Science and Technology Facilities Council

UK XFEL

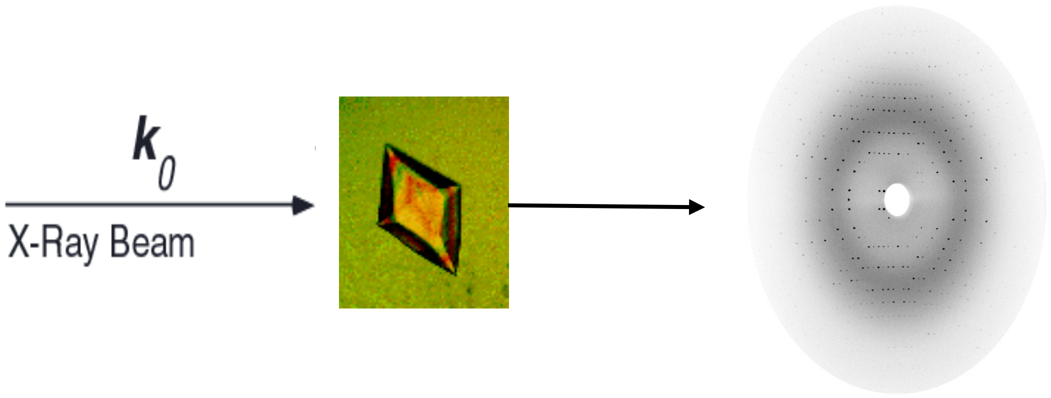
Science and Technology Impact of XFELs and Opportunities with a Next Generation Facility

xfel.ac.uk

X-ray probing of the nanoscale structure of matter

X-ray diffraction

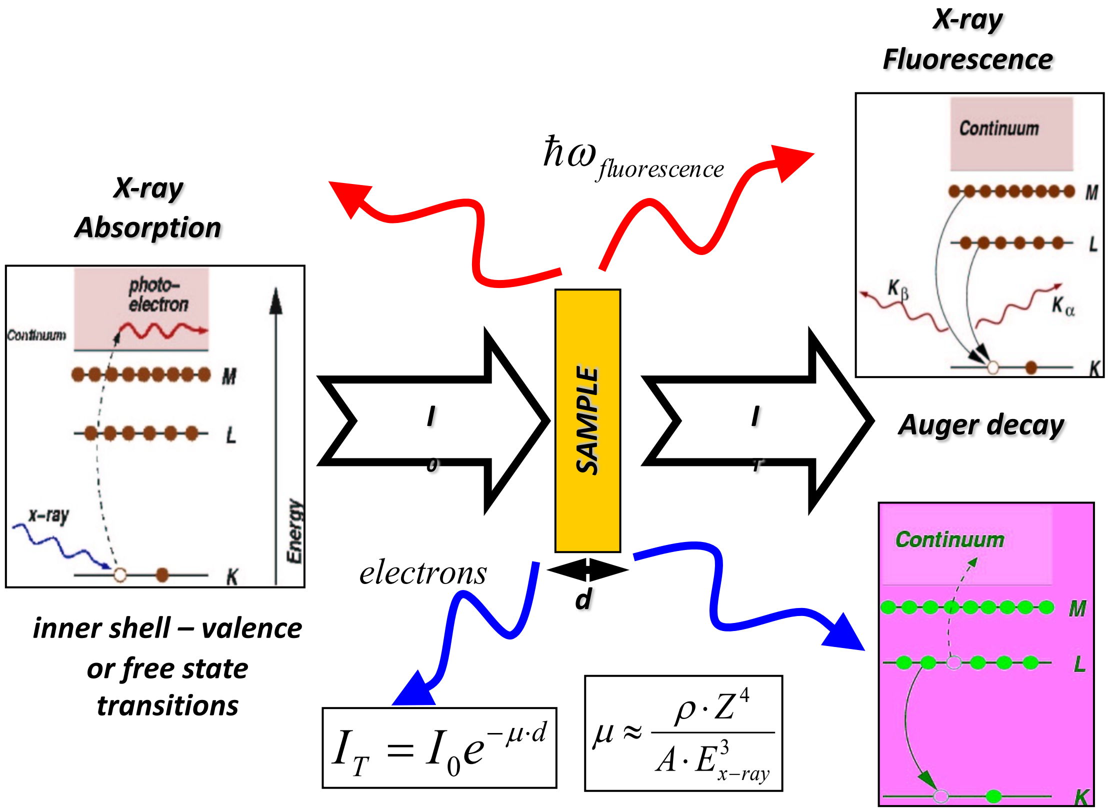
provides atomic structure



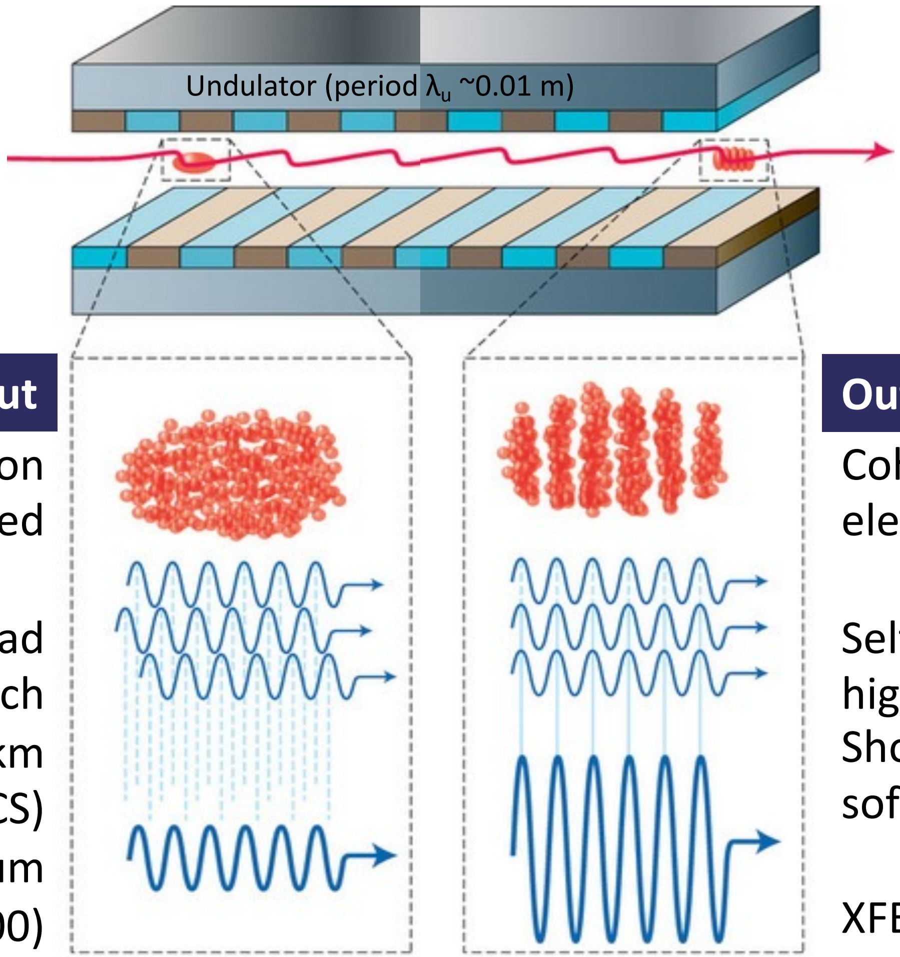
$\Delta \mathbf{k} = \mathbf{k}_0 - \mathbf{k}_S$ $\quad I(\Delta \mathbf{k})$

X-ray spectroscopy

provides electronic states with atomic specificity



XFEL Self-Amplified Spontaneous Emission (SASE)



Input

Incoherent emission
electrons randomly phased

Low emittance, narrow energy spread
relativisitic electron bunch
4 – 15 GeV accelerated in 100 m - > 1 km
electron linear accelerators (LINACS)
(relativistic electrons are the gain medium
with a Lorentz factor Υ ~ 2000)

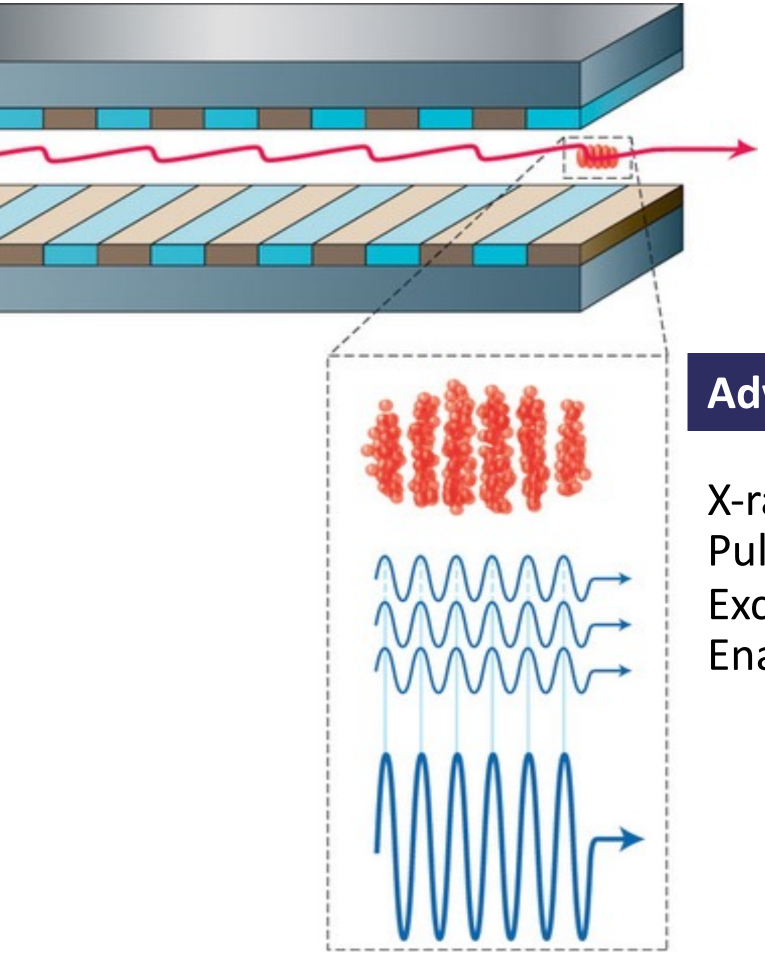
Output

Coherent emission
electrons bunched at radiation wavelength

Self-Amplified Spontaneous Emission (SASE)
high brightness,
Short Pulses
soft to hard X-rays

XFEL radiation wavelength $\lambda_r \sim \lambda_u\ \Upsilon^{-2}$

XFEL Self-Amplified Spontaneous Emission (SASE)

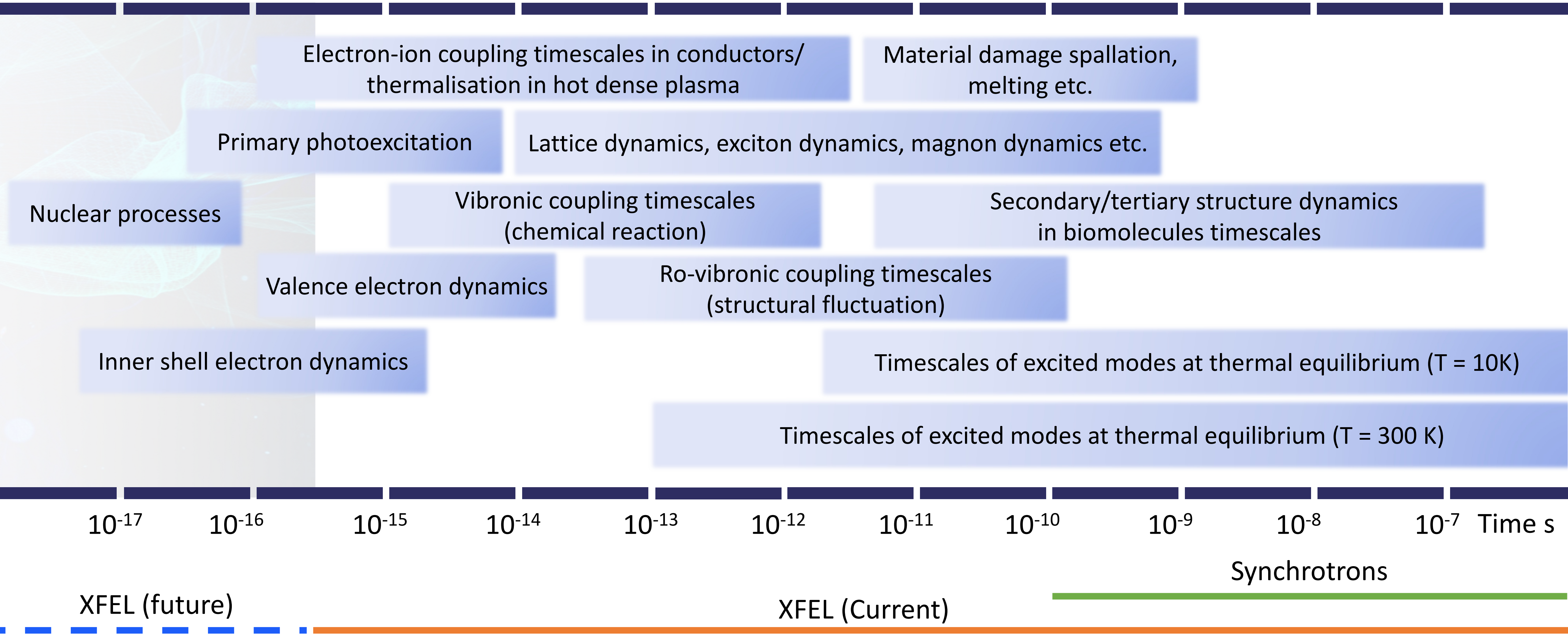


Advantages

X-rays from 10 eV to > 10 keV photon energies (100 nm to < 0.1 nm wavelength)
Pulses 0.3 fs – 100 fs duration
Exceptional brightness
Enable time resolved x-ray scattering and x-ray spectroscopy measurements

Real-time access to the characteristic processes and fluctuations in matter down to the quantum scale

Science drivers



XFELs Enable: Time-resolved X-ray measurements by the pump-probe methodology

Pump (X-ray to THz) – activates the sample:

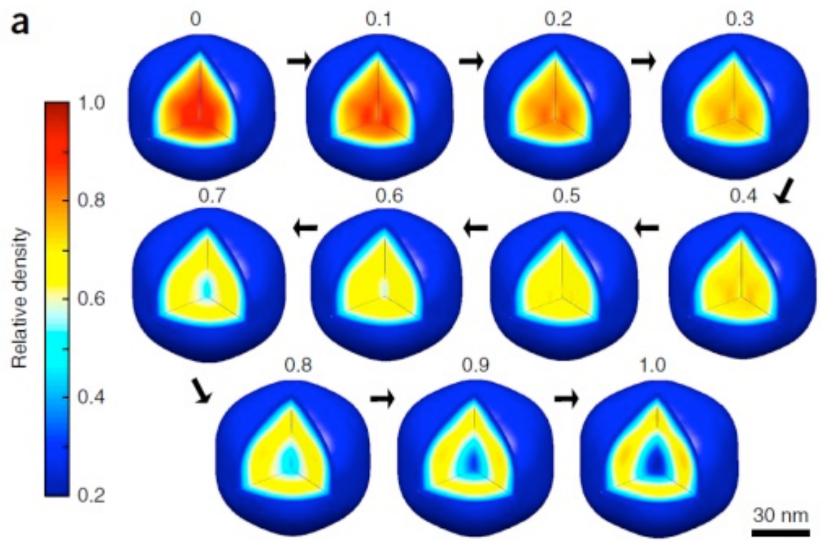
Sudden heating, injection of hot electrons, electronic state photoexcitation/photoionisation, excitation of vibrational/phonon or rotational modes etc.

