UK XFEL Science Case Exercise

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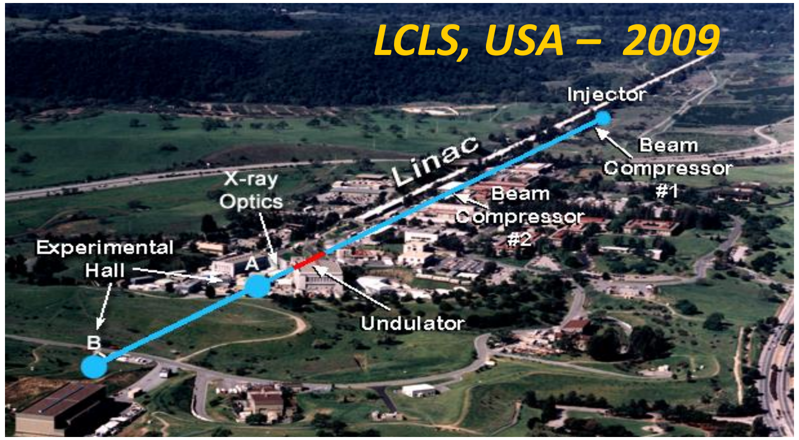
in partnership with STFC

Royal Society July 16th 2019

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

- Commissioned by STFC on behalf of UKRI
- A series of subject area workshops will follow in autumn 2019
- We anticipate the Science Case will be published in mid-May 2020
- Will support in the consideration of “Mission Need” (CD0) by UKRI
- We will be seeking engagement with Academia, UK Government (AWE, Facilities, Research Councils, DSTL, DBEIS), Industry, Learned Societies & Research Charities etc.

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)

Other projects under consideration

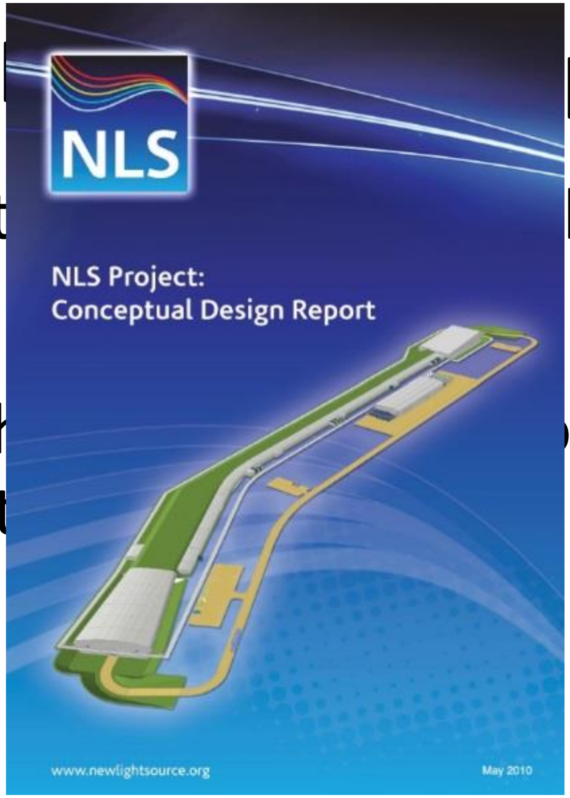
This is a Long Range Science Planning Exercise

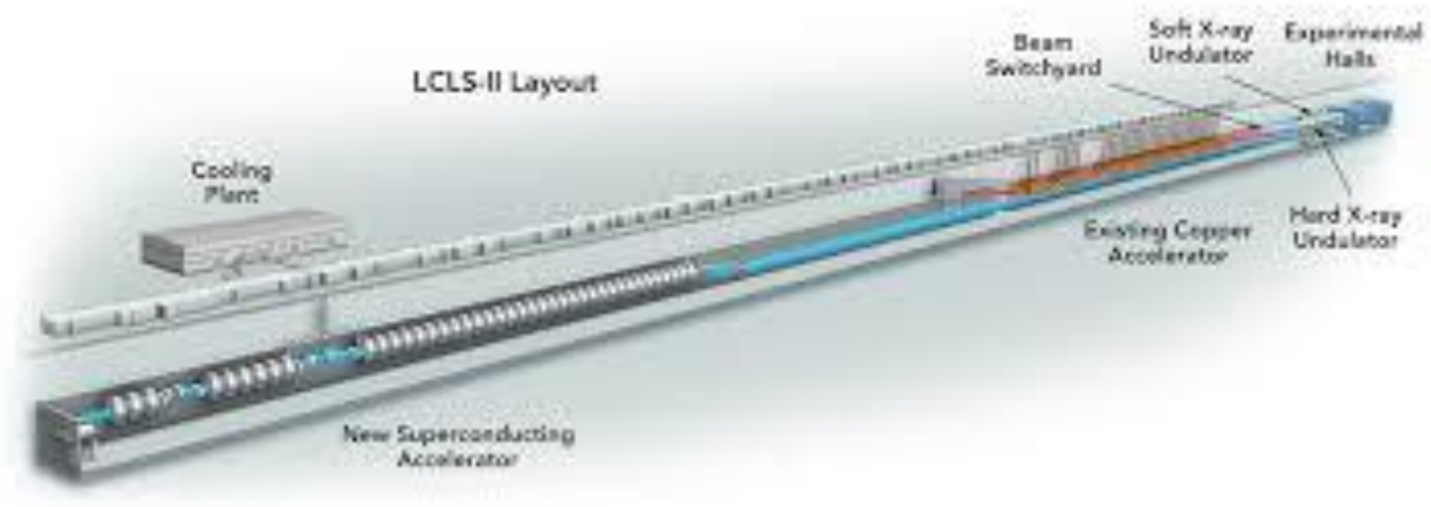
- It will deliver science for the late 2020's, 2030's, 40's & 50's
- It had better be a cutting edge machine at first light or it will soon be obsolete
- We should think long range and about things that NO current or planned XFELs can do
- We need to take a wide view of where there will be science impact
- We need to consider the full range of advanced industries in the UK that this facility will serve
- 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)

And if UK … pport CD0 ?

A good chance we won't … but still worth doing:

- Last time it informed th… on by DOE to build LCLS II (shame we don't own t…





And if UKRI doesn't support CD0 ?

A good chance we won't get CD0 approval but still worth doing:

- Last time it informed the eventual decision by DOE to build LCLS II

  (shame we don't own that one though)
- This exercise will boost the building of the science community and get more people actively using these resources in their research (as it did 10 years ago)
- It will provide a strong case for making appropriate UKRI investments into the science and the community, with additional long-term support for using international facilities
- It may motivate increased UK investment in other infrastructure opportunities e.g. "empty tunnel" at Euro XFEL, Swiss FEL or LCLS II end-stations

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 (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)
- **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)

















Science Opportunities with XFELS

High brightness ultra-fast x-ray pulses from an X-ray FEL provide the capability for time-resolved imaging of atomic scale structure and electronic states in a material using X-ray scattering and X-ray spectroscopy

