Science and
Technology
Facilities Council

UK XFEL

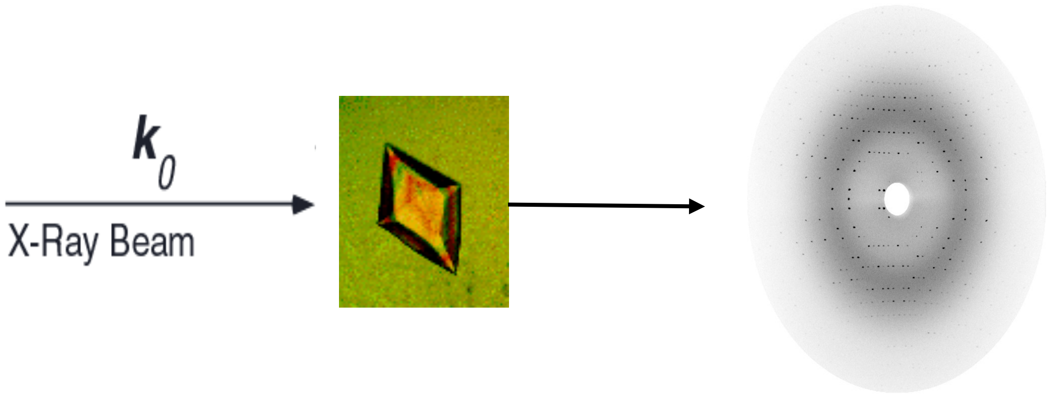
Science and Technology Impact of XFELs and Opportunities with a Next Generation Facility