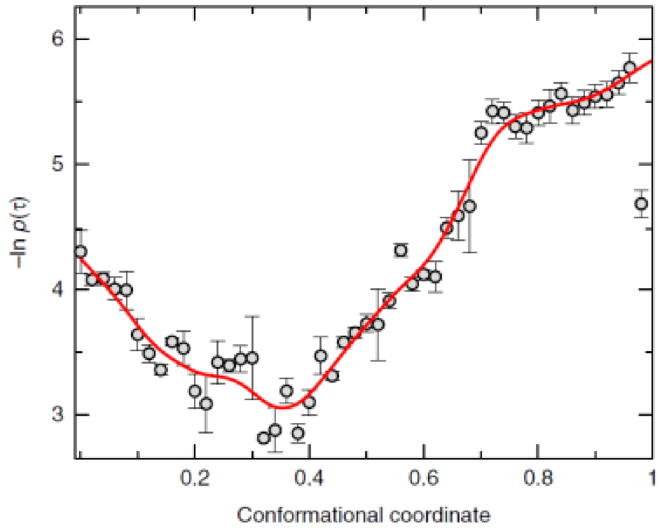
Probe (X-ray) – interrogates the sample after delay time τ by generating a suitable observable:

X-ray scattering/diffraction, resonant inelastic X-ray scattering (RIXS), X-ray spectroscopy (absorption (XAS) and emission (XES), X-ray photoelectron spectroscopy (XPS) etc.)

Data Volume Approach

Scattering from "identical" single systems with a large number of shots, coupled to advanced analysis methods, is enabling mapping of conformational dynamics, i.e. brief rare events (such as barrier crossings etc.)





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

Conformational dynamics from data driven approaches *Nature Methods* 14 877 (2017)

High brightness scattering can outrun destruction

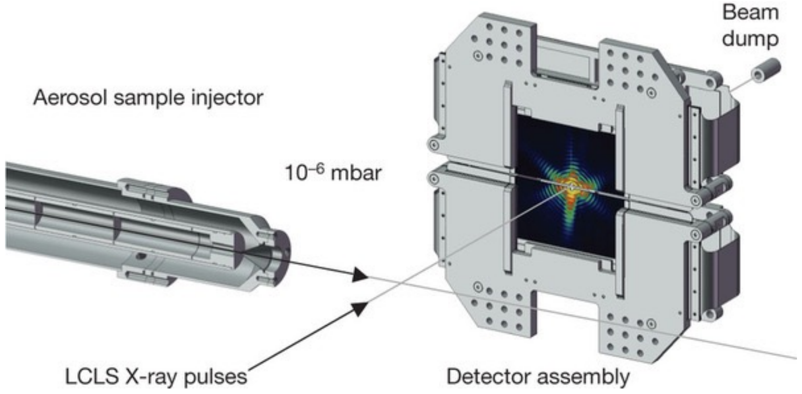
Diffract and Destroy

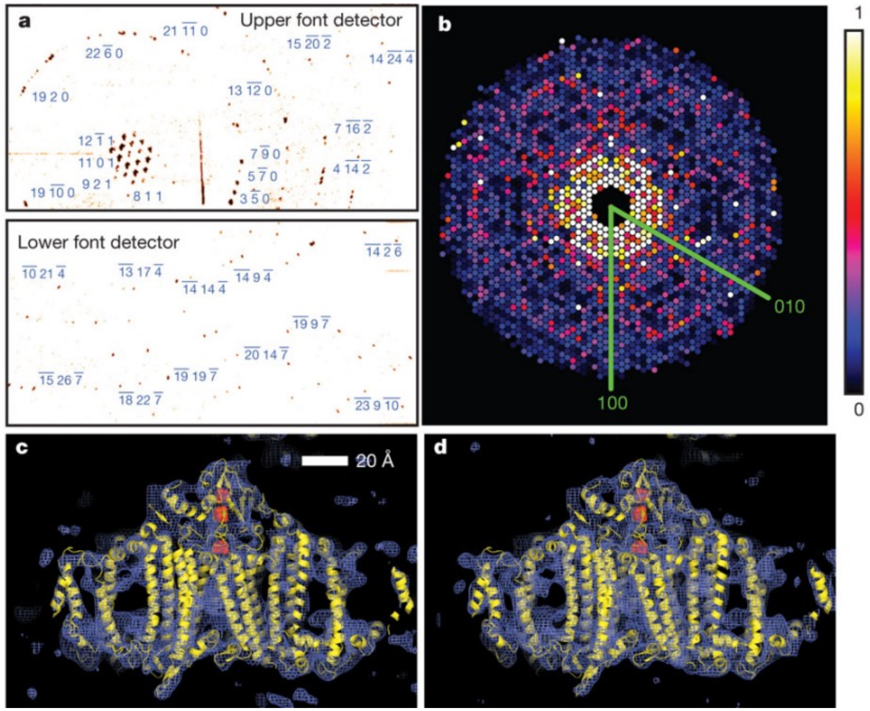
Conventional X-ray sources non-crystal samples destroyed before signal enough to determine structure.

Diffract before Destroy

Possible with the very short and very bright pulses from an XFEL!

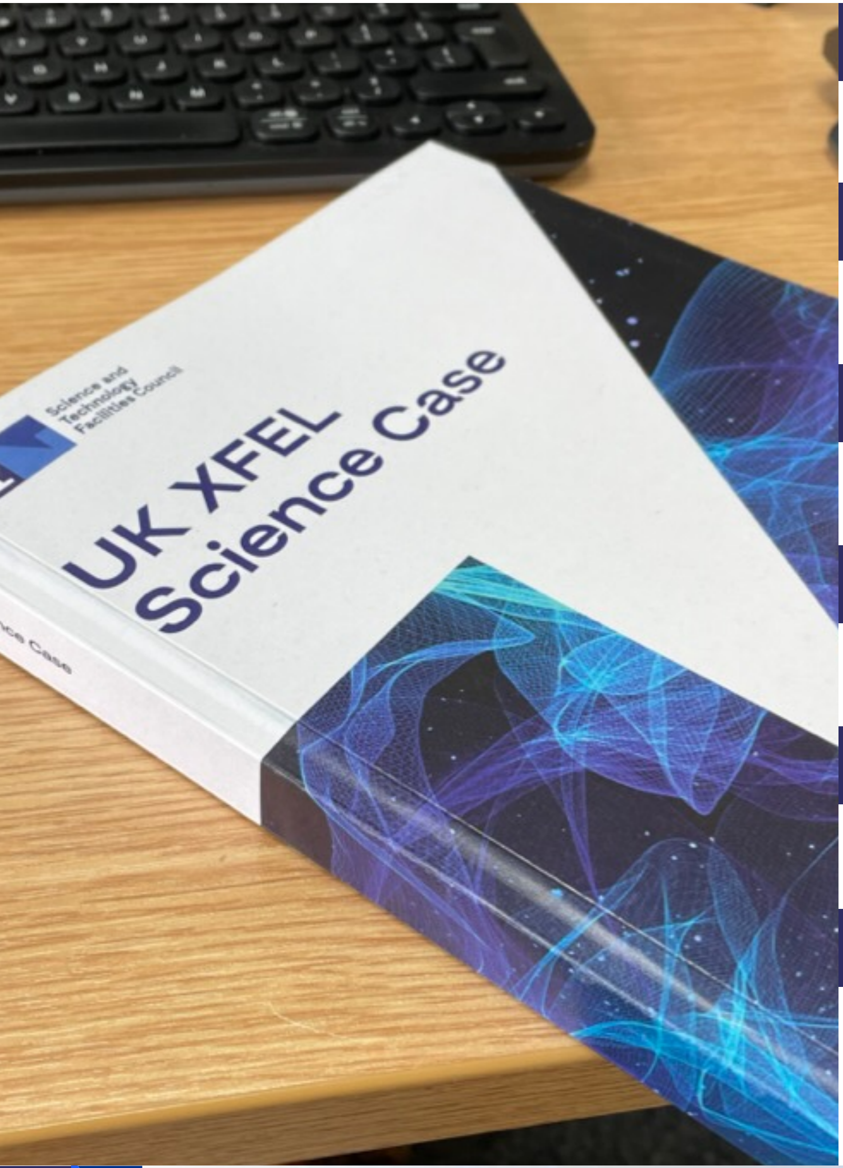
Non-crystal sample can be imaged before destroyed.





Chapman et al, *Nature 470, 73 (2011)*

Expert Science Team



Matter in extreme conditions

Andy Higginbotham (York), Andy Comley (AWE), Emma McBride (QUB), Sam Vinko (Oxford), Marco Borghesi (QUB), Malcolm McMahon (Edinburgh), Justin Wark (Oxford)

Nano/Quantum materials

Anna Regoutz (UCL), Marcus Newton (Soton), Ian Robinson (UCL/Brookhaven), Mark Dean (Brookhaven), Awan Shakil (Plymouth), Paolo Raedelli (Oxford), Simon Wall (Aarhus), Sarnjeet Dhesi (Diamond),*

Engineering/Materials/Applications

*David Rugg (RR), Sven Schroeder (Leeds), David Dye (IC) Dan Eakins (Oxford), Mike Fitzpatrick (Coventry) +**

Life sciences:

Allen Orville (Diamond), Jasper van Thor (IC), Xiaodong Zhang (IC), Shakil Awan (Plymouth), Adrian Mancuso# (Diamond), Tian Geng (Heptares)*

Chemical sciences:

Julia Weinstein (Sheffield), Russell Minns (Soton), Sofia Diaz-Moreno (Diamond), Alex Baidak (Manchester), Andrew Burnett (Leeds), Tom Penfold (Newcastle), Rebecca Ingle (UCL), Mark Brouard, Claire Vallance (Oxford)*

Physical sciences:

Amelle Zair (KCL), Adam Kirrander (Edinburgh), Jason Greenwood (QUB), Jon Marangos (IC), Elaine Seddon (Cockcroft) + #

+ around 100 additional experts from around the world contributing to Science Case

UK XFEL

An exciting opportunity for science and innovation

Key next-generation capabilities identified in the UK XFEL Science Case:

- Transform limited operation across entire X-ray range
- High efficiency facility with a step-change in the simultaneous operation of multiple end stations
- Evenly spaced, high-rep rate pulses to match samples & detectors
- Improved synchronisation/timing data with external lasers to < 1 fs
- Multiple colour X-rays at one end-station
- Full array of synchronised sources:
  XUV-THz, e-beams, high power & high energy lasers at high rep-rate

Science and Technology Facilities Council

Thank You

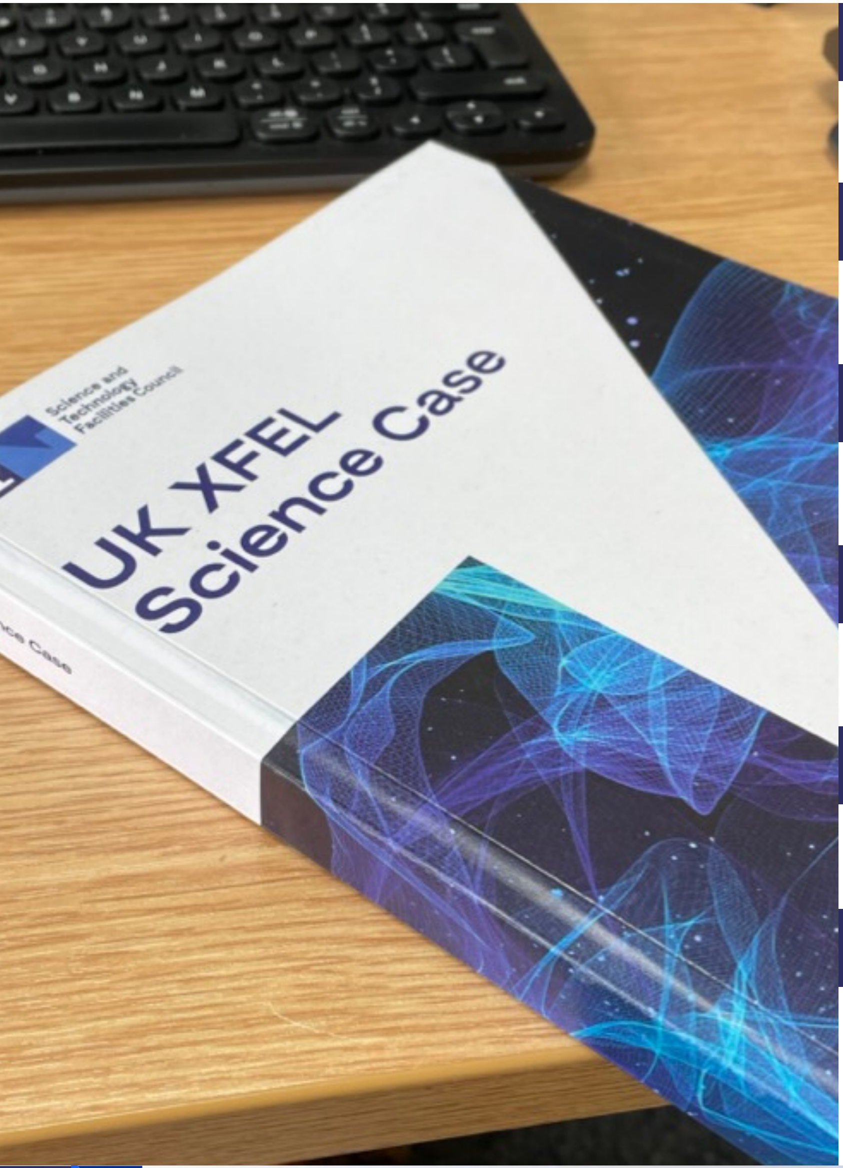
Slides and References available at

xfel.ac.uk

UKRI Science and Technology Facilities Council

The Science Case

Expert Science Team



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Science and Technology Facilities Council