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

This will be 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

Access to structural dynamics

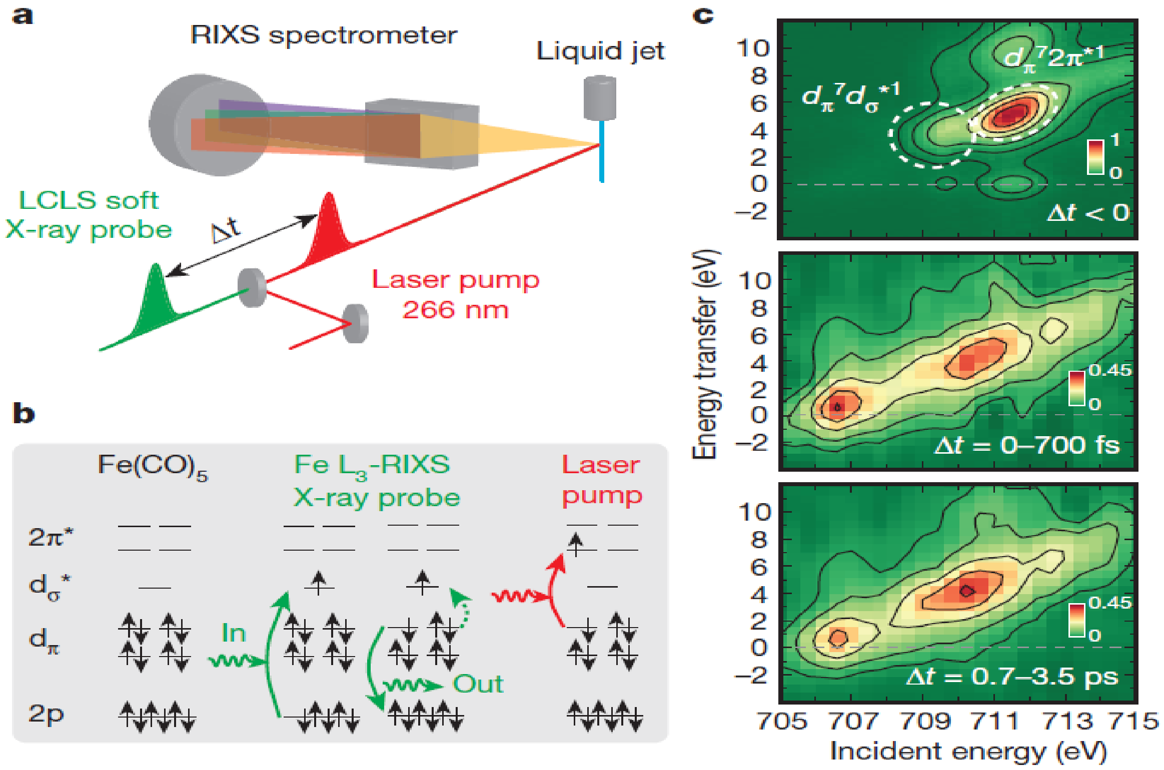
Transient phenomena can be probed after laser excitation on a time scale down to femtoseconds thus covering electronic dynamics, lattice dynamics and chemical bonds breaking/forming.

Catalysis and chemistry in solution phase:

“Orbital-specific mapping of the ligand exchange dynamics of $Fe(CO)_5$ in solution” ***Nature*** 520, 78 (2015)

“Tracking excited-state charge and spin dynamics in iron coordination complexes” ***Nature*** 509, 345 (2014)

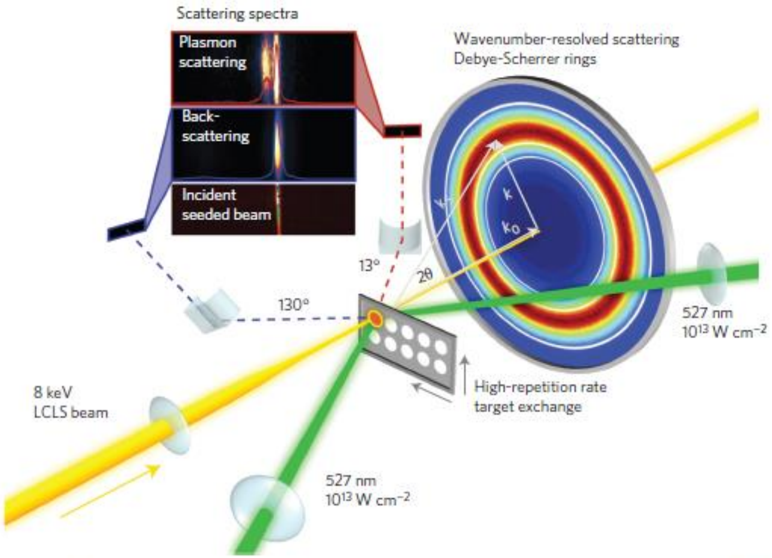
Time resolving surface catalysis ***Science*** 347,978 (2015)

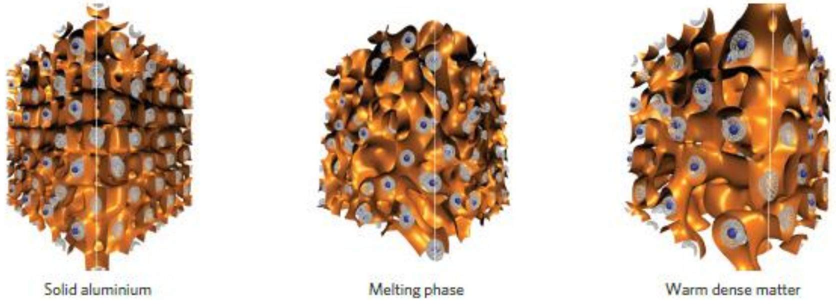


Important to chemical reactions (e.g. catalysis, water-splitting, hydrogen storage mechanisms), energy materials (e.g. photovoltaics, battery technology), engineering materials (e.g. to understand/ mitigate mechanisms of corrosion, radiation damage, shock damage), and biochemistry (e.g. to unravel photosynthesis, light sensitive protein activity).

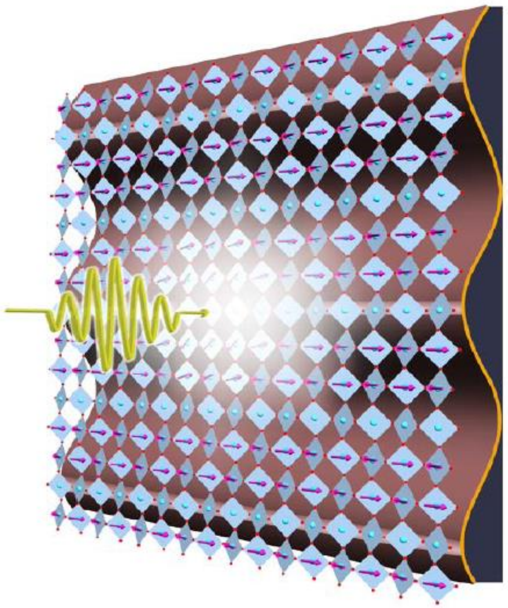
Access to transient states

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





"Direct observation of melting in shock compressed bismuth with fs X-ray diffraction
PRL 115, 095701 (2015)
Probing laser generated dense matter:
"Ultra-bright X-ray laser scattering for dynamic warm dense matter physics"
Nature Phot. 10, 1038 (2015)

