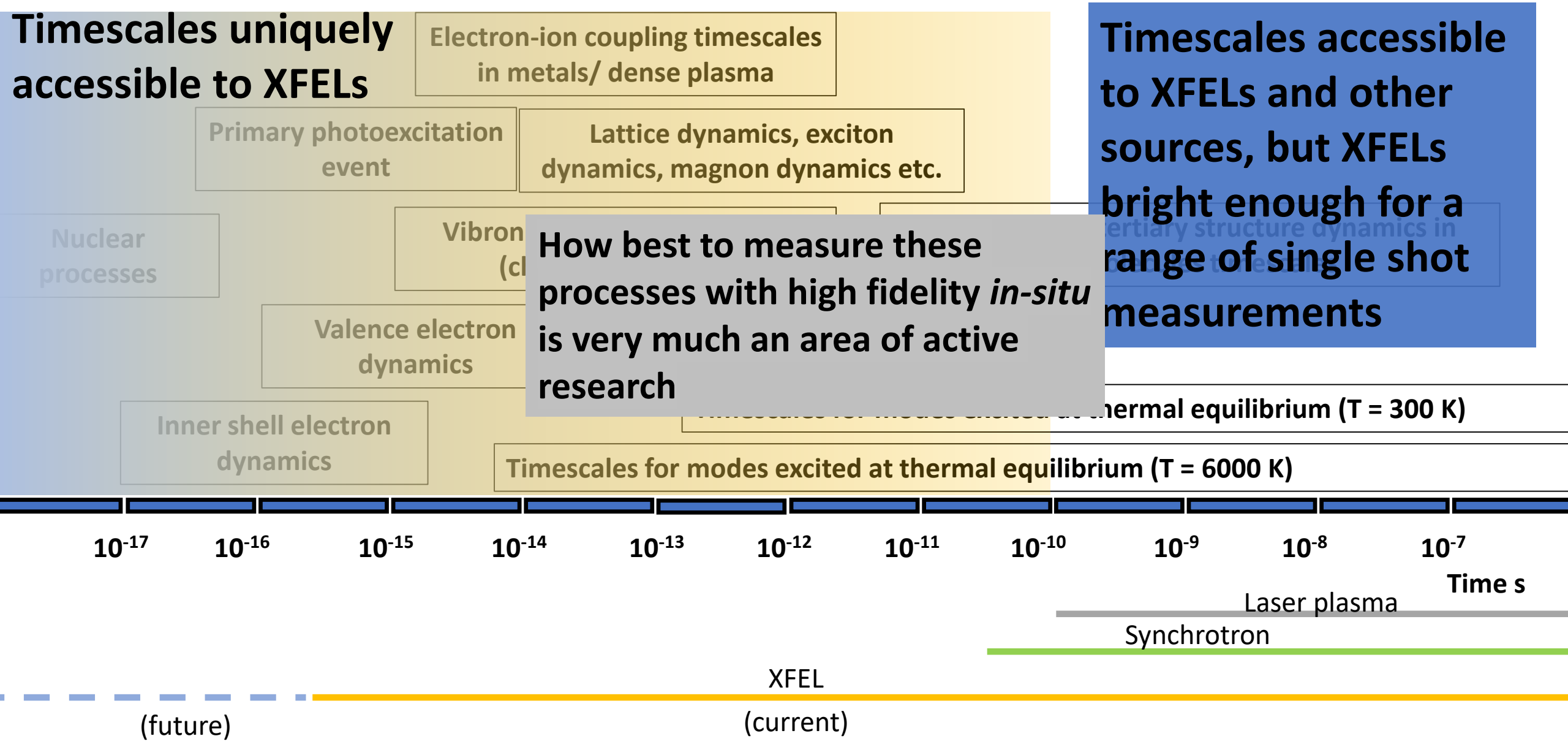
Science Opportunities with XFELS

X-ray FELs give ***bright*** and ***ultrafast*** **pulses** that provide the capability for ***snap-shot*** imaging and ***time-resolved*** determination of atomic scale structure and electronic states in matter using ***X-ray scattering*** and ***X-ray spectroscopy***

This is a unique, incisive, capability that opens a window into ***structure*** and ***dynamics*** with impact across a wide landscape of science and technology