xfel.ac.uk

X-ray probing of the nanoscale structure of matter

X-ray scattering

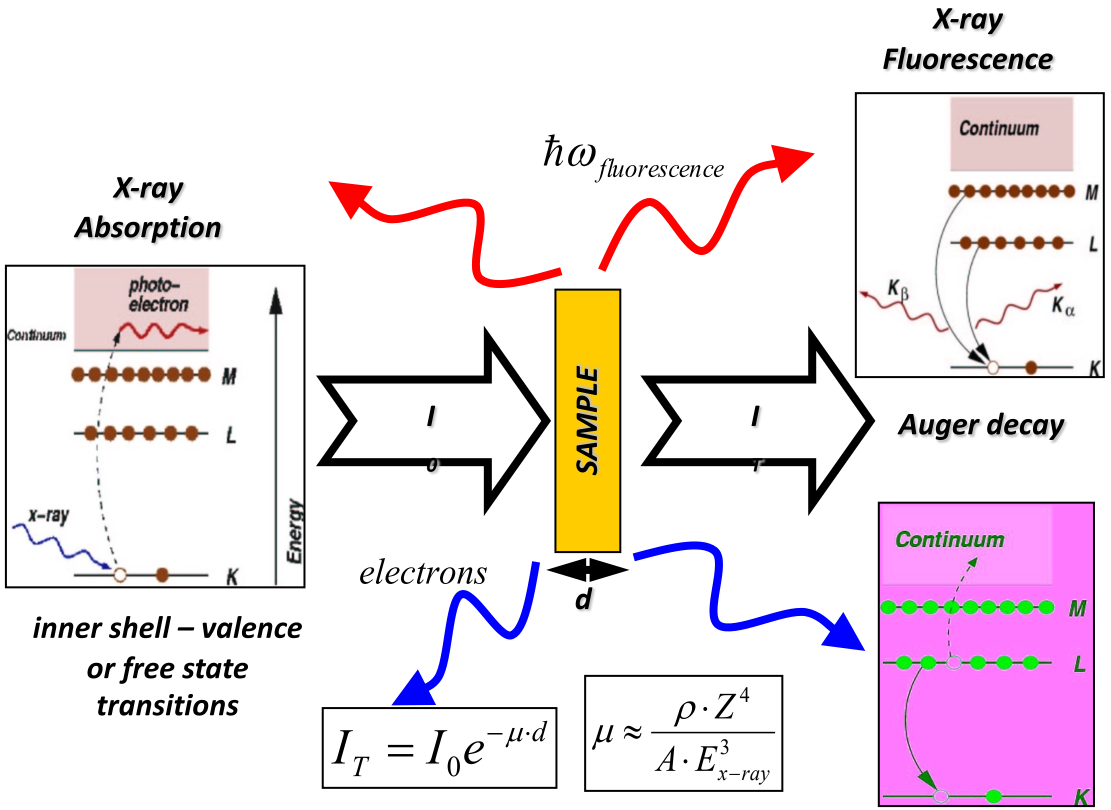
provides atomic structure



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

X-ray spectroscopy

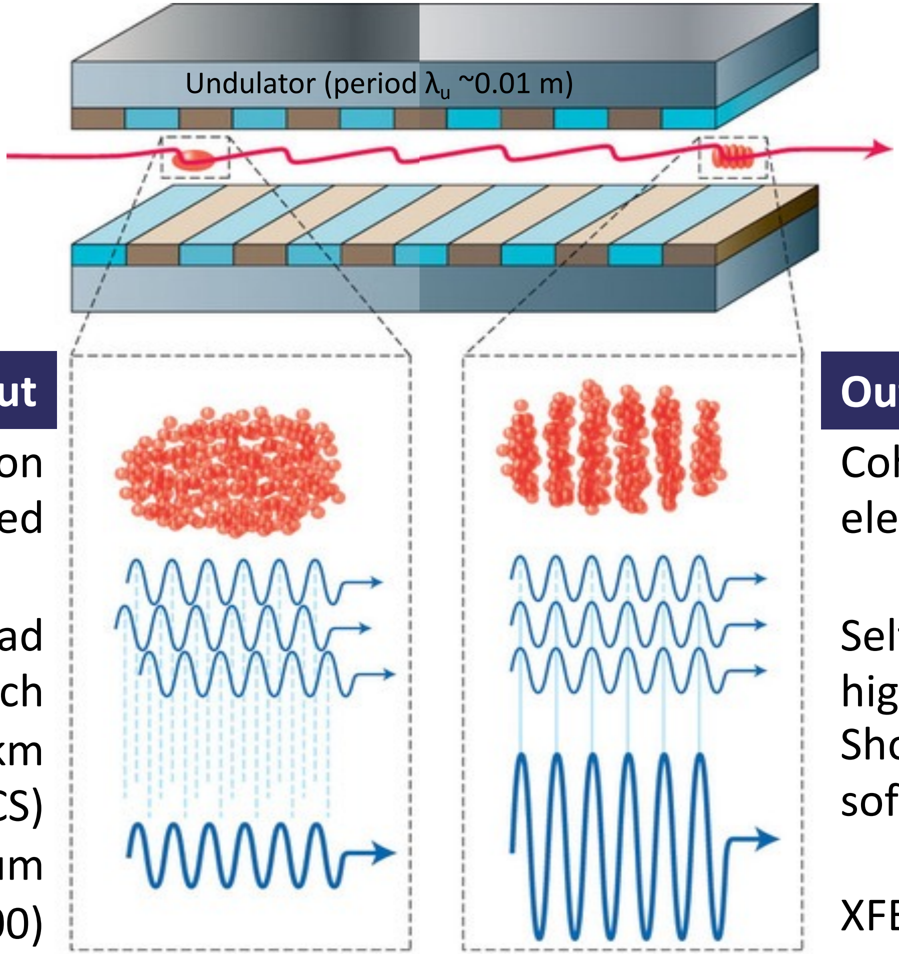
provides electronic states with atomic specificity



$$I_T = I_0 e^{-\mu \cdot d}$$

$$\mu \approx \frac{\rho \cdot Z^4}{A \cdot E^3_{x-ray}}$$

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 $\Upsilon > 2000$)