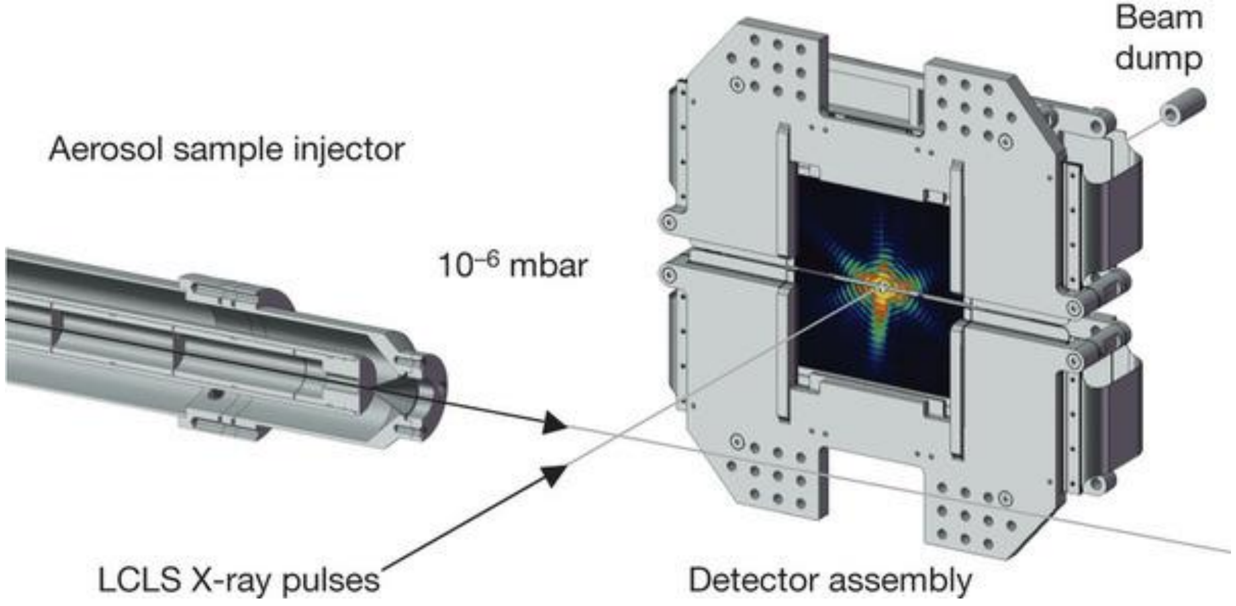


Optical/THz dressed materials
Foerst et al, ***PRL*** 112, 157002 (2014)
Mankowski et al, ***Nature*** 516, 71 (2014)

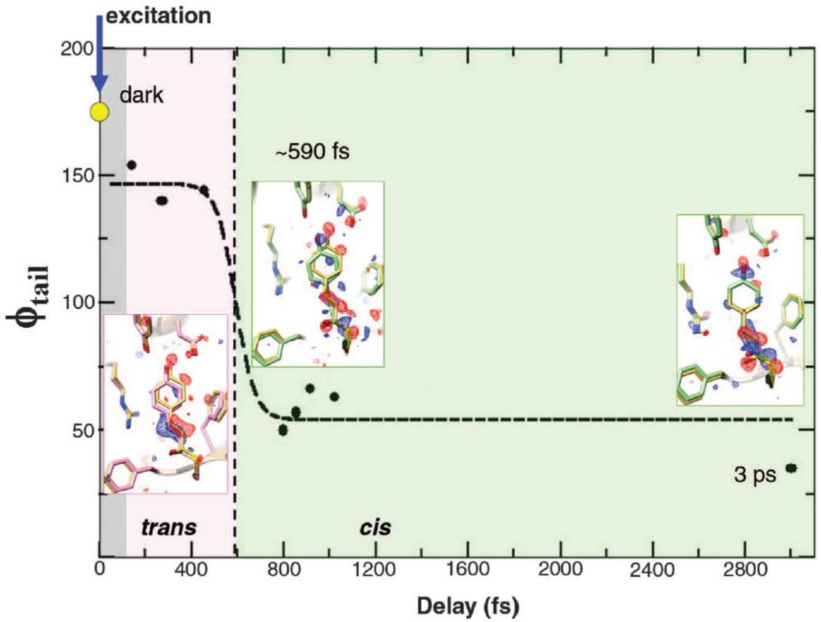
Important to astrophysics, planetary science, geophysics, defence and quantum materials

New modes of nanoscopic imaging

For seeing the nanoscopic arrangements in nanotechnology and life-sciences free from radiation damage and adverse effects of sample preparation.



Serial nanocrystallography, many examples e.g.
Kuptiz et al, ***Nature*** **513**, 261 (2014)
TbCatB protein of the *Trypanosoma brucei* protozoan – critical agent in sleeping sickness ***Science*** 10, 1126 (2012)
Architecture of the synaptotagnmin- SNARE machinery for neuronal exocytosis ***Nature*** 525, 62 (2015)



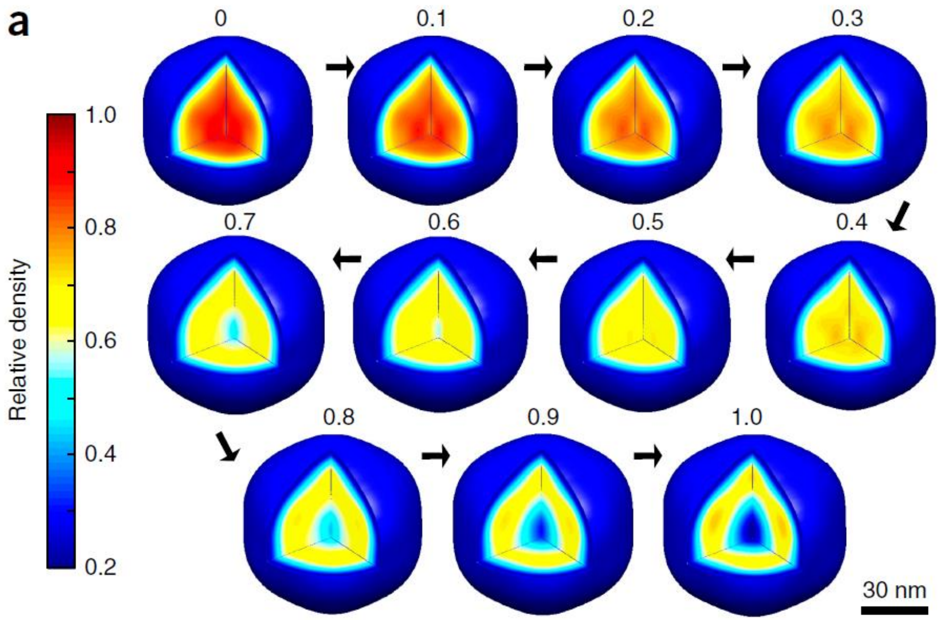
Femtosecond structural dynamics drives the trans/cis isomerization in photoactive yellow protein

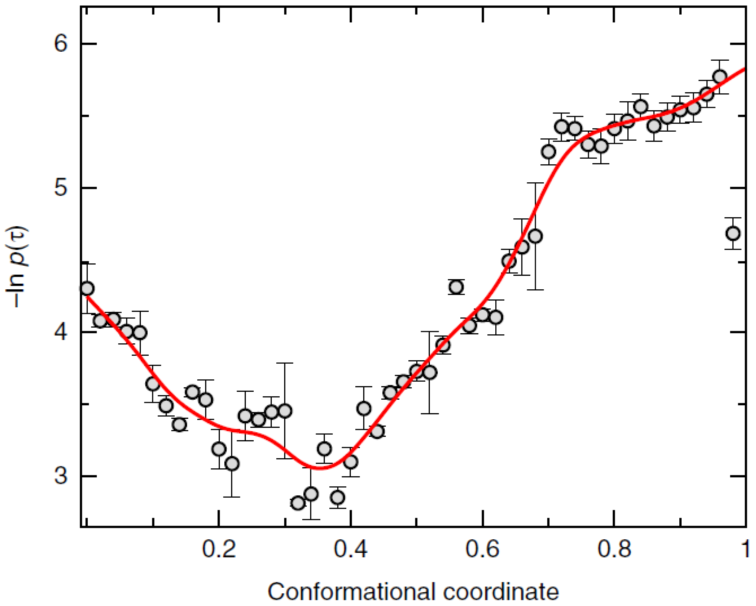
Pande et al, ***Science,*** **352**, 725 (2016)

Important to nano-crystallography and in-situ imaging of the function of biomolecular assemblies at operating temperature

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.