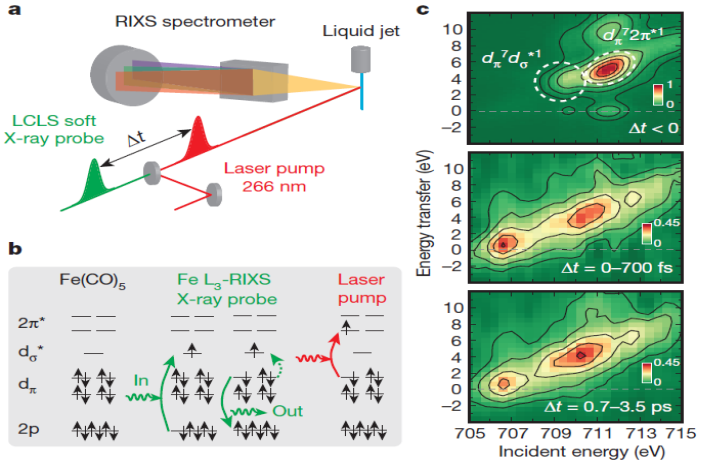
This is being used alongside other powerful modalities (*optical (UV-THz), neutron, cryo EM, UED, synchrotron X-ray, NMR etc*.) to give us the best tools to probe and control matter

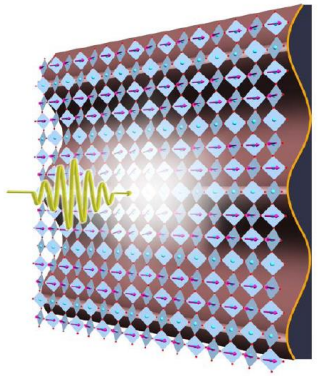
Primary science driver is access to timescales not accessible to other x-ray photon sources



Science Opportunities with XFELs

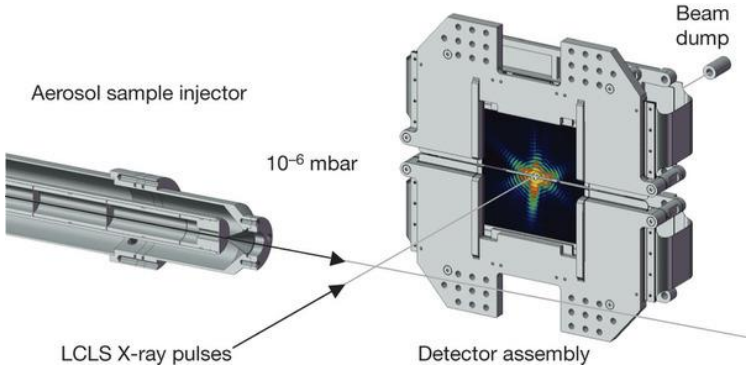
Access to structural dynamics: Dynamical phenomena can be probed after laser excitation on a time scale down to femtoseconds thus covering electronic dynamics, lattice dynamics and chemical bonds breaking/forming.

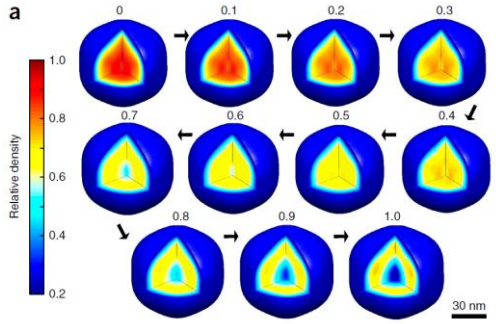




Access to transient states: Matter can be probed under only transiently attainable conditions of extreme pressure, high E & B fields, laser dressing and high energy density.

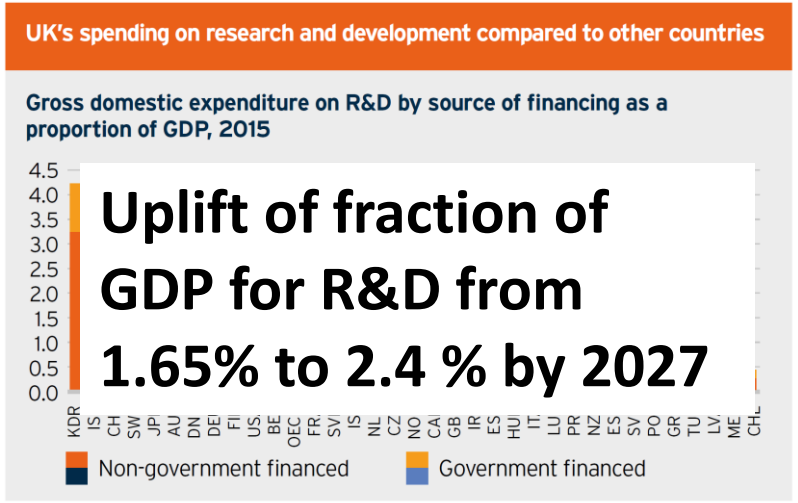
New modes of crystallography & nanoscopic imaging: For seeing the nanoscopic arrangements relevant to nanotechnology and life-sciences free from radiation damage and adverse effects of sample preparation.