The Science Case

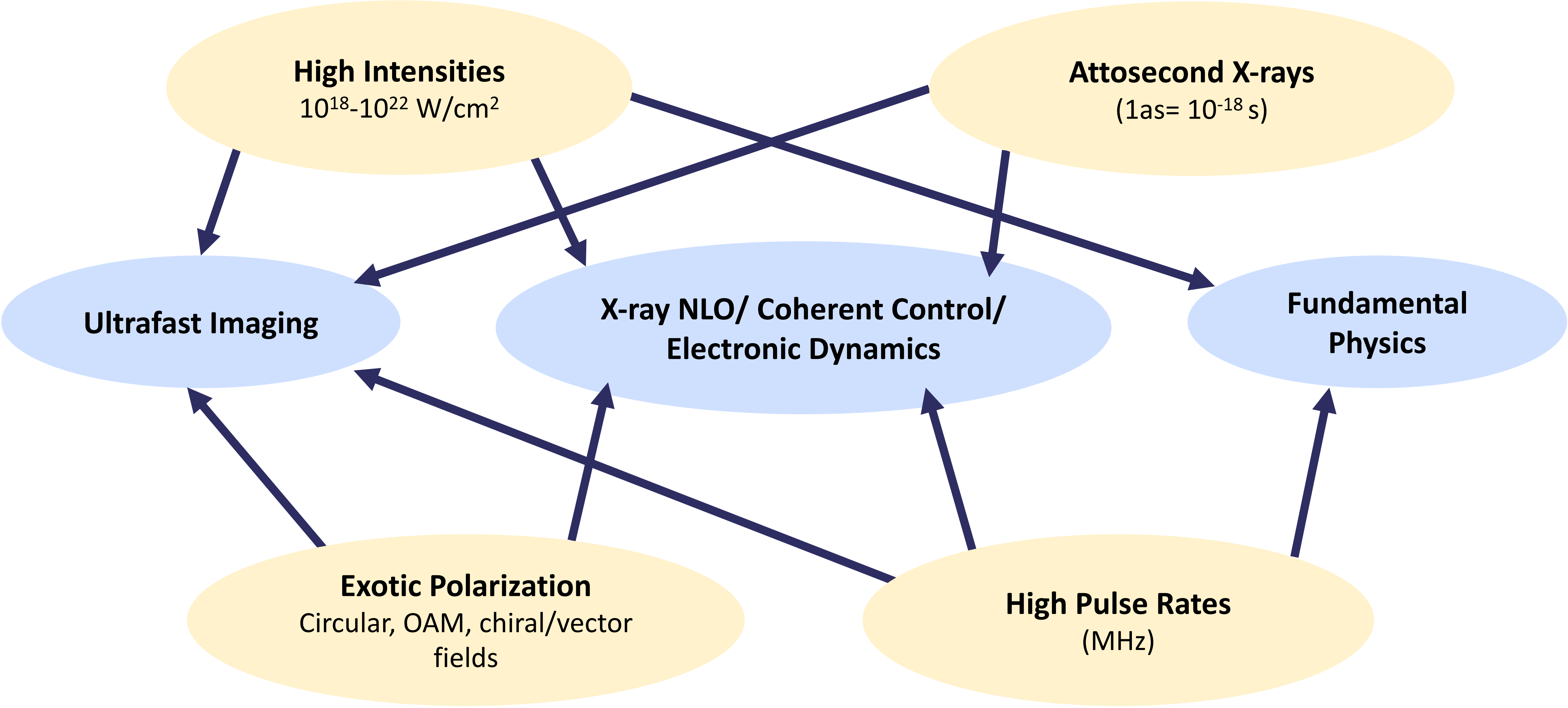
1. Physics and X-ray Photonics
2. Chemical Sciences
3. Life Sciences
4. Condensed Matter, Quantum and Nanomaterials
5. Matter at Extreme Conditions
6. Industrial Applications
7. Future Directions

Science and Technology Facilities Council

Physical Sciences

Amelle Zair (KCL), Adam Kirrander, (Oxford), Jason Greenwood (QUB),
Jon Marangos (IC), Elaine Seddon (Manchester)

New Physics and X-ray Photonics

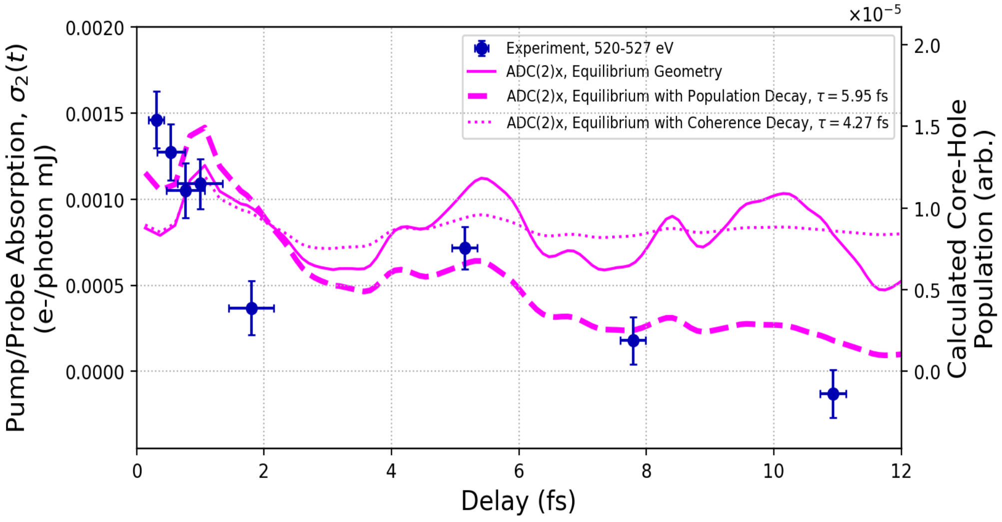


New Physics and X-ray Photonics

Attosecond electron dynamics

New tools to reveal electron dynamics, electron-phonon and photon-electron coupling in molecules, metals, semiconductors, dielectrics, 2D materials, liquids and amorphous systems

Charge migration damping in **aminophenol**

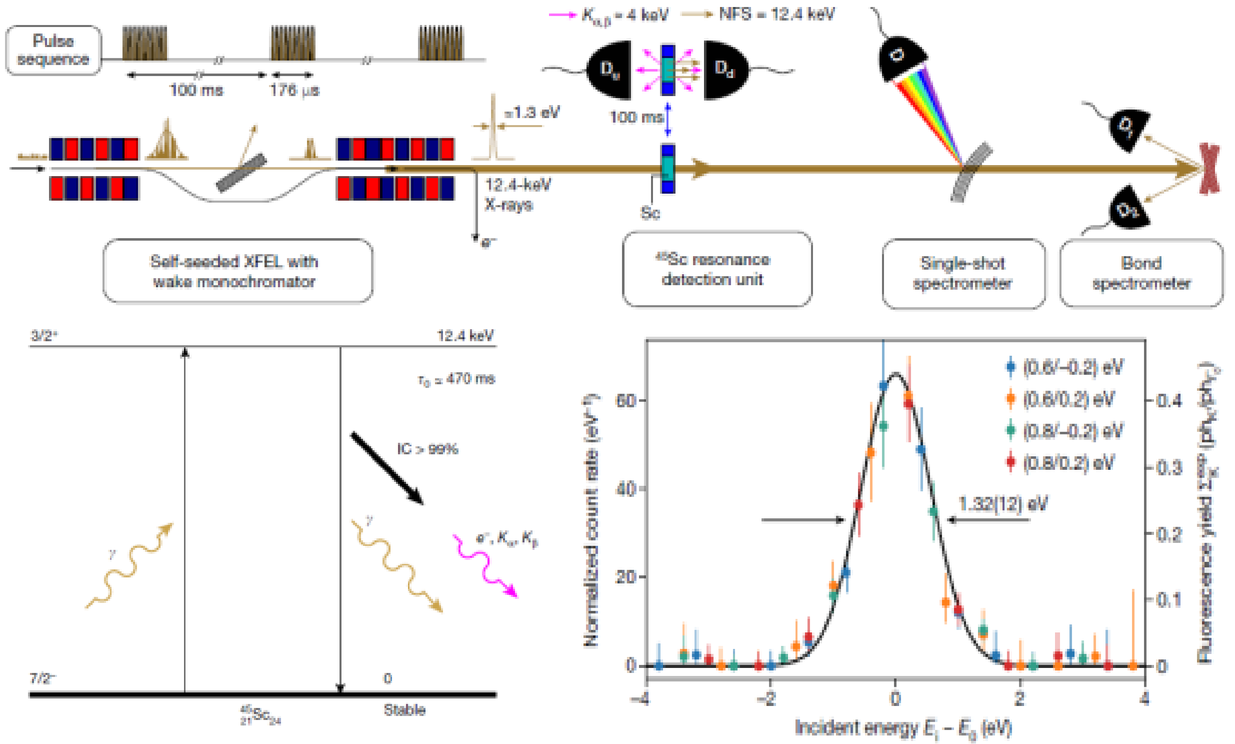


Charge migration and electron-nuclear coupling in glycine *Science Advances* 8 (2022)
Isolated attosecond pulses *Nature Photonics* 14 30 (2020)
Impulsive stimulated x-ray Raman scattering *PRL* 99 073203 (2020)
Core electronic wave packet dynamics *Science* 375 285 (2022)

Explore fundamental physics

Future opportunities to explore fundamental physics eg: strong field QED, CP violations, axions, dark matter

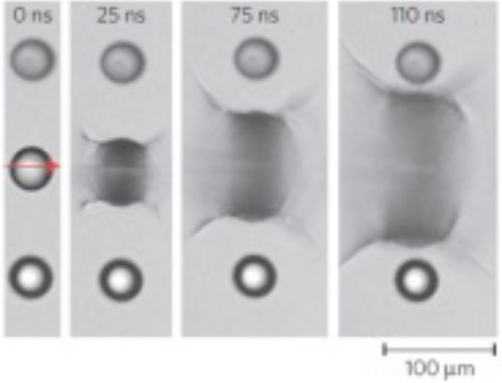
Resonant x-ray excitation of nuclear clock isomer ^{45}Sc



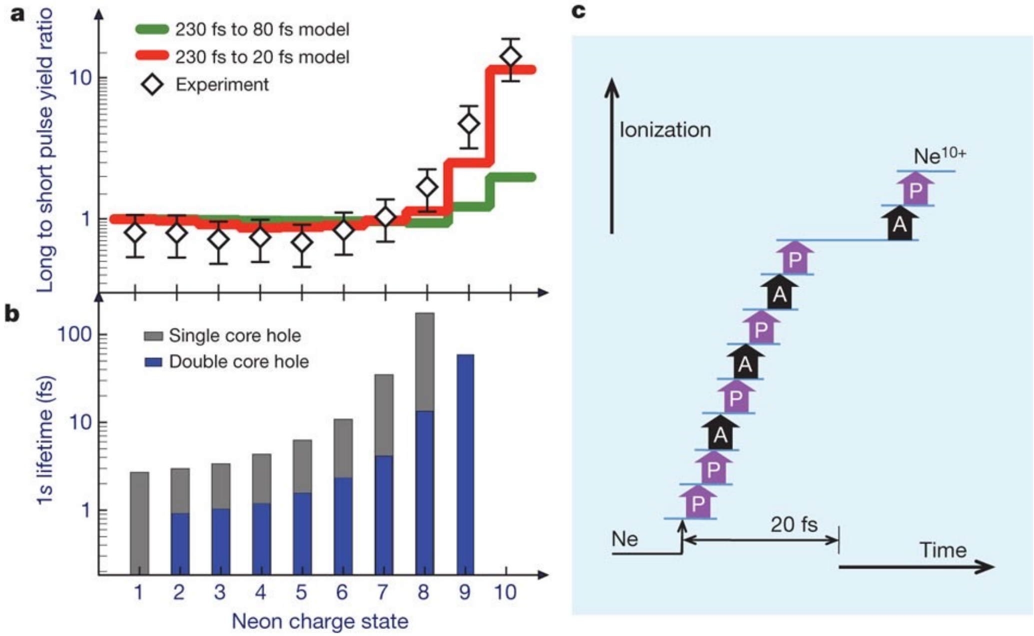
Nature 622 471 (2023)

New Physics and X-ray Photonics

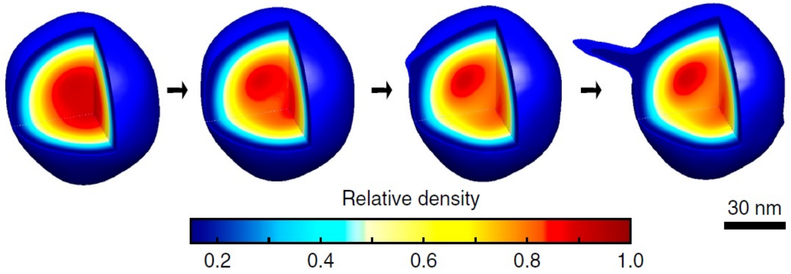
X-ray - matter interaction



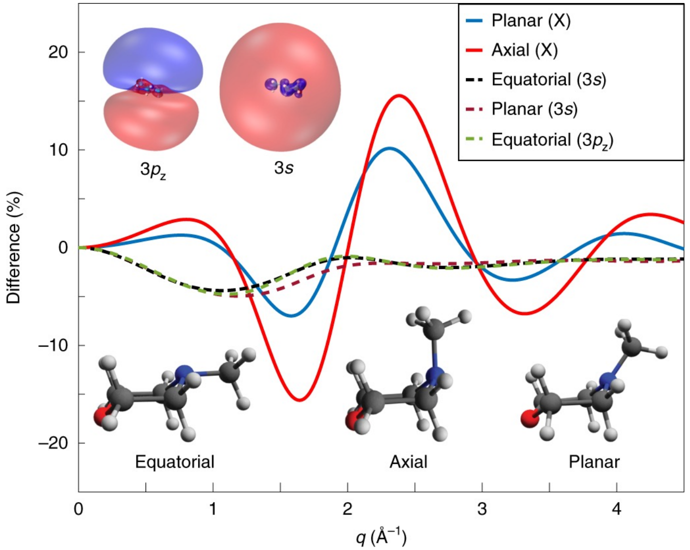
Response to ultra-intense X-rays *Nature* 466 56 (2010)
Interaction with liquids *Nature Physics* 12 966 (2016)
Ultrafast radiolysis *Science* 367 179 (2020)



New directions in x-ray scattering



Conformational dynamics from data driven approaches *Nature Methods* 14 877 (2017)
Ultrafast coherent dynamics in isolated molecules *Nature Chemistry* 11 716 (2019)



Future Opportunities for Physical Sciences

New linear and non-linear x-ray spectroscopies

Probe dynamics, charge, and energy transfer in matter
(intense, high rep-rate, attosecond pulses, soft to hard x-rays, multi-colour x-rays)

Sensing chirality and tracking chiral dynamics

ultrafast pulses, polarisation control, high rep-rate, soft x-rays

Biomolecular and nanosystems

Conformational dynamics across wide spatial and temporal scales (high rep rate, hard x-rays)

Extreme x-ray interaction with matter and vacuum

x-ray nanoscale high fields, formation virtual electron-positron pairs (high rep-rate/high intensity/hard x-rays)

Material processing

New opportunities with atomic scale resolution/atomic specificity (nanofocusing, high rep-rate, short pulses)

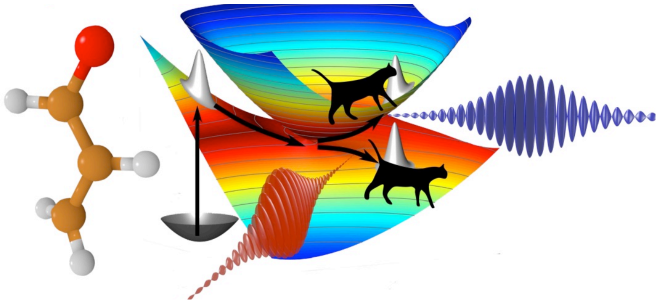
Chemical Sciences, Catalysis, Energy

Julia Weinstein (Sheffield), Russell Minns (Soton), Sofia Diaz-Moreno (Diamond), Andrew Burnett (Leeds), Tom Penfold (Newcastle), Rebecca Ingle (UCL), Mark Brouard, Claire Vallance (Oxford), Alex Baidak (Manchester)*