Conformational landscape of a virus by single-particle X-ray scattering
Abbas Ourmazd group ***Nature Methods***, 14, 877 (2017)

But far more opportunities at high (> 100 kHz – MHz) rep-rate

Capturing natural chemical/biochemical reactions in the act

What capability is the science likely to demand?

- Soft to hard x-ray (0.1 – 10 keV), (maybe harder, maybe VUV)
- Short X-ray pulse available (< 0.5 fs)
- Two pulse/two colour with delays over sub-fs to ns
- Synchronised or tagged to lasers to high precision (< 5 fs)
- High spectral brightness/narrow-bandwidth available (< 50 meV)
- High rep-rate is mandatory for much advanced science (chemical, quantum materials, rare events …) (> 1 kHz maybe > 1 MHz)
- High photon pulse energy (~ 10^{12} photons/pulse, maybe not at full rep-rate)
- Polarisation control (Linear, circular, OAM)
- ………..

The science case will help define the scientific and therefore the facility technical priorities

Other facility features

- Data rates enormous – must have the infrastructure !
- Sample delivery (all phases, sample on demand, active tracking)
- Advanced X-ray detectors
- High resolution RIXs capability
- Multi-hit particle detection
- Pump lasers on all end-stations
- A BIG laser for MEC
- Other beams at interaction point (not just laser, but maybe synchrotron X-rays, relativisitic electrons, high Z ions, neutrons….)
- Off-line preparation labs (chemistry, biology, nanofab, target prep etc.)
- End-station upgradability through facility lifetime

Advanced concepts include …..

- Attosecond modes (XLEAP, Attosecond pulse trains,….)
- Increased spectral brightness (e.g. RAFEL or X-ray oscillator)
- Increasing rep-rate (non-SC limits ~ 1 kHz, new concepts ~10 MHz)
- Super-radiance schemes to increase power and shorten pulse
- X-ray seeding (e.g. using an "Arizona" type device to seed with super-radiant incoherent Compton X-rays)
- Increased photon energy via non-conventional electron energy boost:

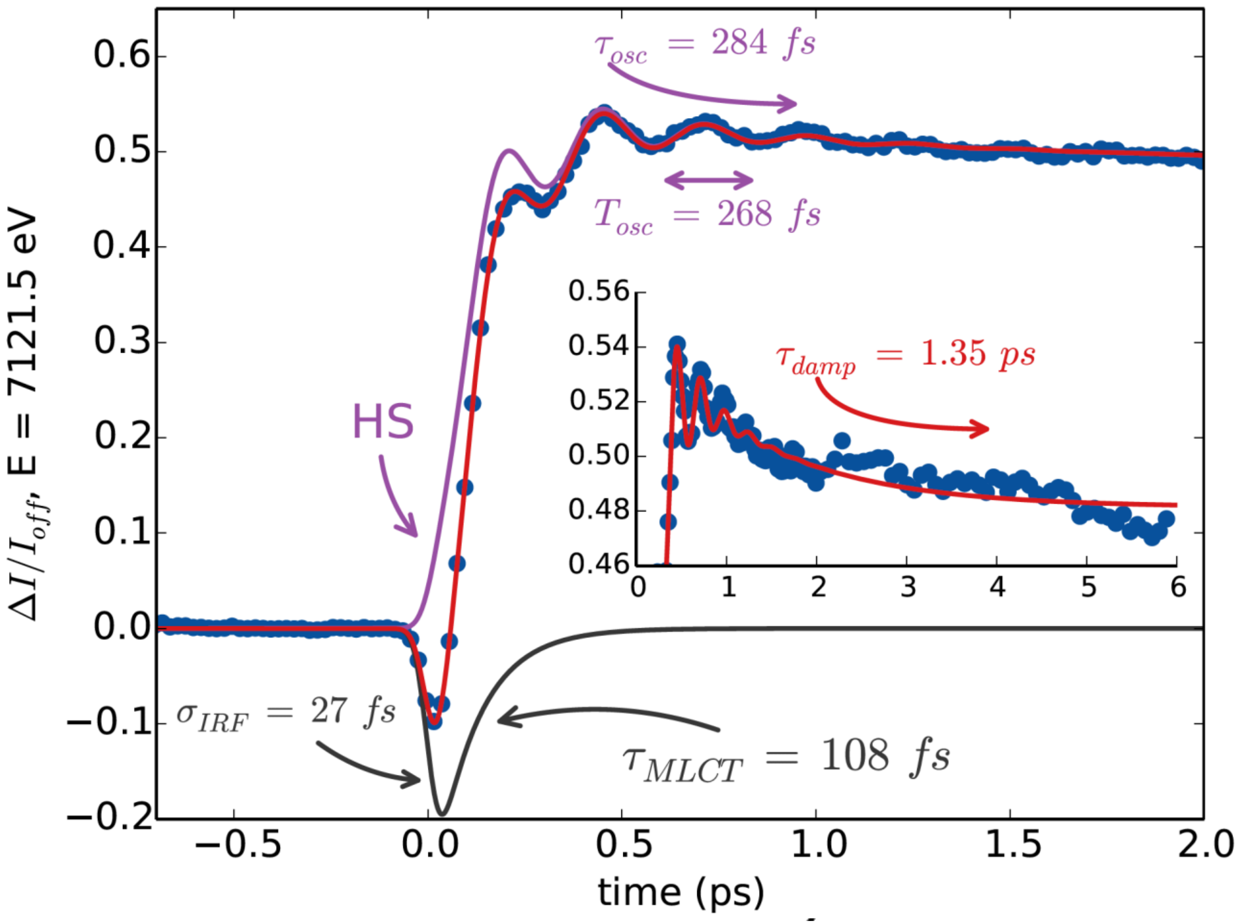
- Multi-pass linac
- PWFA

Already we have seen enormous advances in capability over last 10 years. For example in reaching the sub-femtosecond regime…..

XFELs have driven massive improvements in time resolved X-ray spectroscopy

In time resolving dynamics in metal-ligand complex $Fe(bpy)_3^+$

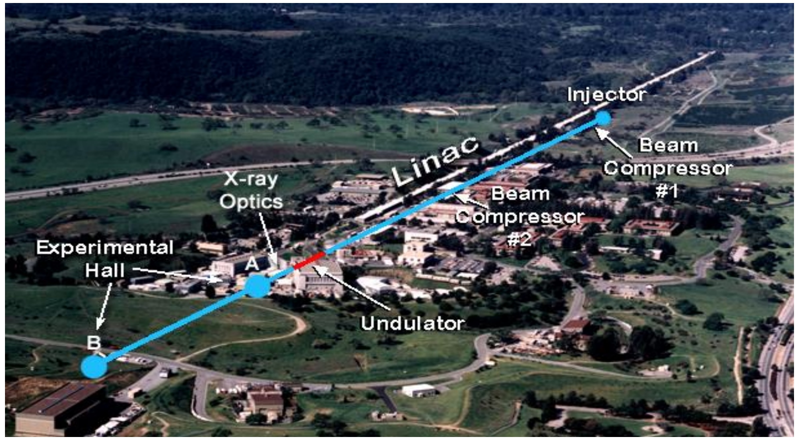
(Fe K edge absorption change at 7121.5 eV)