Capturing rare events: In physical, chemical and biological systems critical processes can proceed through brief rare events (e.g. barrier crossings) arising from intrinsic fluctuations.

We are developing project alignment to: Industrial Strategy & Grand Challenges



Source: OECD (2017) *"OECD Economic Surveys: United Kingdom 2017"*. *2014 data for France, Ireland, Italy, Portugal and OECD aggregate. 2013 data for Belgium, Israel, Luxembourg and Sweden. Non-government financed includes finance from higher education, which may be partly government-financed; and from the rest of the world, which may include foreign and supranational government finance

Uplift of fraction of GDP for R&D from 1.65% to 2.4 % by 2027

Anticipate a national XFEL providing substantial direct investment into UK economy via construction, procurement and jobs

Anticipate an XFEL boosting science, technology and know-how:
Advanced Materials
Energy and Sustainable Chemistry
New Therapies & Drugs
Training at all levels:
Research, Technology, IT & Apprenticeships

and services move

of an ageing society

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.

Impact of space-time resolved X-ray studies

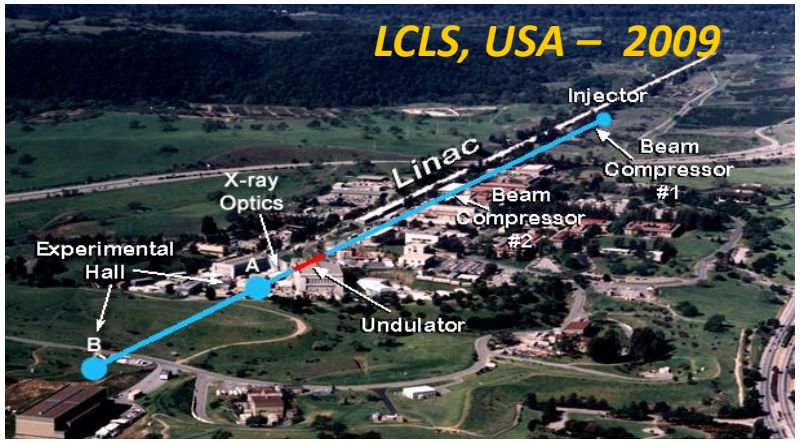
- **New energy materials (e.g. PV's)** can be created based on our emerging understanding of nanoscopic mechanism and quantum scale dynamics
- **Optimised function of catalytic processes** higher efficiency and better use of rare materials, acceleration of recycling of materials through full mechanistic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

Existing X-ray FELs: Anticipate 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)

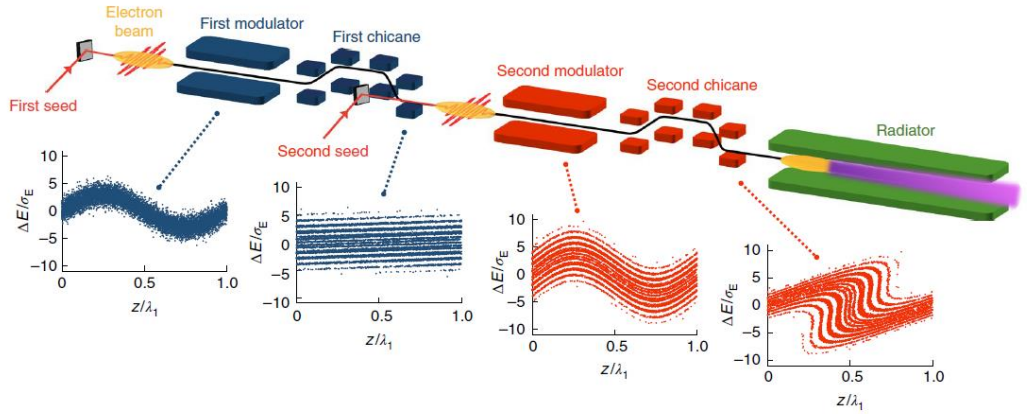
Large investments are being made, e.g. in USA via Basic Energy Sciences of DOE