Chemical Sciences, Catalysis, Energy

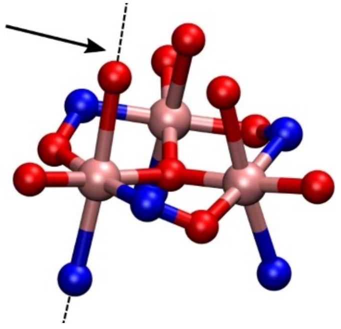
Transient electronic coherence

(attosecond X-Ray Raman)



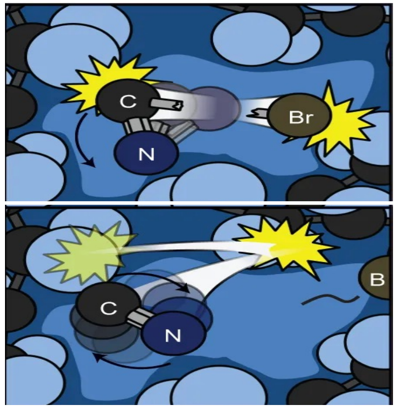
Phys Rev Lett 2015, 115, 19003

Spin dynamics



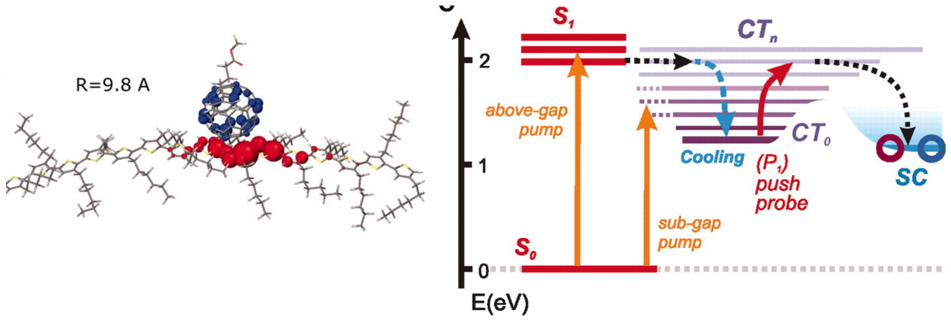
Vibrational coherence in
single-molecule magnets, «Mn3»
Nature Chem. 2020, 452

Solvent-Solute interaction



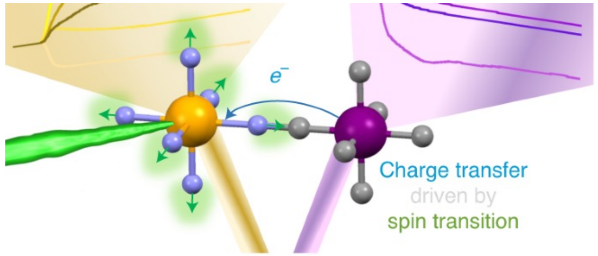
Nature Chem.2016, 242

Exciton Dynamics



Science 2012, 335, 1340

Charge transfer dynamics



Charge transfer driven by ultrafast spin transition
in a CoFe Prussian blue analogue. *Nature Chem 2021, 10.*

Towards molecular movie in chemistry and biochemistry

The Science Question

Fundamentals of reaction dynamics, the interplay of spin, charge, structure.

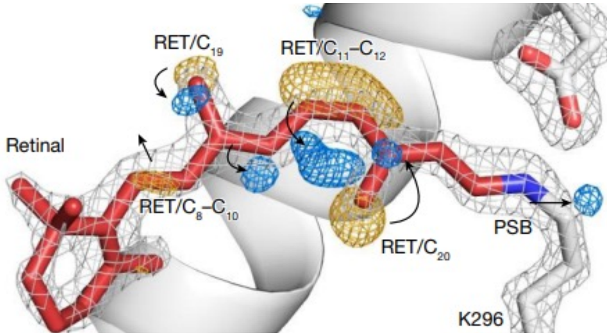
The Movie

Ligand dissociation
Primary steps in protein dynamics

The Applications

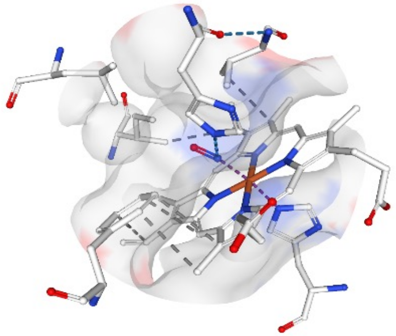
Enzyme catalysis
Photoprotection
Drug-target interaction

Ultrafast structural changes direct the first molecular events of vision



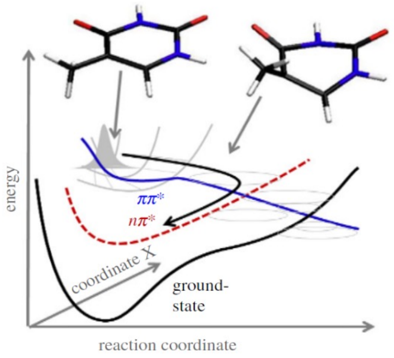
Nature, 615, 939 (2023)

Correlated spin & structural dynamics



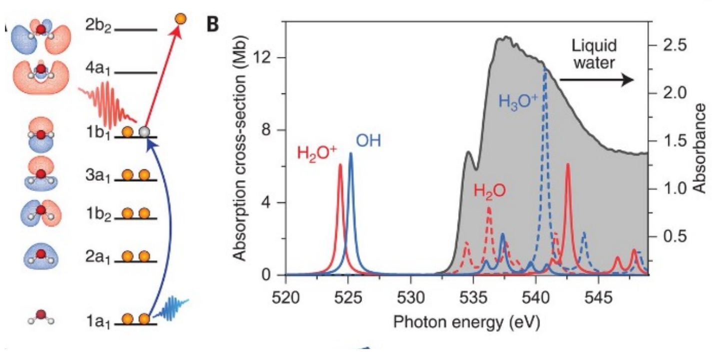
Nat. Comm. 11, 4145 (2020)

Photochemistry of DNA



Nat. Comm. 8, 29, (2017)

Observation of the fastest chemical processes in the radiolysis of water



Science, 367, 179 (2020)

Fundamentals of reaction dynamics

The Science Question

Fundamentals of reaction dynamics, the interplay of spin, charge, structure.

The Movie

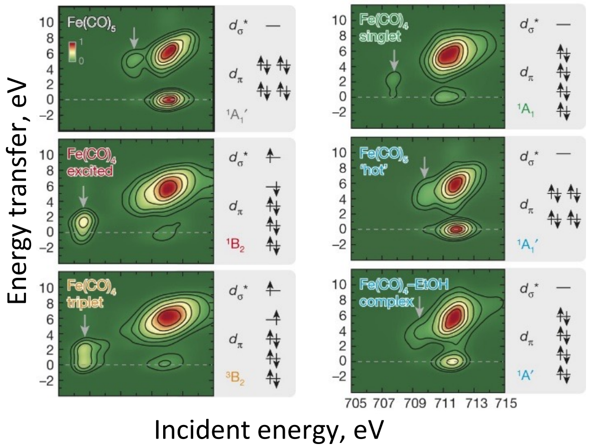
Ligand dissociation
Primary step in catalysis

The Applications

Magnetic materials, Information storage
Fundamentals of chemical reactivity

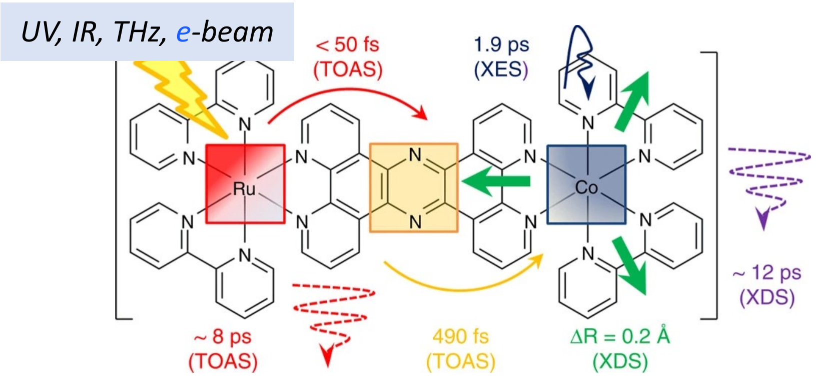
Element- and site-specific probing:

Time-resolved RIXS *at the Fe L_3 edge, $Fe(CO)_5$*

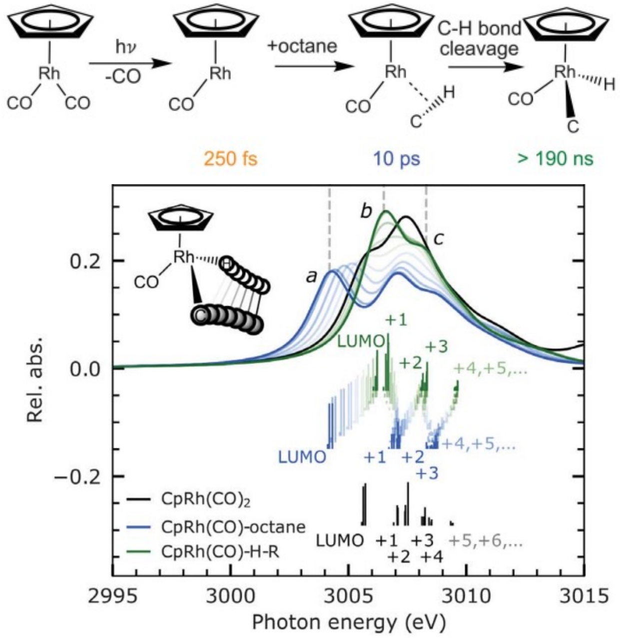


Orbital-specific mapping of the ligand exchange dynamics of $Fe(CO)_5$ in solution *Nature 520, 78 (2015)*

Homogeneous catalysis

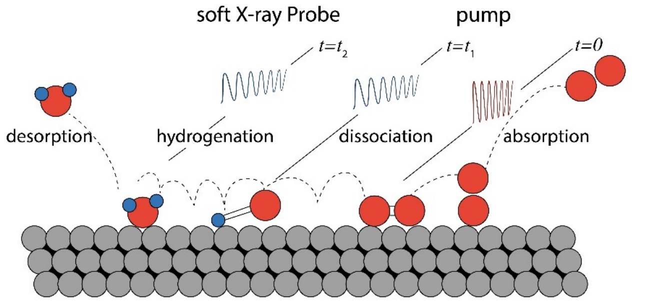


Photocatalysis, Enzyme catalysis



Tracking C–H activation with orbital resolution provides opportunities for manipulating C–H reactivity in transition metals *Science 380, 955 (2023)*

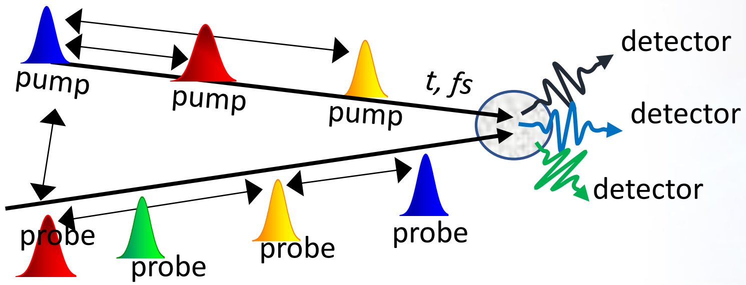
Controlling catalytic reactions with THz excitation



Chem Phys Lett 675, 145 (2017))

Chemical Sciences and Energy with XFELs: fs, <0.01 Å, real-time "movie"

Chemistry: all states of matter, decades of time-scale and energies, and dimensions from atomic to protein to whole organisms.



- Predict and control photochemical reactions
- Fundamentals of reaction dynamics: nuclei, electrons and spin
- Exploring complex energy landscapes through chemical activation
- Energy materials and devices
- (Photo)(electro)catalysis *in operando*
- Environment: aerosols, space, combustion, corrosion
- Photodynamics in biomolecules, therapies, diagnostics

Game Changer

Combine X-rays with *e*-beam, VUV, UV, Vis, IR, THz excitation and detections: mix-and-match, multicolour, multi-parameter space, multidimensional methods

- High repetition rate
- High photon flux
- Broad X-ray energy range – soft/hard; light and heavy elements
- Synchronisation as required
- *Whole system in one snap-shot*

Science and Technology Facilities Council

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Life Sciences

Allen Orville (Diamond), Jasper van Thor (IC), Xiaodong Zhang (IC), Shakil Awan (Plymouth), Adrian Mancuso (Diamond), Tian Geng (Heptares)

Opportunities for Life Science

1. Atomic resolution structures of biomolecules w/o X-ray dependent artifacts via serial femtosecond crystallography (SFX) methods using nano- to microcrystal slurries.
2. Obtaining deep functional insights through time-resolved crystallography, scattering, and/or imaging of biomolecules in crystalline and/or solution states that can also be correlated with spectroscopy derived from the same sample and X-ray pulse.

The Era of *Dynamic* Structural Biology (at XFELs & synchrotrons)

NEW SCIENCE

- Time-Resolved SFX / SSX
- General and Widespread
- High Temporal (fs) and Spatial (~ 1 Å) Resolutions
- Correlated with one/more Spectroscopies (tr-XES …)

NEW CAPABILITY

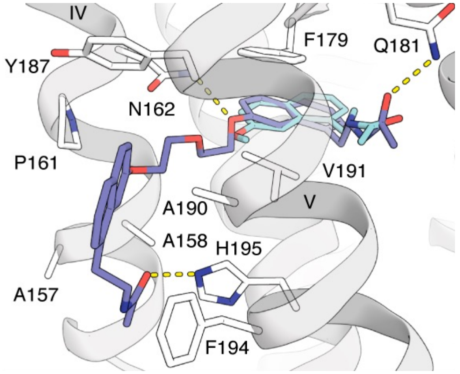
- High rep. rate detectors → more time points / Rxn
- Spatially Resolved Anomalous Dispersion → status of intermediates
- SASE -*vs*- Seeded → tr-SFX ± tr-XES ± ΔE across metal(s) absorption edge(s)

IMPACT

- **Stop-motion movies of functional systems**
- **Detailed mechanistic insights, less ambiguity**
- **New drugs, therapies**
- **New catalysts for global energy challenges**

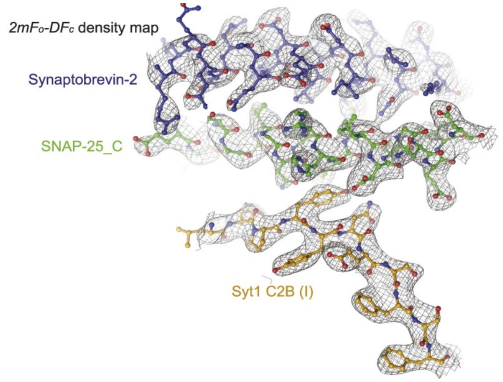
Atomic resolution structures without artefacts