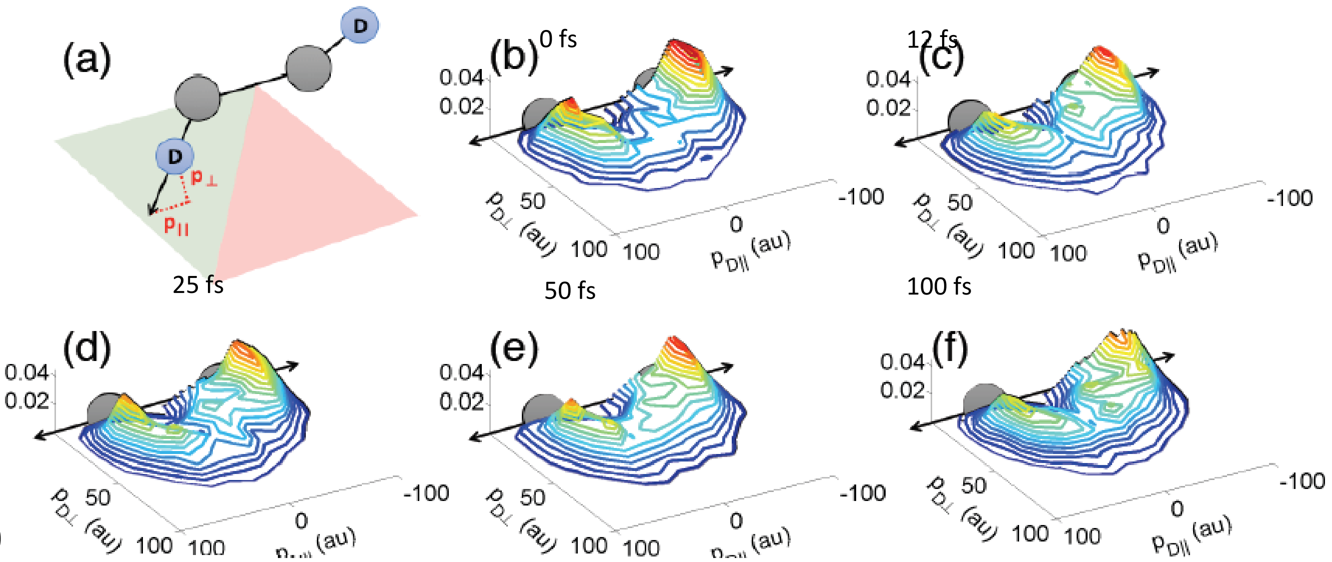


Lemke et al 2017 Resolving coherence and intermediate HS state using time-sorting with LCLS

Courtesy of Marco Cammarata

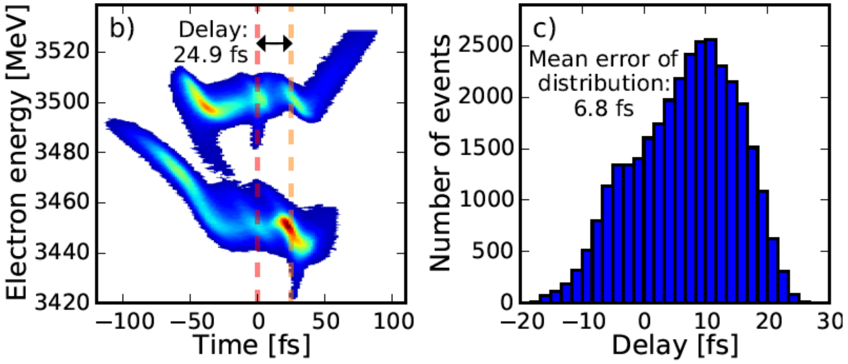
Few- to Sub-Femtosecond Time Resolution with XFELs





Fundamental events in chemistry resolved to 10 fs:

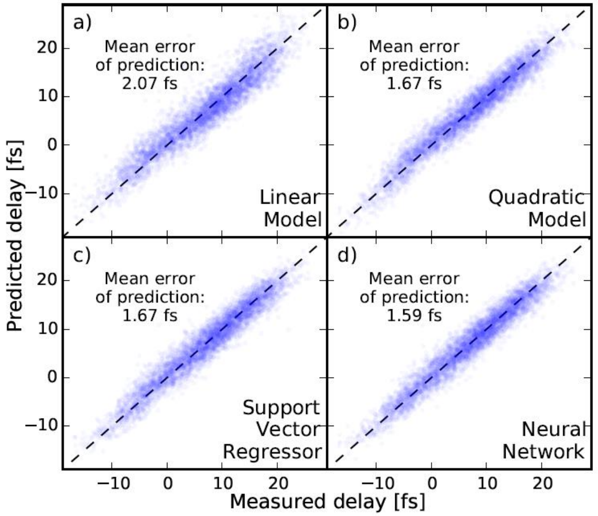
"X-ray induced ultrafast isomerization acetylene - vinyldiene" *Nature Comm.* , 6, 8199 (2015)



Improving the technology: Using machine-learning

A.Sanchez-Gonzalez et al, *Nature Communications* (2017)

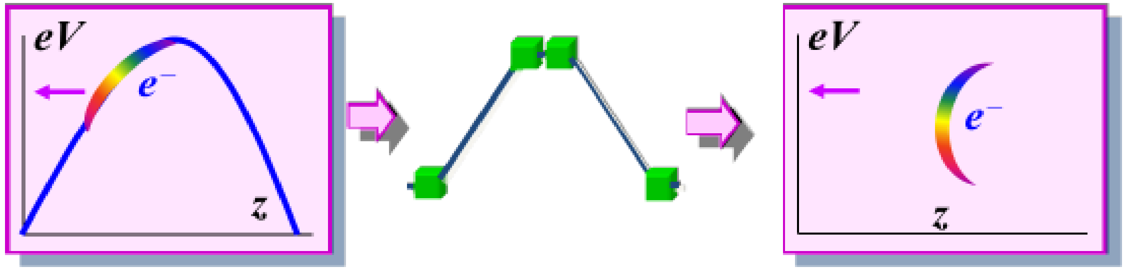
DOI 0.1038/NCOMMS15461 (2017)



Attosecond X-ray Pulses from XFELs

Led by Agostino Marinelli (SLAC)