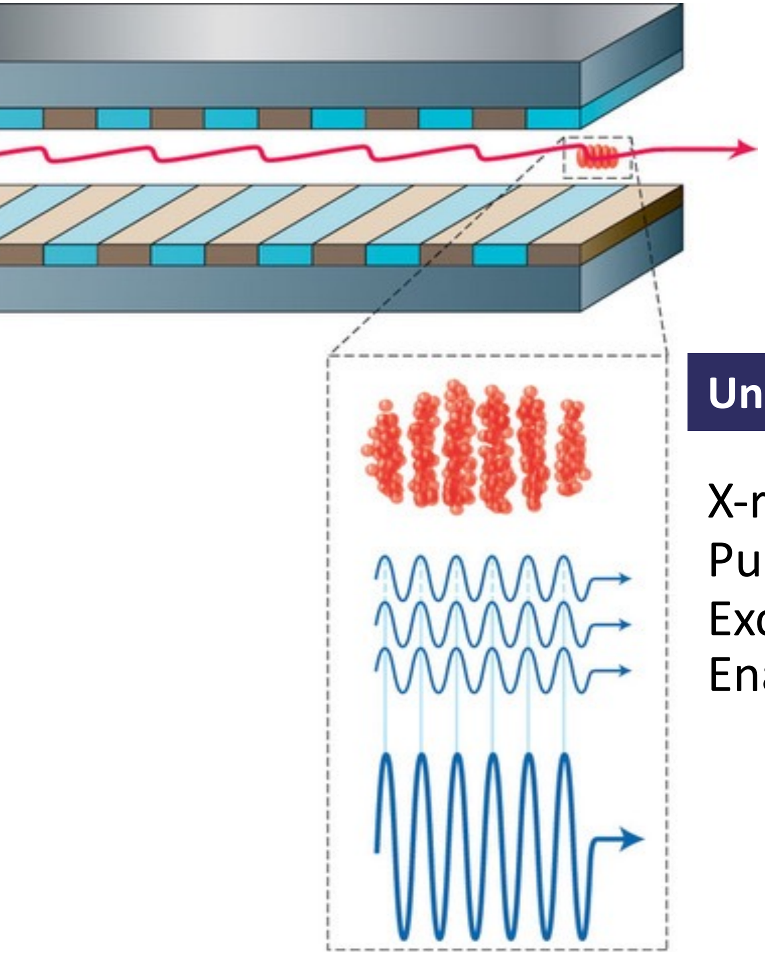
Output

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)

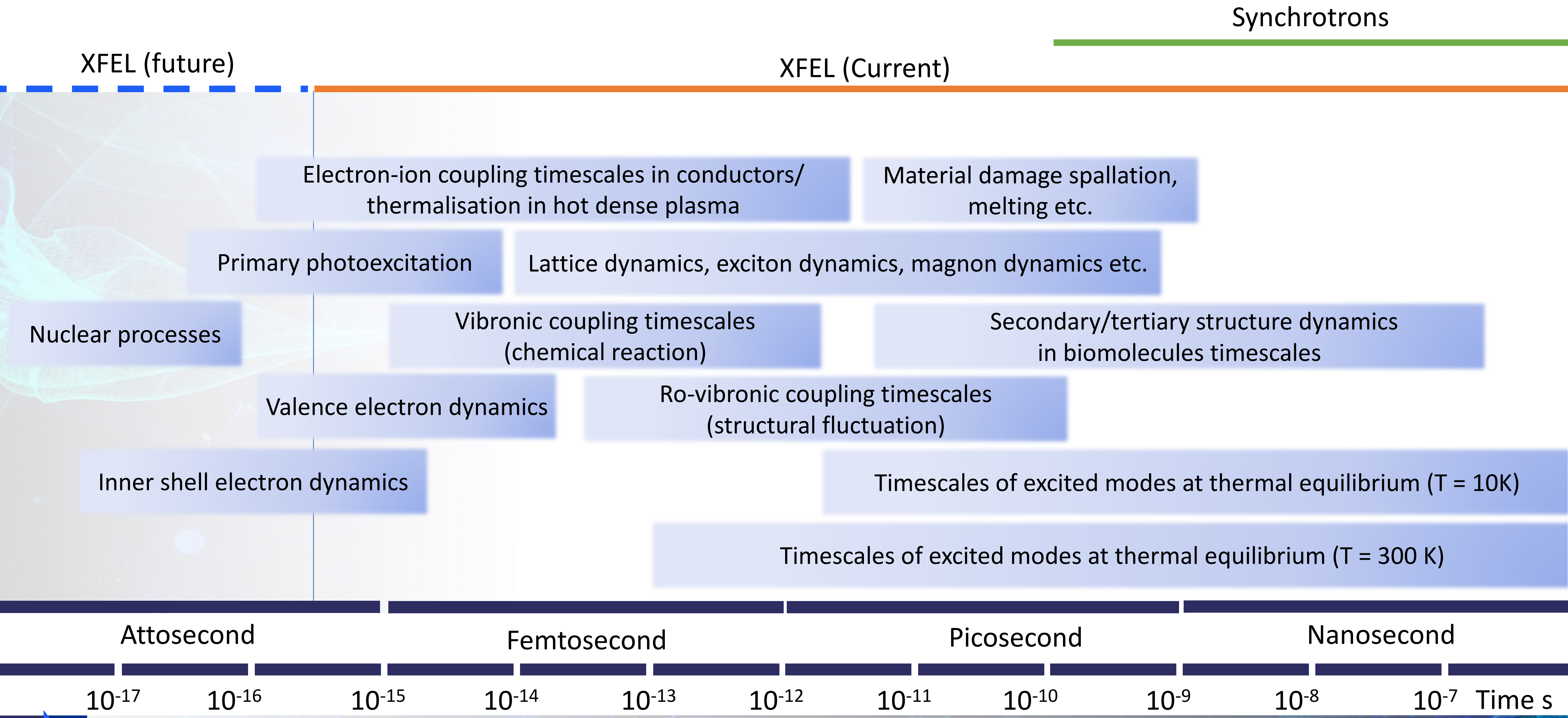


Unique Features

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

Real-time access to structural and electronic dynamics



Synchrotrons

XFEL (future)