UK XFEL is a long range science planning exercise

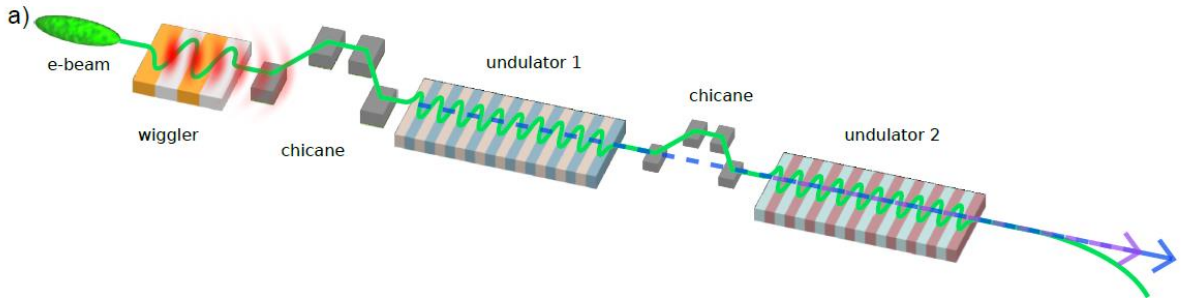
- It would deliver science for the late 2020's, 2030's, 40's & 50's
- It should be a cutting edge machine at first light or it could soon be obsolete
- We need to take a wide view of where there will be science impact
- We need to consider the full range of industrial impact in the UK
- Need to see it as an important part of the international network of Light Source provision (not necessarily doing everything – but certainly doing some things better than anywhere else)

Anticipating further advances and future opportunities

- The technology is not static – already in 10 years there have been remarkable improvements of performance and instrumentation
- Now non-linear/multidimensional X-ray spectroscopy is in reach and first pioneering work on X-ray holography, quantum imaging, attosecond science etc. are underway
- Methods beyond SASE are likely to become widely available (seeding - e.g. at FERMI, enhanced SASE - e.g. XLEAP, superradiance schemes, chirped schemes, XFELO and RAFEL under development etc..)



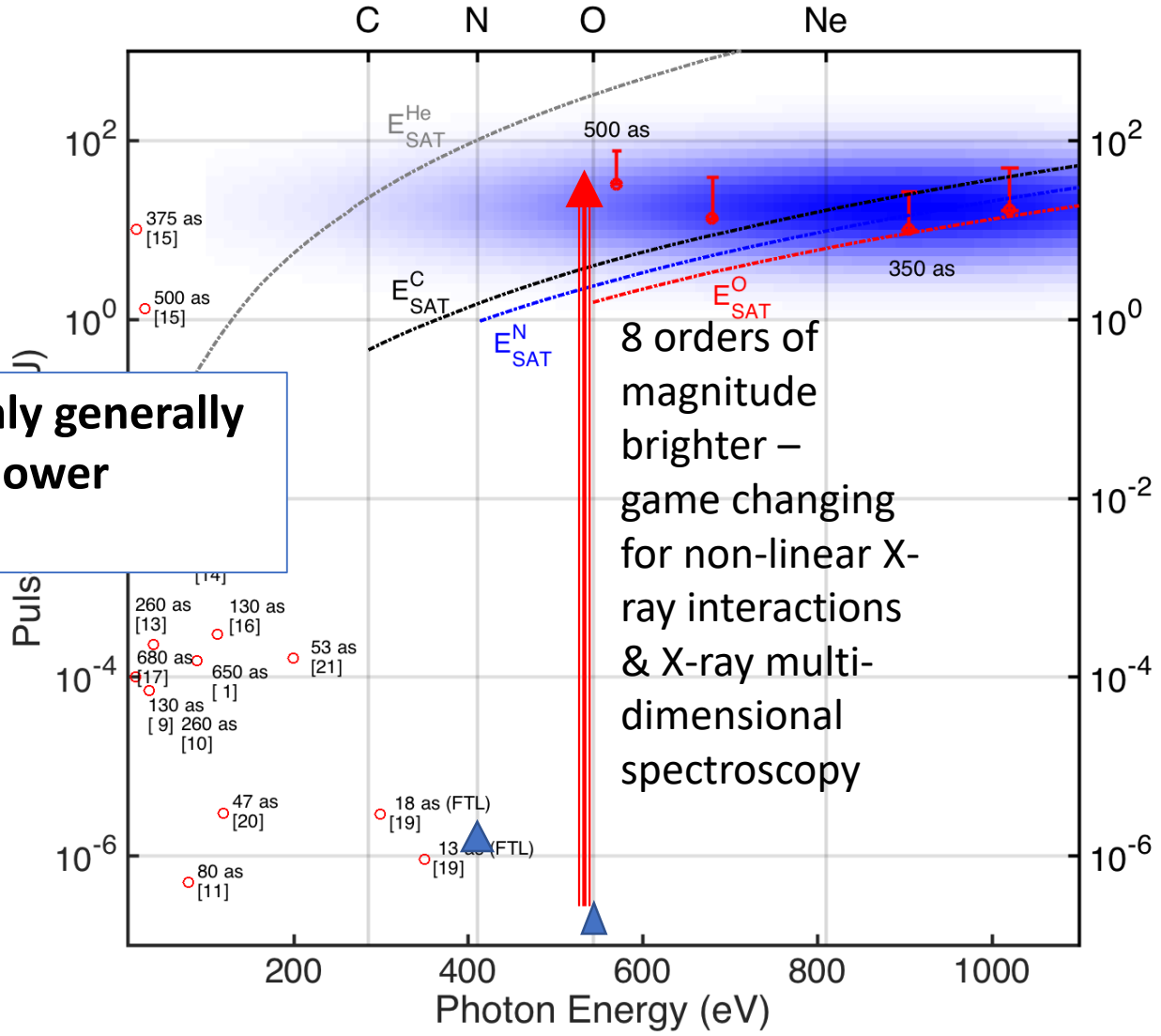
Echo enhanced seeding @ FERMI (2019)