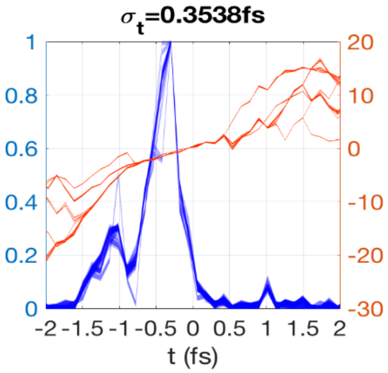
HXR: Isolated 200 as pulse produced

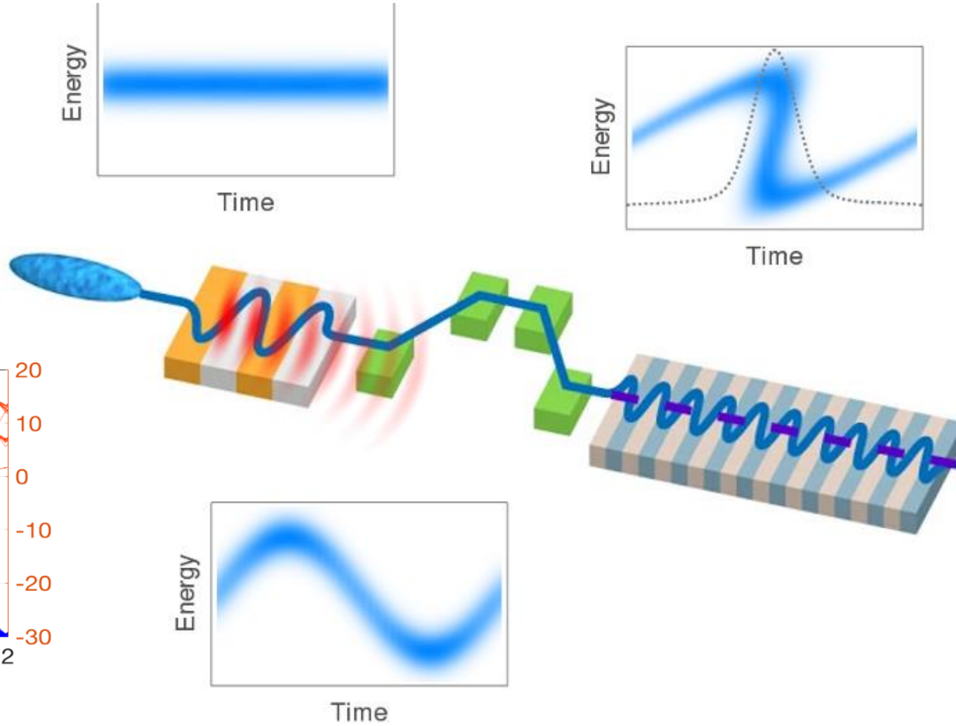


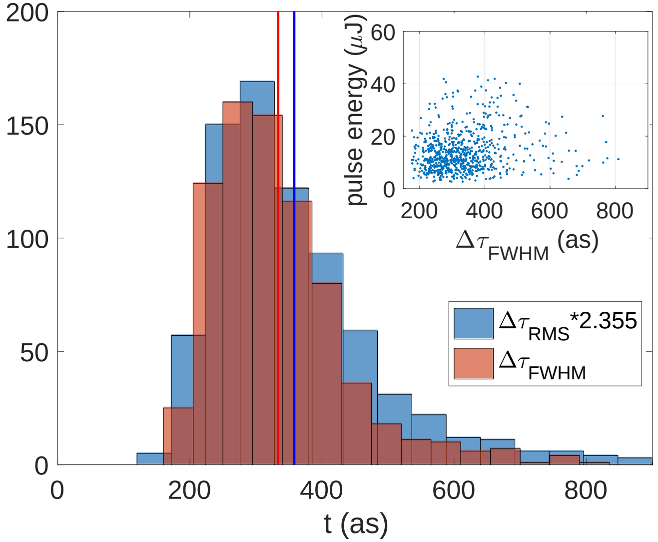
Nonlinear compression produces
High density head with low density tail

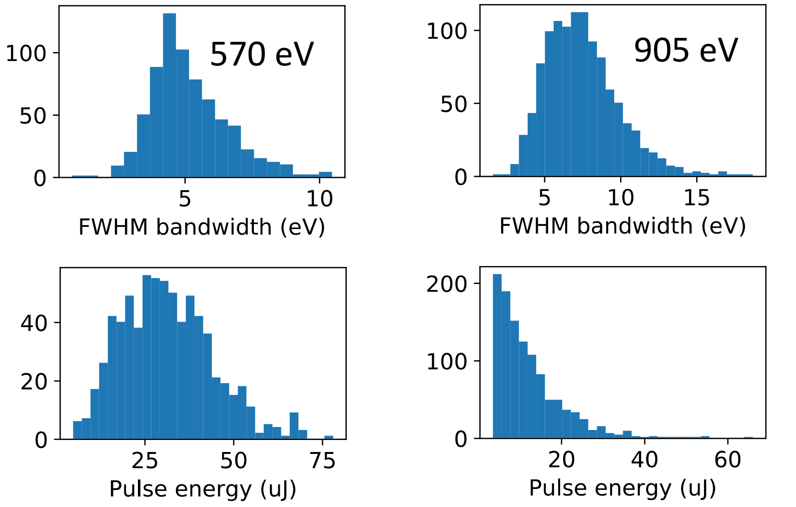
Huang et al, PRL, 119, 154801 (2017)

XLEAP for controlled SXR to HXR attosecond pulses



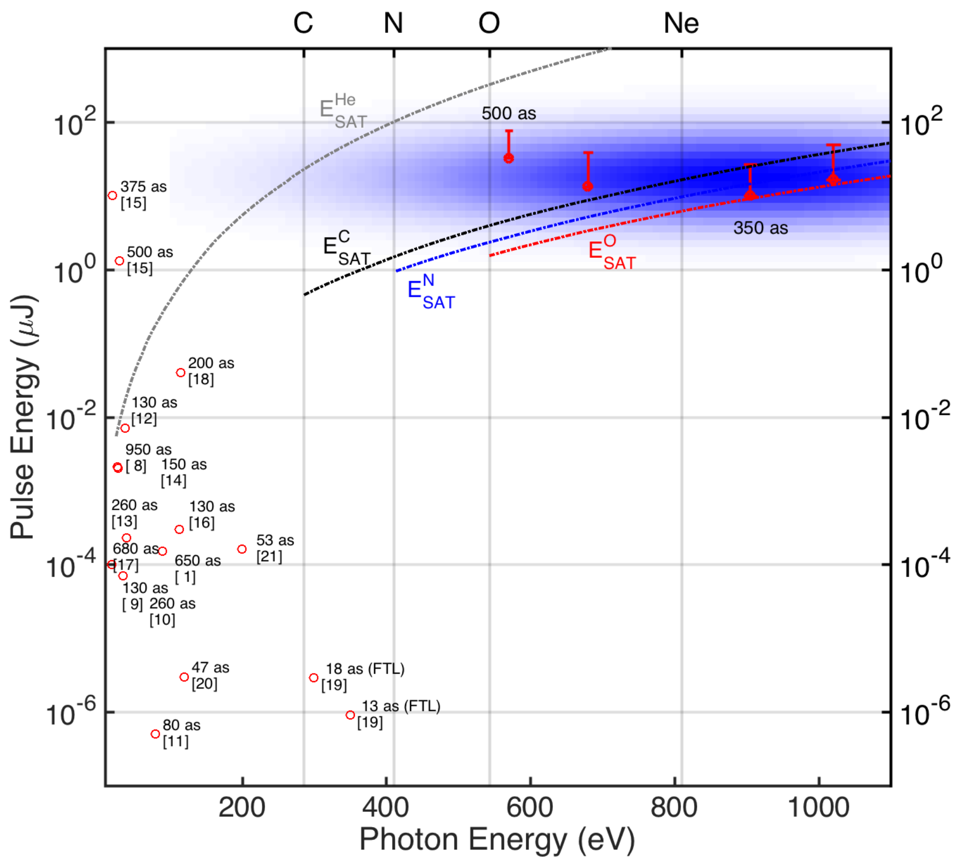


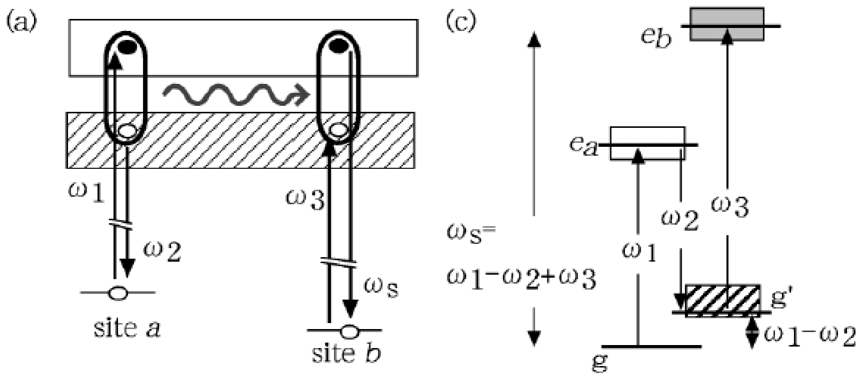




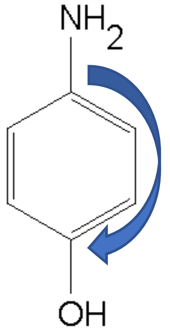
Recent results with XLEAP

collaboration led by James Cryan SLAC





I.V. Schweigert and S. Mukamel, *PRL* **99**, 163001 (2007)