Structural basis of ligand recognition at the human MT1 melatonin receptor

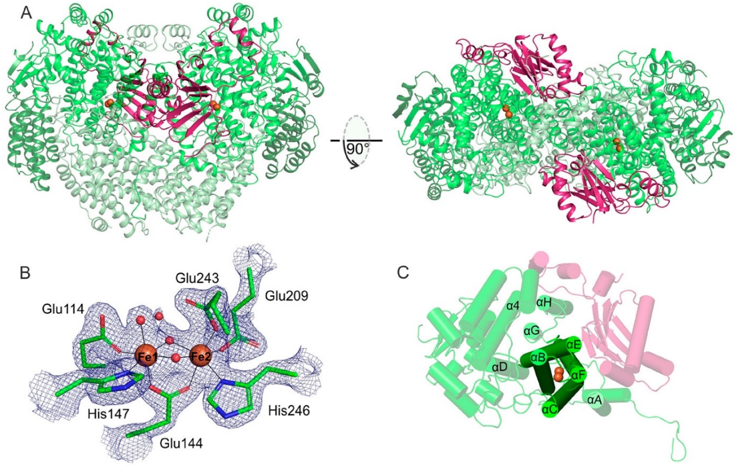


Stauch et al *Nature 569, 284-288 (2019)*

Architecture of the synaptotagnmin- SNARE machinery for neuronal exocytosis

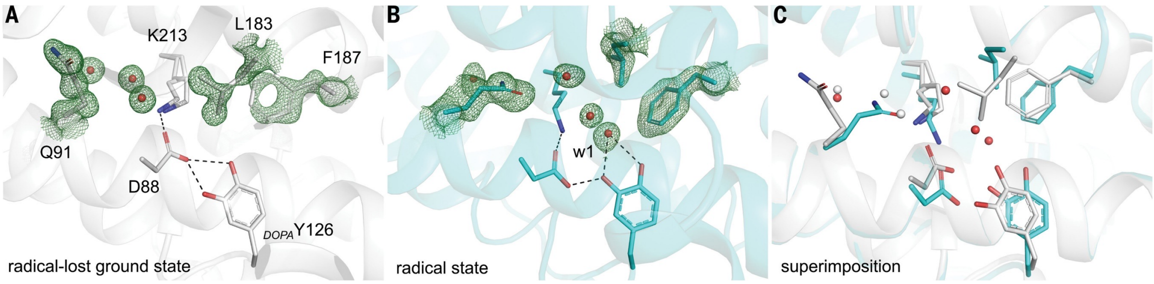


Structure of methane monooxygenase



Srinivas et al *J Am Chem Soc 142, 14249-14266 (2020)*

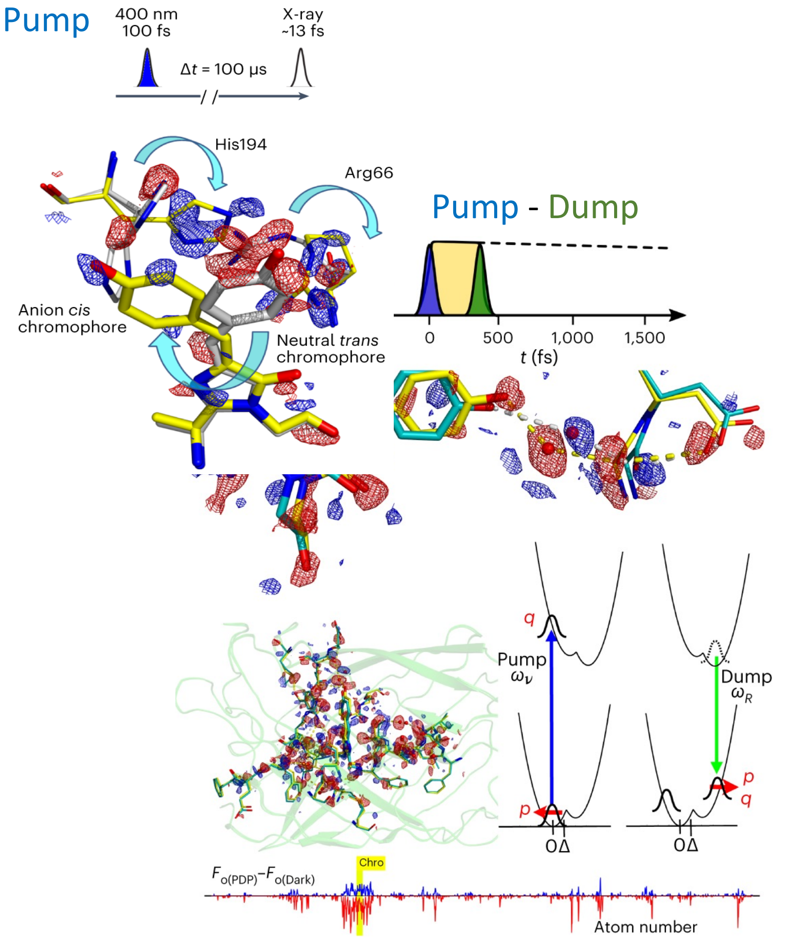
Structure of a ribonucleotide reductase R2 protein radical



Lebrette et al. *Science 382, 109-113 (2023)*

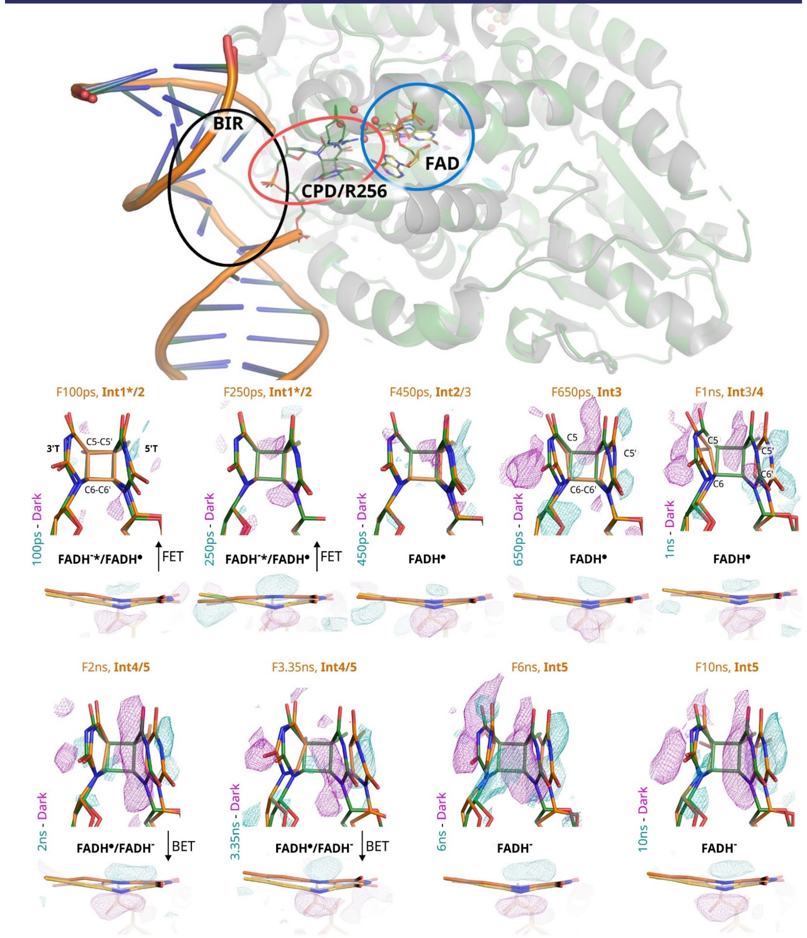
Dynamic structural biology

Optical control of ultrafast structural dynamics in a fluorescent protein.



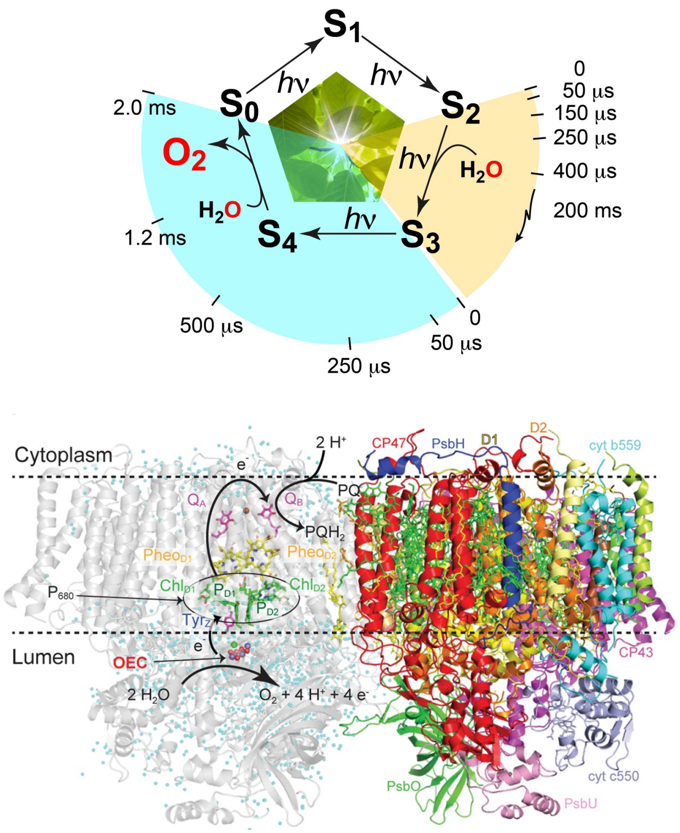
Hutchison et al *Nature Chem. 12, 1607 (2023)*

Visualizing the DNA repair process at atomic resolution



Maestre-Reyna et al *Science 382, eadd7795 (2023)*

Structural evidence for intermediates during O2 formation in photosystem II



Kern et al *Nature 563:421 (2018)*
Bhowmick et al *Nature 617:629 (2023)*

Future Opportunities for Life Sciences

High throughput SFX enabling new structures for life-sciences and pharma

(*high rep-rate x-rays, matched rep-rate of detectors and sample deliver*

High data volume CDI and tomographic XRD

(*average x-ray flux orders of magnitude higher than DLS II, nanofocusing)*

Conformational dynamics in viruses and sub-cellular assemblies

(*high rep rate, hard x-rays*)

Mapping drug activity in real time

(*high rep-rate/high intensity/hard x-rays)*

Dynamic structural biology capturing dynamics across many timescales

(high rep-rate x-rays, samples and detectors, synchronised laser and activation sources)

Radiation biology and medicine

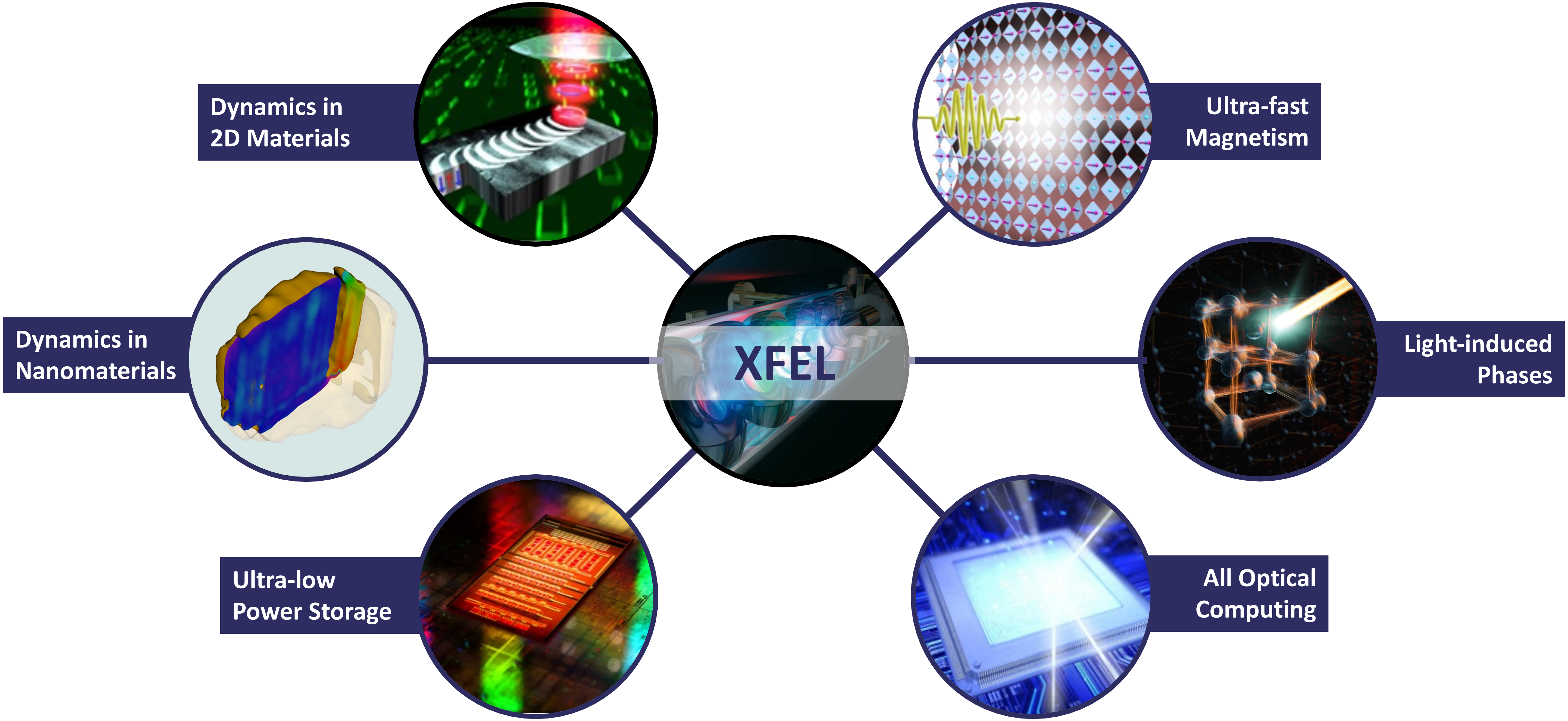
(hard x-rays synchronised to soft x-rays, electron, proton and ion pulses)

Science and
Technology
Facilities Council

Condensed Phase, Quantum Materials and Nanotechnology

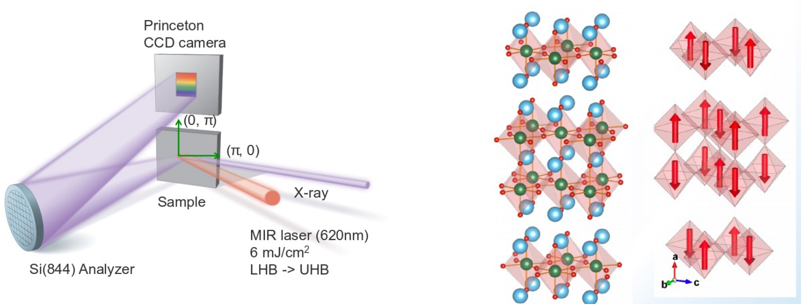
Anna Regoutz (UCL), Marcus Newton (Soton), Ian Robinson (UCL/Brookhaven), Mark Dean (Brookhaven), Awan Shakil (Plymouth), Paolo Raedelli (Oxford), Simon Wall (Aarhus), Sarnjeet Dhesi (Diamond),*

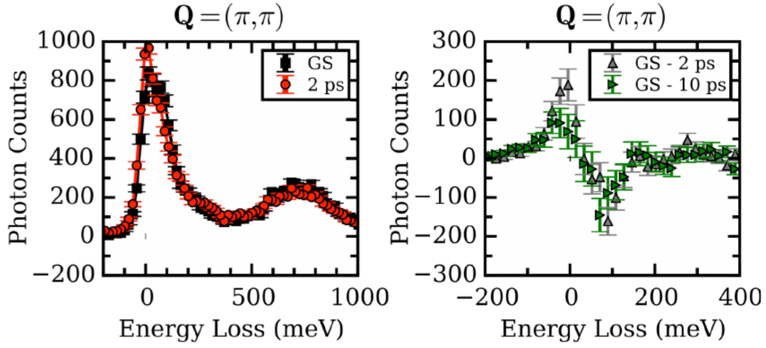
Condensed Phase, Quantum Materials and Nanotechnology