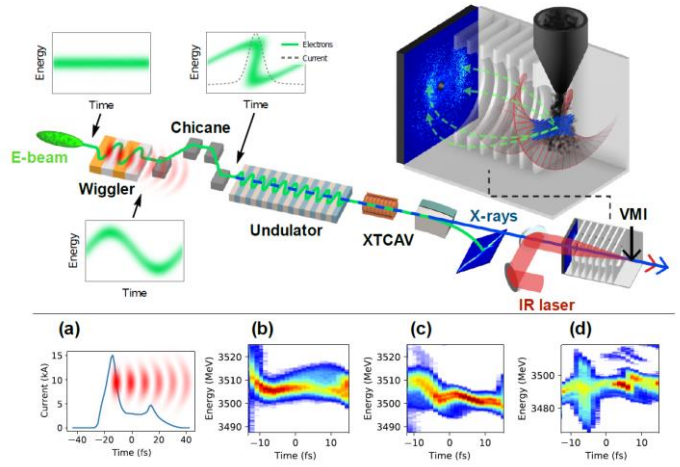
XLEAP two-colour attosecond pulses @ LCLS (2019)

XFELs high brightness attosecond X-ray sources

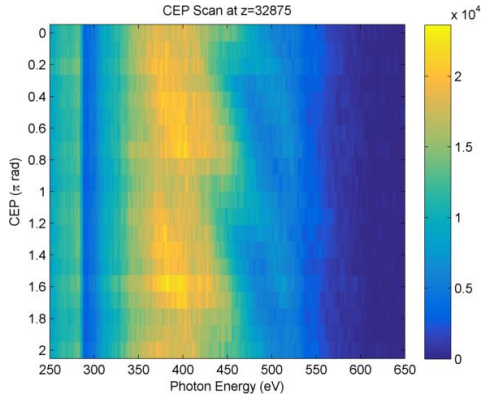
HHG sources only generally competitive at lower photon energy



XLEAP demonstration
Nat.Photonics Dec 2 (2019)



A.Johnson et al *Science Advances* ***4, 3761*** (2018)



Options might include:

- **Build a unique UK XFEL optimised for new capability**
- **Build a UK XFEL providing capacity well beyond 10 years**
- **Invest more in dedicated UK facilities at existing XFELs**
- **Increase investment to support users in exploiting existing opportunities (e.g. long term grant funding schemes, CDT's, "UK XFEL Institute")**
- **Dedicated R & D effort towards a future XFEL ("test facility")**
- **Extend activities of existing Life and Physical Sciences Hubs**
- **A combination of the above……**

Next Steps

- We start this exercise with an open mind as to the most exciting science that might be prioritised and the accompanying machine specification
- We have opened a free format consultation with the UK science and technology community to gather information and ideas
- https://www.clf.stfc.ac.uk/Pages/UK-XFEL-science-case.aspx
- A science case will be drafted through early 2020 with possibilities for continued input from the UK community

Oct 2nd *Matter at Extreme Conditions (Edinburgh)*
Nov 5th *Life Sciences (Crick)*
Nov 13th *Frontiers in Physical Sciences (Imperial)*
Nov 27th *Quantum Materials & Nanotechnology (Southampton)*
Dec 4th *X-ray FEL Applications (Warwick)*
Dec 11th ***Chemical Dynamics & Energy (Newcastle)***