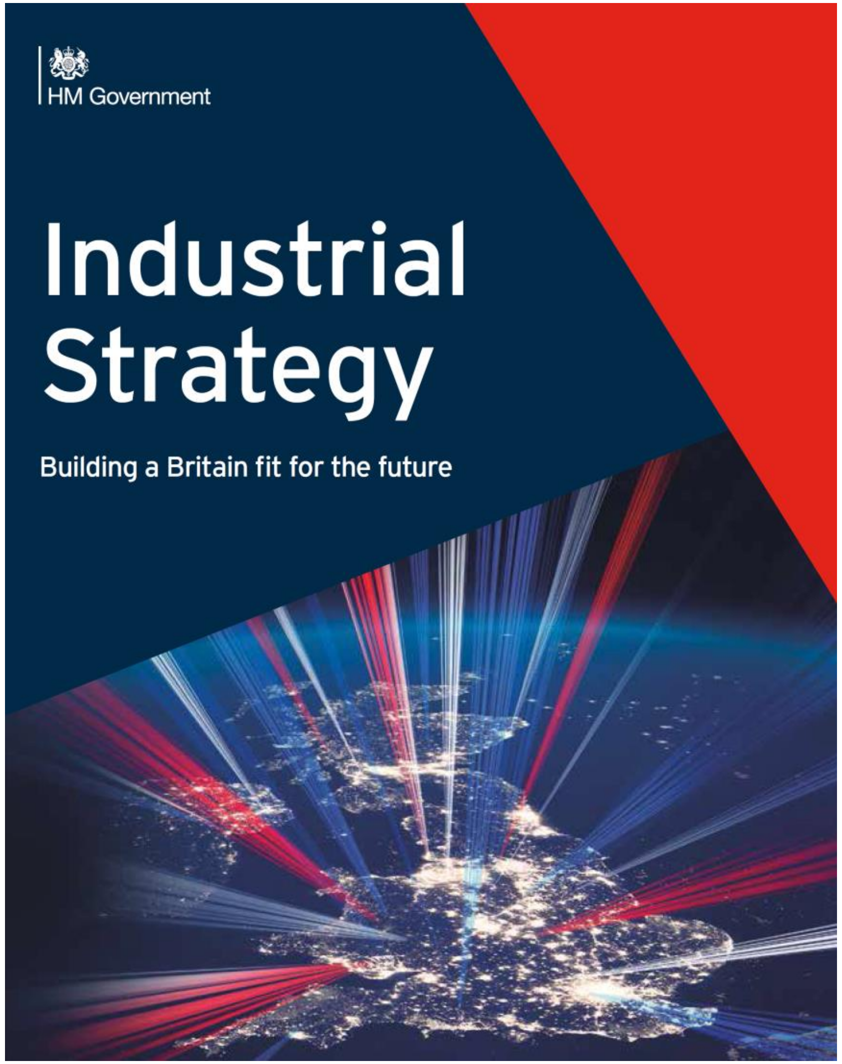
XLEAP intense enough to drive non-linear interactions across the SXR range. First evidence that it can drive electronic impulsive X-ray Raman recently seen.

An enabling step for attosecond multi-dimensional spectroscopy – with creation and probing of localised electronic wavepackets in neutral molecules ….

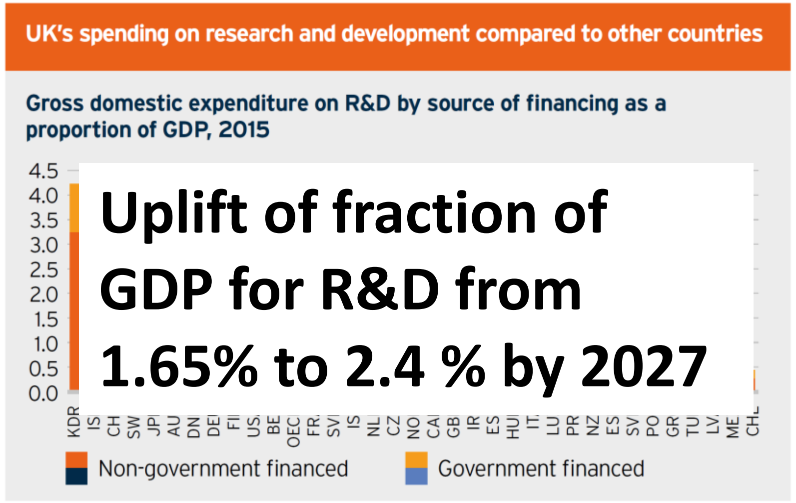
Anticipating further advances and future opportunities

- We can see the technology is not static – already in 10 years there have been remarkable improvements of performance
- Methods beyond SASE are likely to become widely available (seeding - e.g. at FERMI, enhanced SASE - e.g. XLEAP)
- Now non-linear/multidimensional spectroscopy is in reach and first pioneering work on X-ray holography, quantum imaging etc. are underway
- Impact on science beyond those areas already actively using XFELs must be anticipated – our case must capture these too

The Case Must Strongly Align with the HM Government Industrial Strategy



We must demonstrate our alignment to: Grand Challenges & other Objectives



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

Ancipate an XFEL providing substantial direct investment into UK economy via construction, procurement and jobs

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

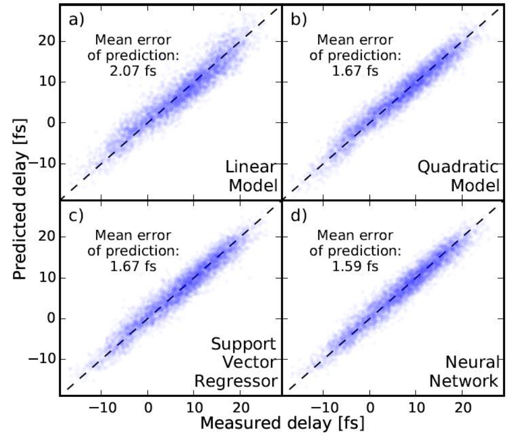
and services move

of an ageing society

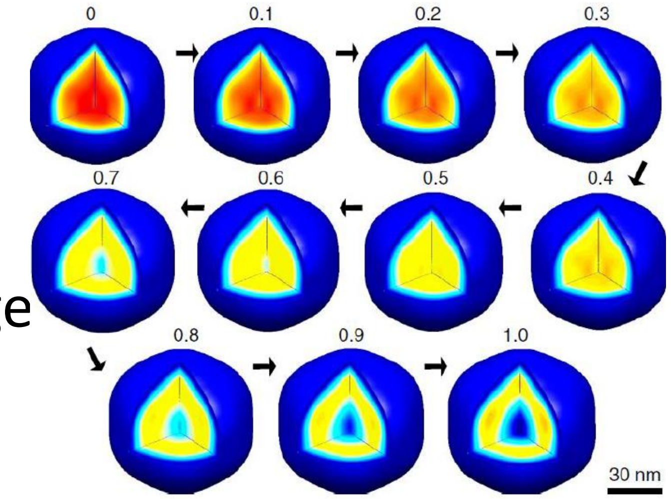
Growing the AI & Data-Driven Economy

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

- We will need to solve problems in an innovative way on: **Data flow & reduction, AI/Machine Learning & novel optimized hardware systems** that will feed directly into Industry relevant problems and train the workforce