Recent work

Time-resolved Resonant Inelastic X-ray Scattering (Tr-RIXS)

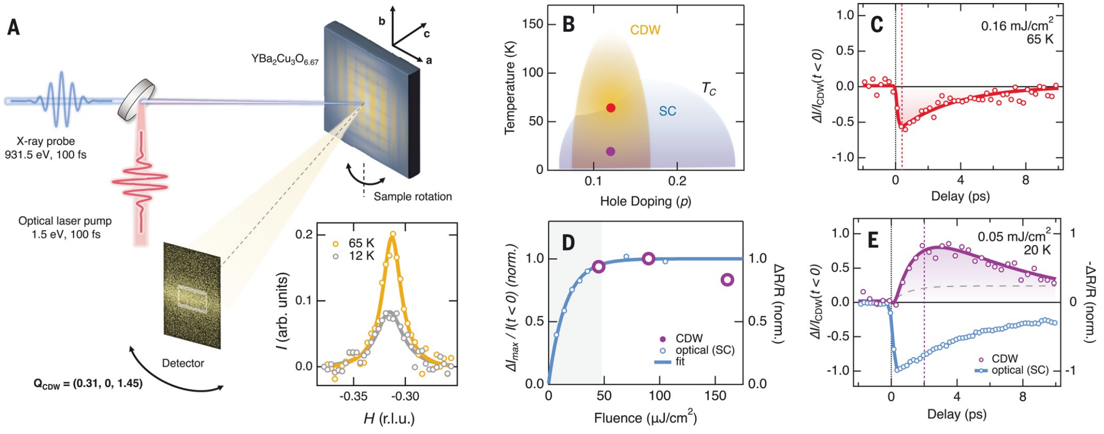


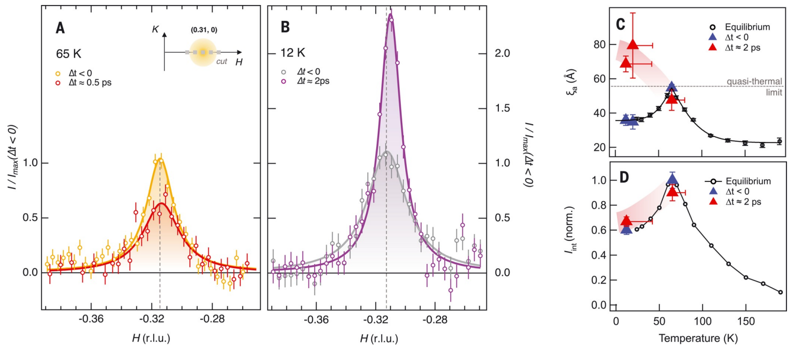


Tr-RIXS resolves spin, orbit charge contributions in magnetic materials out of equilibrium.

M. P. M. Dean et al., *Nature Materials 15, 601–605 (2016)*

Laser pump, X-ray probe of Superconductivity and CDW Interactions



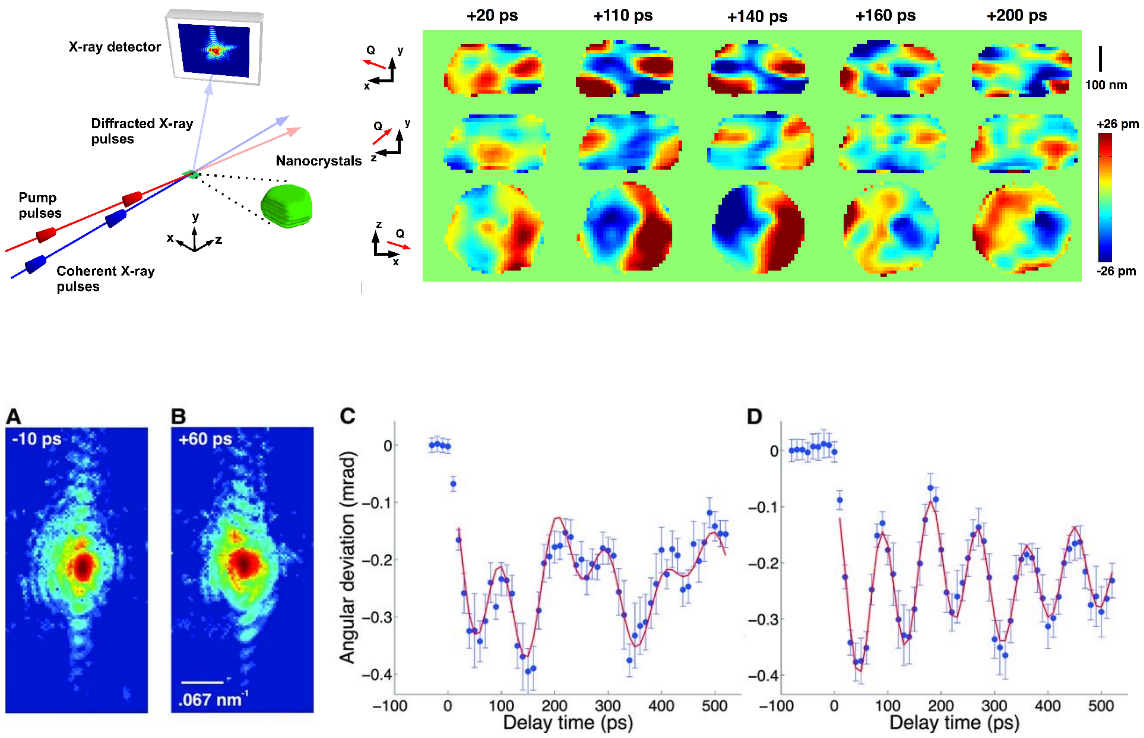


Superconductivity stabilises CDW topological defects that are removed by suppressing superconductivity.

R. Mankowsky et al. *Nature 516, 71-73 (2014)*
S. Wandel et al., *Science 376, 860 (2022)*

Recent work

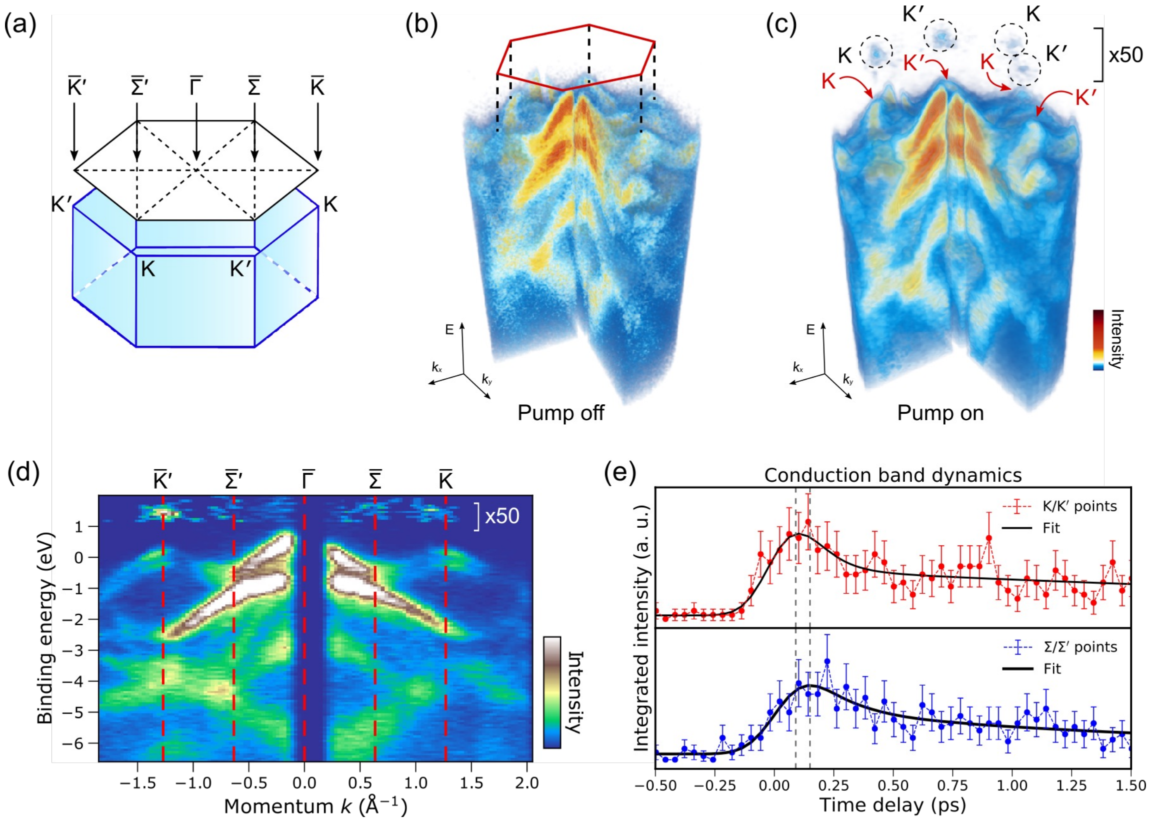
Time-resolved Bragg Coherent Diffraction Imaging (Tr-BCDI)



3D images of acoustic phonons in a nanocrystal. Orthogonal cut planes through the nanocrystal showing the projected displacement as a function of delay time.

J.N. Clark et al. *Science 341, 56–59 (2013)*

Photoelectron Momentum Microscopy of 2D Material



Combining valence-band and core-level spectroscopy with photoelectron diffraction for electronic, chemical, and structural analysis.

D. Kutnyakhov, et al. *Rev. Sci. Instrum. 91 (1): 013109 (2020)*

Future Opportunities

Ultrafast Magnetism

Femto/atto second pump-probe scheme in THz/mid-IR to couple to phonon modes

Imaging Dynamics in Nanomaterials

Femto/atto second time-resolution to unambiguously probe each stage during a structural phase transition in three-dimensions

Electronic Dynamics in Quantum Materials

Access to electronic dynamics in the time-domain with atto second time resolution

Disorder in Quantum Materials

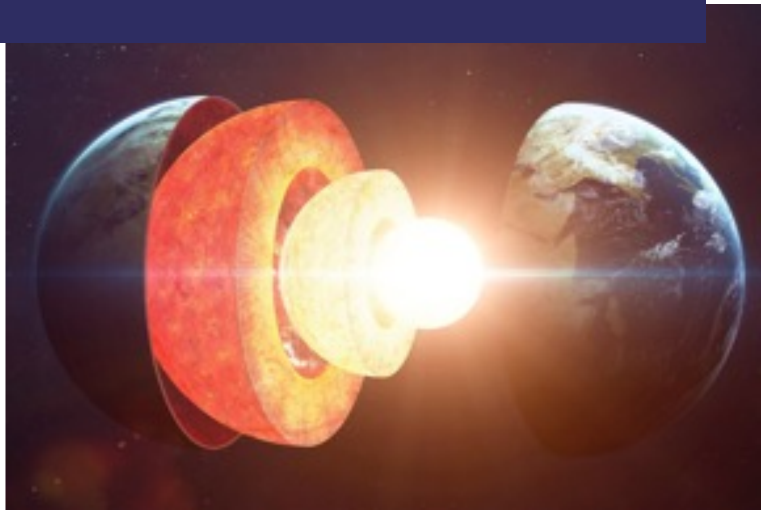
Probing disorder in broad range of materials with femto/atto second time resolution
Utility of high energy x-rays, for time-resolved pair distribution function (tr-PDF) measurements upto 50 keV.

Matter at extreme conditions

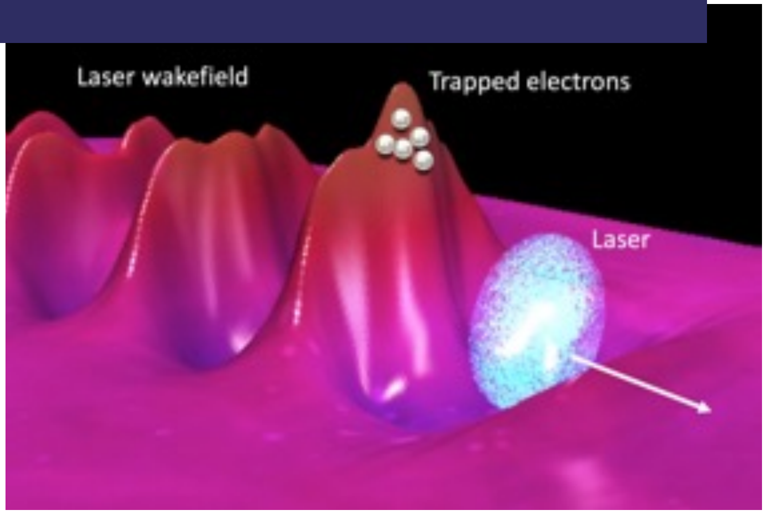
Andy Higginbotham (York), Andy Comley (AWE), Emma McBride (QUB), Sam Vinko (Ox), Marco Borghesi (QUB), Malcolm McMahon (Edinburgh), Justin Wark (Ox)

Matter at Extreme Conditions

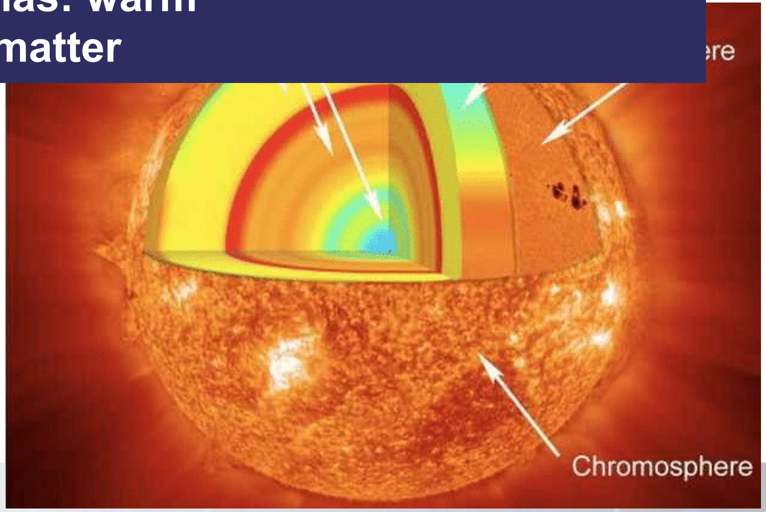
Shocked materials and matter at extremes



Interactions with energetic electron and ion beams



Quantum plasmas: warm and hot dense matter



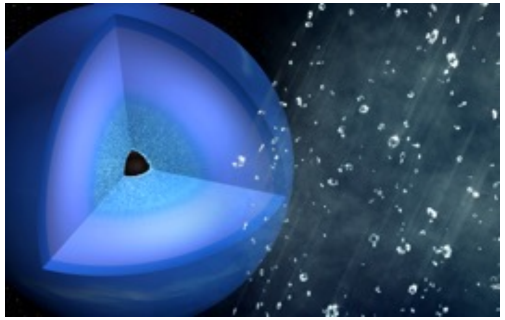
Even more extreme conditions at a spherical compression facility

Shocked materials and matter at extremes

At extreme pressures matter undergoes complex low-symmetry phase transformations including melting. Understanding this behaviour is important for many different scientific fields