- **XFEL data will feed into the biomolecular data bases** with new insights for drug discovery & healthcare

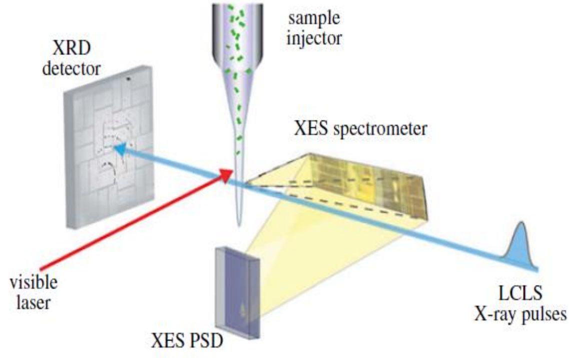


- **New ultrafast electronic/optoelectronic devices for advanced information processing (both classical and quantum)** will emerge from research into the nanoscopic dynamics in nanomaterials & quantum materials

Industrial partners in: IT Sector, Health Sector, Defence Sector, Nanofab/Nanotechnolgy Sector

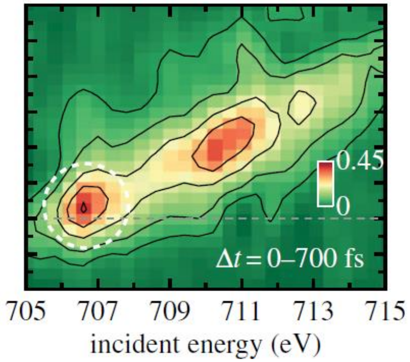
Clean Growth

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.



- **New energy materials (e.g. PV's)** will be created based on our emerging understanding of nanoscopic mechanism and dynamics, optimised materials for nuclear fission and fusion

- **Understanding mechanisms of corrosion and chemical change** to improve: resilence of materials to degradation (e.g. durability against corrosion) or acceleration of their degradation in the environment (e.g. bio-degradable)

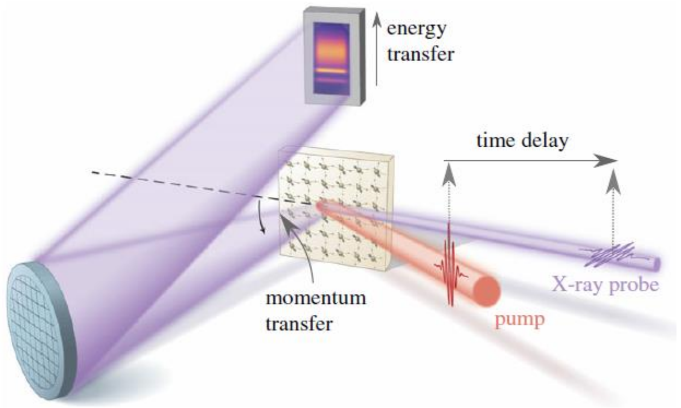


- **Optimised function of catalytic processes** for more efficiency and better use of rare materials, acceleration of recycling of materials

Industrial partners in: Chemical & Metals Sectors, Engineering Sector, Energy & Nuclear Sector, Electronics Sector

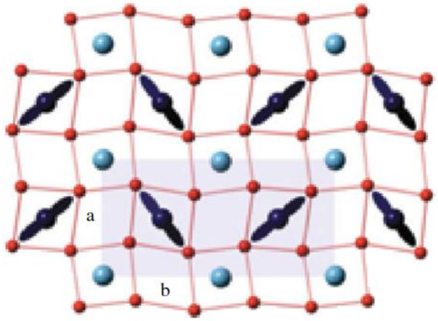
The Future of Mobility

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



- Basic research to **improve batteries and other energy storage materials** from the atomistic level up with full mechanistic understanding

- **Lighter and more durable engineering materials** for transportation (marine, land and aviation)

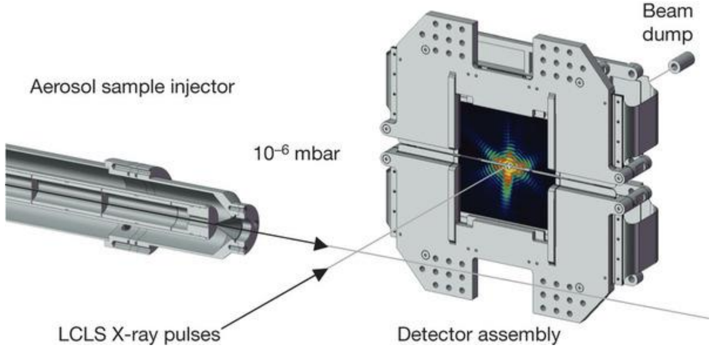


- **More efficient use of energy & distribution** e.g. via new classes of quantum materials with optimized performance

Industrial partners in: Chemical & Metals Sectors, Engineering Sector, Energy & Nuclear Sector, Electronics Sector

Ageing Society

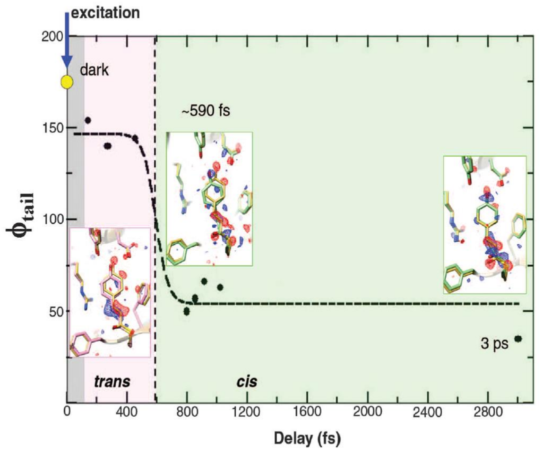
We will harness the power of innovation to help meet the needs of an ageing society.



- **Protein structure** (from nanocrystallography) leads to drug discovery

- **Deeper understanding of biomolecule processes in living cells** will lead to new concepts in healthcare & therapy, advanced therapy and diagnostics through novel developments of accelerators and detectors

- Research e.g. in HEDs & materials will lead to support for **better defence technology**



Industrial partners in: Pharmaceutical Sector, Heathcare Sector, Defence Sector,……

The Facility will Address Future Science & Technology Questions

- **There will be other/different challenges** and strategies that emerge over the next decades
- The **cutting edge capability to image matter in *space* and *time*** will remain a core requirement for all scientific and technology problems that require an understanding of **how matter works at the nanoscopic and quantum level**
- It will **underpin our ability to develop new technologies** based upon that understanding

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
- After todays meeting we will open a free format consultation with the UK science and technology community to gather information and ideas
- A series of Workshops will happen through the autumn on:

- Life Sciences
- Chemical Sciences & Energy
- Physical Sciences
- Quantum Materials and Nanotechnology
- Matter at Extreme Conditions
- X-ray FEL Applications to Technology

- A science case will be drafted through early 2020 with possibilities for continued input from the UK community

Thank you for your attention – we look forward to your participation in the UK XFEL science case exercise