Understanding planetary interiors

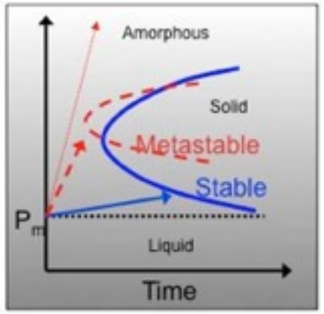
Partial dissociation of C-H and formation of diamond on Neptune



Kraus et al. *Nat. Ast. 1, 606 (2017)*

Novel material synthesis

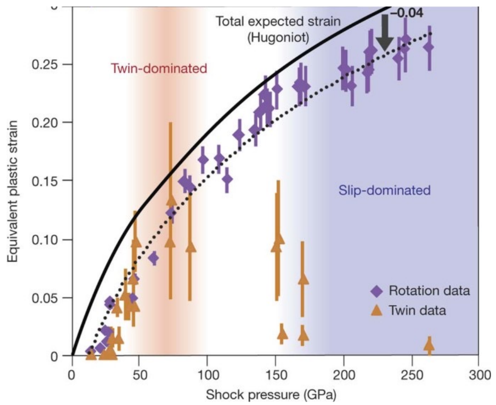
Observation of metastable phase in bismuth



Gorman et al. *APL 114 120601 (2019)*

Dynamic strength of materials

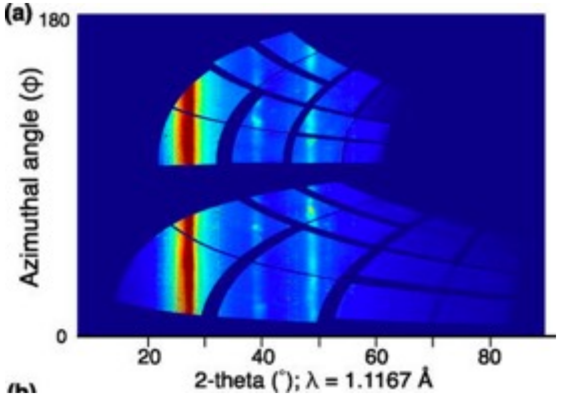
Twinning in dynamically compressed tantalum



Wehenberg, et al. *Nature, 550, 496 (2017)*

Melting at extreme pressures

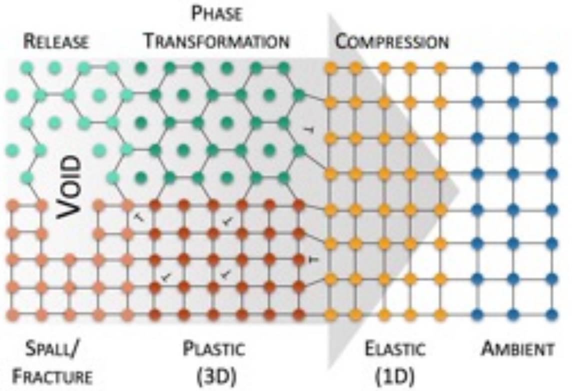
Shock-induced melting in tin



Briggs et al. *APL, 115, 264101 (2019)*

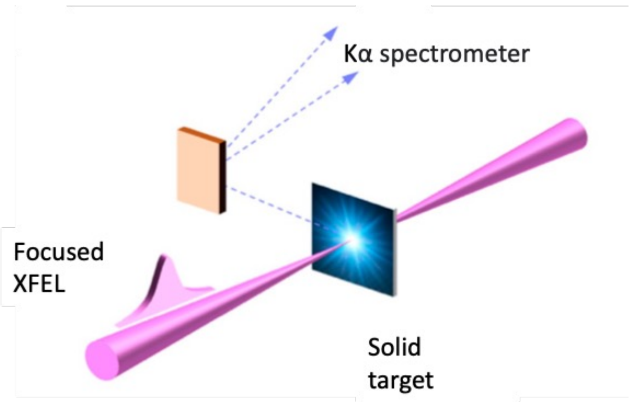
High strain rate phenomena

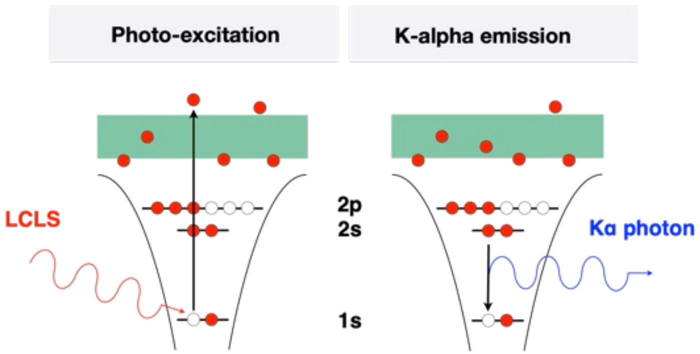
Response of silicon to uniaxial compression



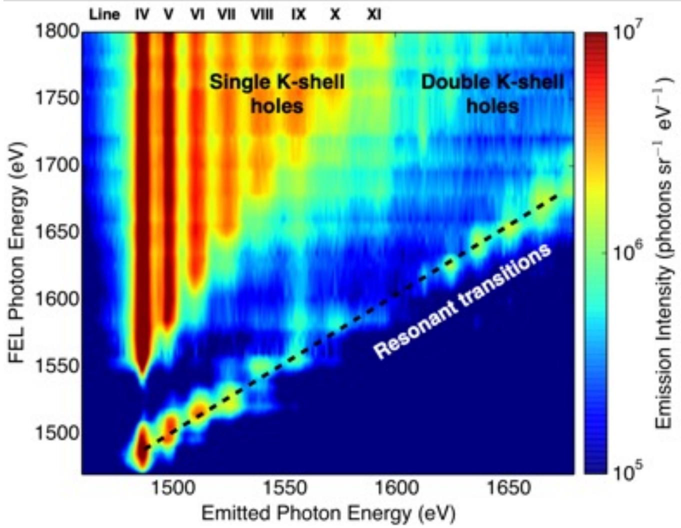
McBride et al. *Nat. Phys 15, 89 (2019)*

Quantum plasmas: warm and hot dense matter



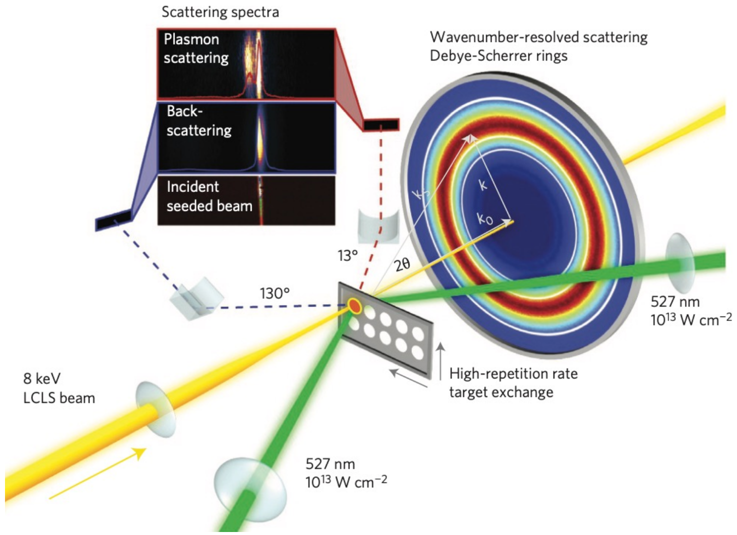


Al solid density plasma at 150eV



Vinko et al. *Nature 482, 59 (2012)*

Inelastic X-ray scattering in warm dense matter



Fletcher et al. *Nature Phot. 9, 274 (2015)*

Higher X-ray pulse energies and nanofocusing will achieve even more extreme states

X-ray pump probe schemes will allow the exploring of volumetrically heated matter

Future Opportunities

Ultrafast Magnetism

Femto/atto second pump-probe scheme in THz/mid-IR to couple to phonon modes

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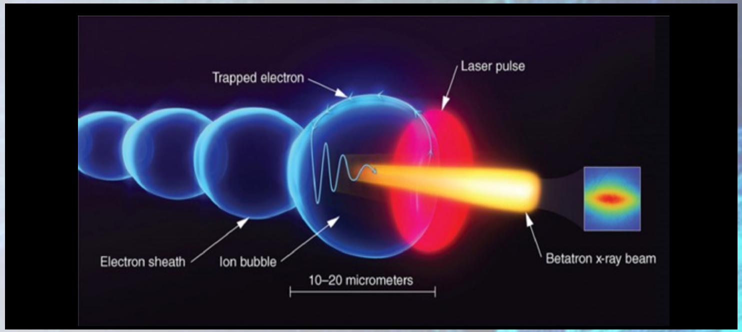
Future Opportunities

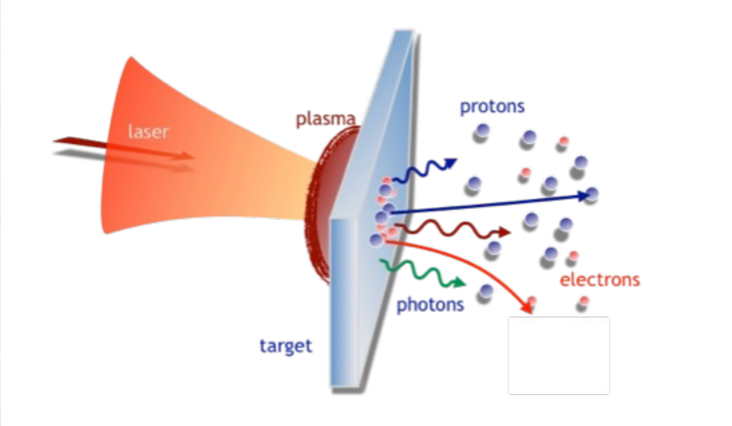
Interaction with laser accelerated electrons

High intensity lasers can be used to produce beams of energetic electrons



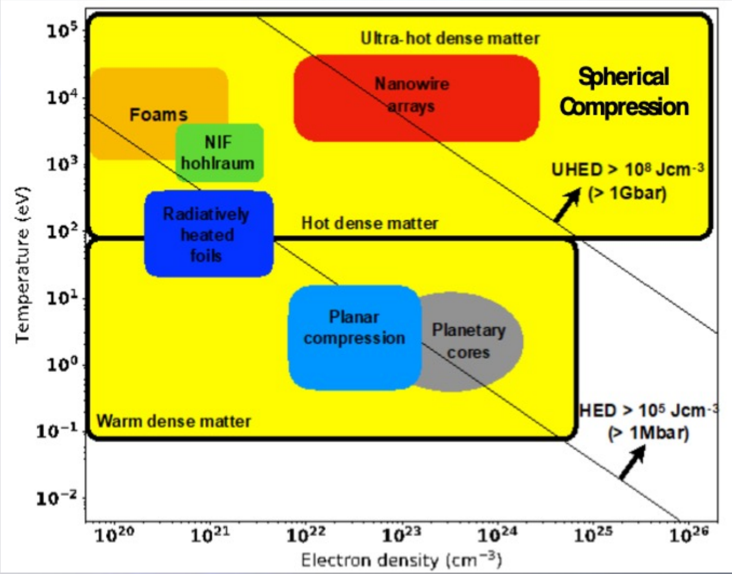
Even more extremes at a spherical compression facility

Laser generated proton and ion beams can be used for in-situ damage studies, as well as isochoric heating



Advances in Fusion energy

Creating and studying matter at stellar core and burning plasma conditions will lead to advances in fusion energy and our understanding of the universe.



The UK has a wealth of expertise in creating diode pumped high rep. rate high intensity lasers and combining these drivers with hard X-rays to investigate matter at extremes

Science and Technology Facilities Council

Science and Technology Facilities Council

Applied and Industrial Research

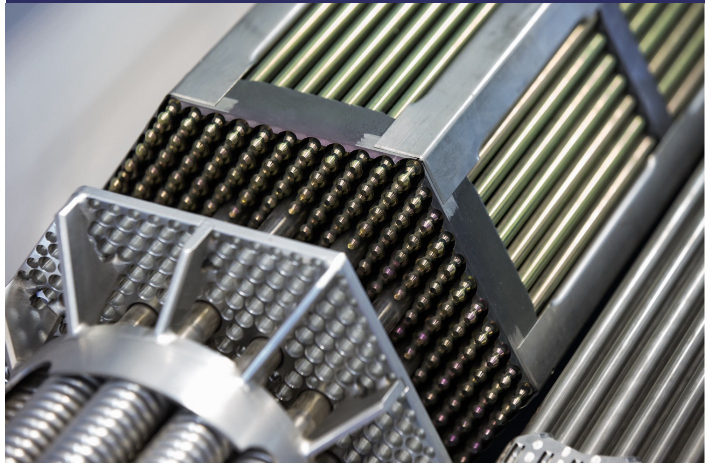
Initial Science Drivers for Applied and Industrial Research

Additive Manufacturing

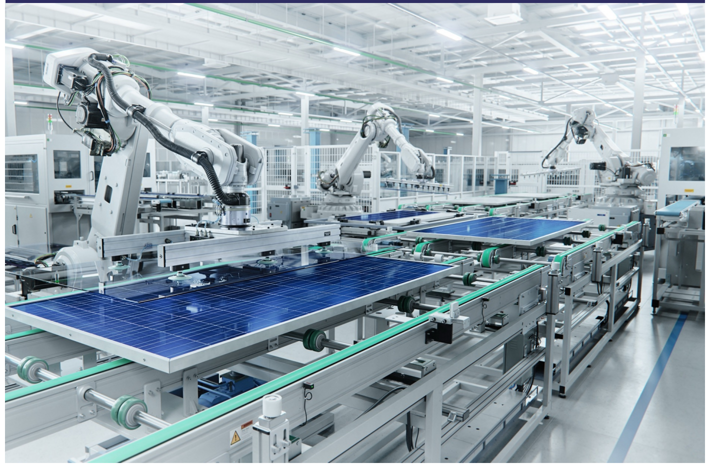
Drug Interactions & Formulation

Shocked Materials

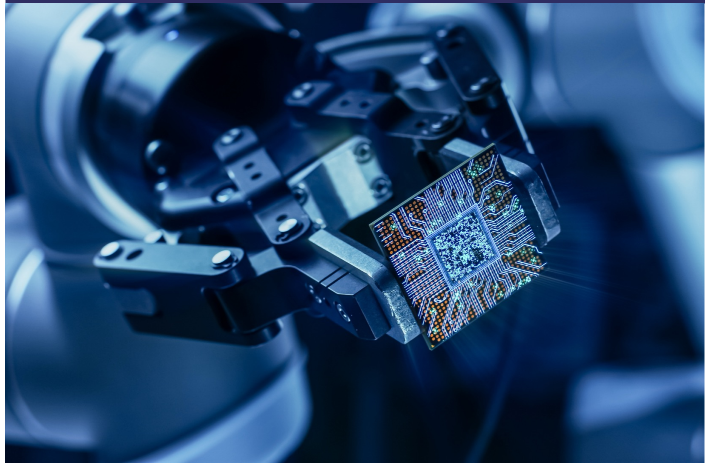
Nucleation



Catalysis

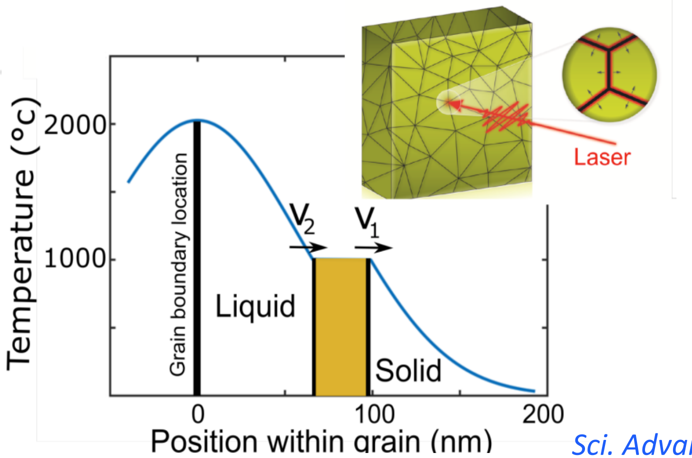


Quantum Tech & Data

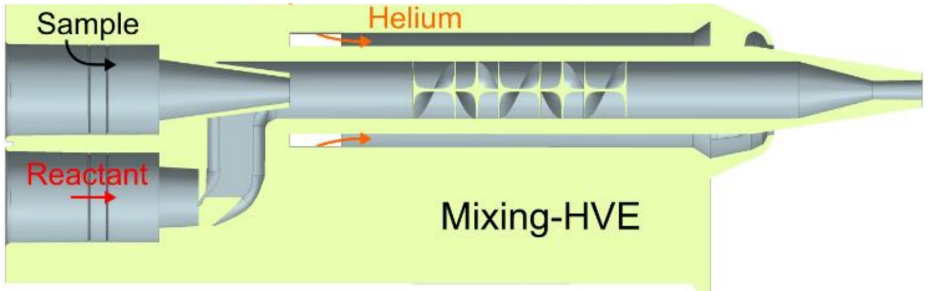


Applications to Laser Processing, Energy Materials, Manufacturing

In-Situ x-ray imaging of additive manufacturing

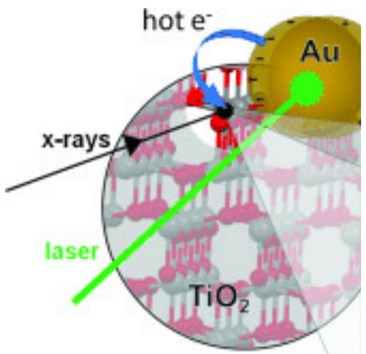


Sci. Advances 6, eaax2445 (2020)
Nat. Comm. 9, 1533 (2018)



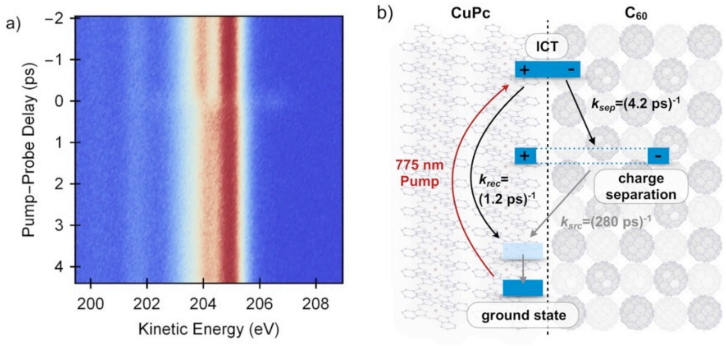
Mix-and-extrude crystallisation dynamics with 3D printed nozzles
J. Appl Cryst 56, 1038 (2023)

Plasmonic Photoctalysis



Plasmonic photocatalysis Angew. *Chem. 54, 5413 (2015)*

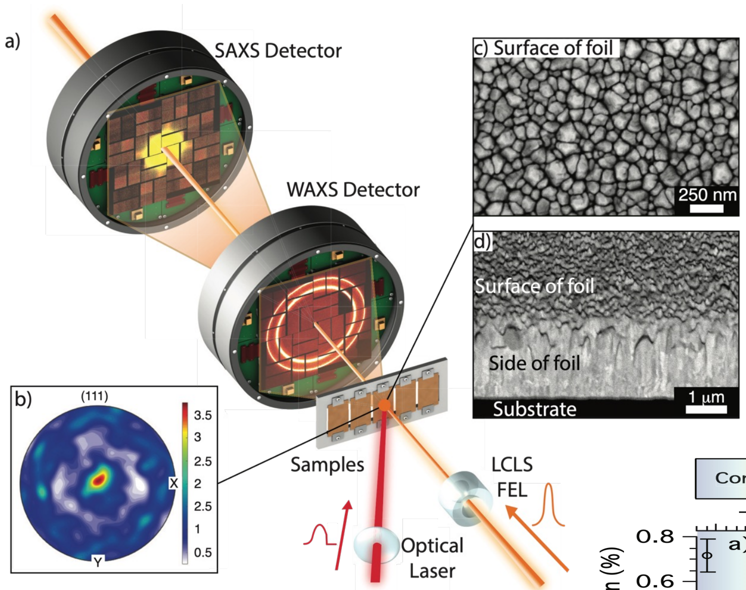
Organic Photovoltaics

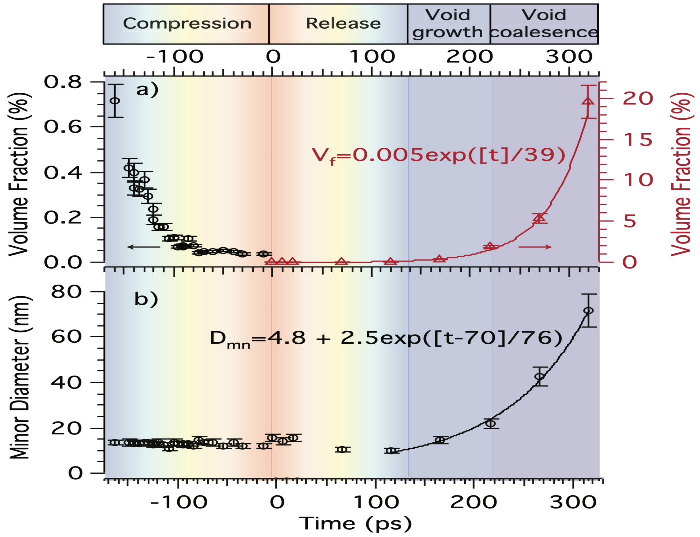


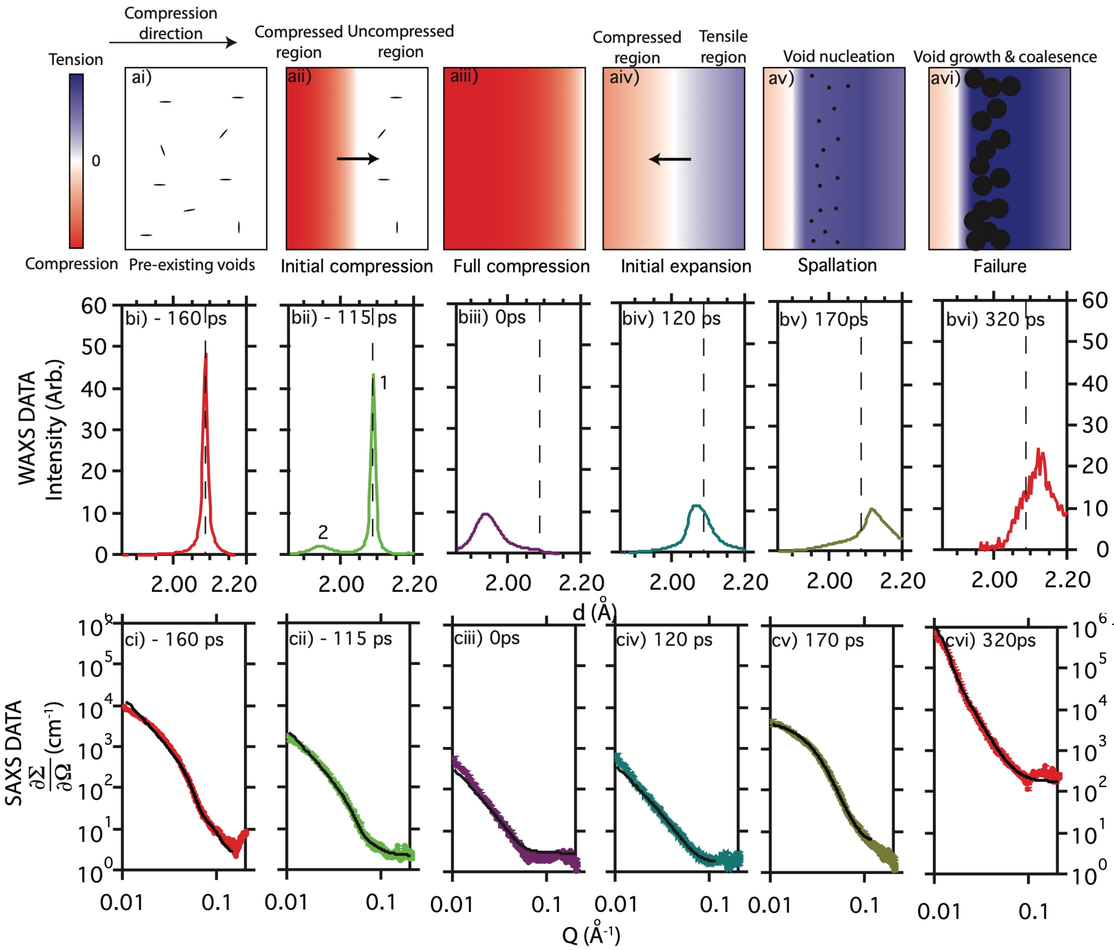
Organic photovoltaics *Nat.Comm. 12, 1196 (2021), Nat.Comm. 13, 3414, (2022)*

Application to Understanding Shocked Materials

Laser Shocked Cu foil, performed on SAXS at CXI, LCLS







Coakley et al, *Sci. Adv., 6(51):eabb4434, 2020.*

Future Opportunities

New biomedical technology

Spatiotemporal structure dynamics in biologically relevant and complex systems;
for example, peptide and protein (mis)folding *(hard x-rays, high rep-rate, solution scattering and spectroscopy)*

Advances in industrial processing

Developing detailed understanding of advanced processes to optimise manufacturing outcomes with the minimum number of empirical trials (from XUV for gas phase processing & photolithography to hard X-rays, at high rep-rate, and coupled to compact process replicators)

Advancing understanding of nucleation, solidification and crystallization in soft-matter

Spatiotemporal dynamics of phase behaviour and reactions: molecular - mesoscale – macroscopic, capturing rare events, non-crystalline phases, nucleation, liquids. (0.2 keV to > 40 keV high rep-rate, compact process replication)

Radiation damage mitigation in space and nuclear industry

(high rep-rate x-rays, synchronised to ultrafast lasers, electron, proton and ion beams)

Science and Technology Facilities Council

Satisfying Future Scientific Research Needs

Future Opportunities

Transform limited operation across entire X-ray range

Spatiotemporal structure dynamics in biologically relevant and complex systems; for example, peptide and protein (mis)folding(hard x-rays, high rep-rate, solution scattering and spectroscopy)

High efficiency facility with a step-change in the simultaneous operation of multiple end stations

Expanding access by providing scope for many hundreds of unique experiments every year

Evenly spaced, high-rep rate pulses to match samples & detectors

Enabling the most advanced measurement methodologies whilst supporting high throughput measurements with standard capabilities

Improved synchronisation/timing data with external lasers to < 1 fs

Realising the full temporal resolution to see dynamics unfold across multiple timescales from sub-femtosecond electronic dynamics to nanosecond thermal relaxation and larger scale structural changes

Multiple colour X-rays at one end-station and full array of synchronised sources:

To interrogate specific electronic, vibronic, excitonic etc. modes to completely uncover the complex dynamical pathways and couplings in matter

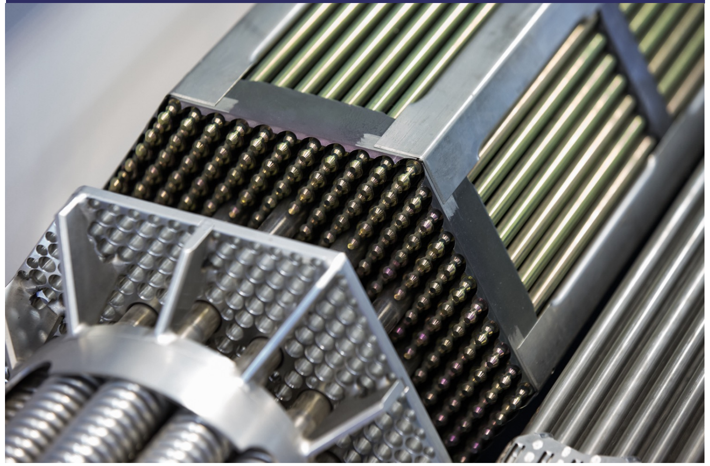
Transformative Impact

Additive Manufacturing

Drug Interactions & Formulation

Shocked Materials

Nucleation



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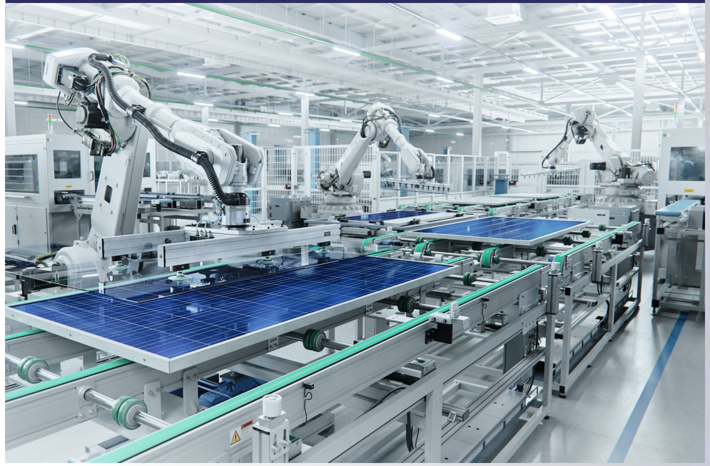

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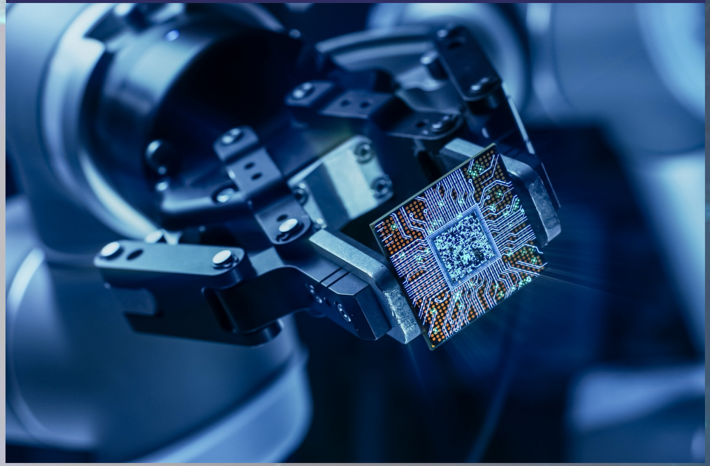

Contributes to generic national strategic themes

Advancing Technology

Through understanding quantum scale structural dynamics

Healthcare

Through advancing dynamical structural biology

Frontiers of Knowledge

Through access to brightest ultrafast X-ray pulses

Net Zero Growth

Through unravelling photo-chemical/catalytic cycles

Economic Strengths

Through skills and research outcomes maintaining competitiveness with China, USA and Europe

UKRI Science and Technology Facilities Council

Thank You

Slides and References available at

xfel.ac.uk