XFEL (Current)

Electron-ion coupling timescales in conductors/ thermalisation in hot dense plasma

Material damage spallation, melting etc.

Primary photoexcitation

Lattice dynamics, exciton dynamics, magnon dynamics etc.

Nuclear processes

Vibronic coupling timescales (chemical reaction)

Secondary/tertiary structure dynamics in biomolecules timescales

Valence electron dynamics

Ro-vibronic coupling timescales (structural fluctuation)

Inner shell electron dynamics

Timescales of excited modes at thermal equilibrium (T = 10K)

Timescales of excited modes at thermal equilibrium (T = 300 K)

Attosecond

Femtosecond

Picosecond

Nanosecond

10^{-17} 10^{-16} 10^{-15} 10^{-14} 10^{-13} 10^{-12} 10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} Time s

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


Probe

τ

Pump

Sample

X-ray observable

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

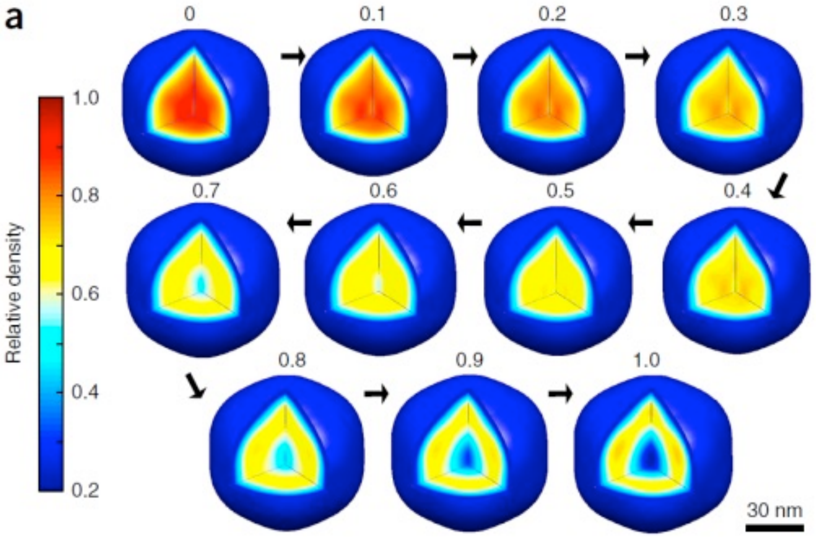
Sudden heating, injection of hot electrons, electronic state photoexcitation/photoionisation, excitation of vibrational/phonon or rotational modes etc.

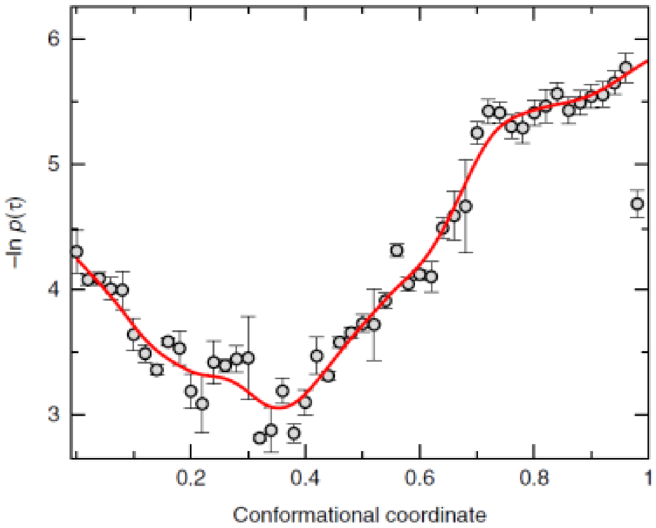
Probe (X-ray) – interrogates the sample after delay time τ by generating a suitable observable:

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

A. Hosseinizadeh, *Nature Methods 14 877 (2017)*

High brightness scattering can outrun destruction

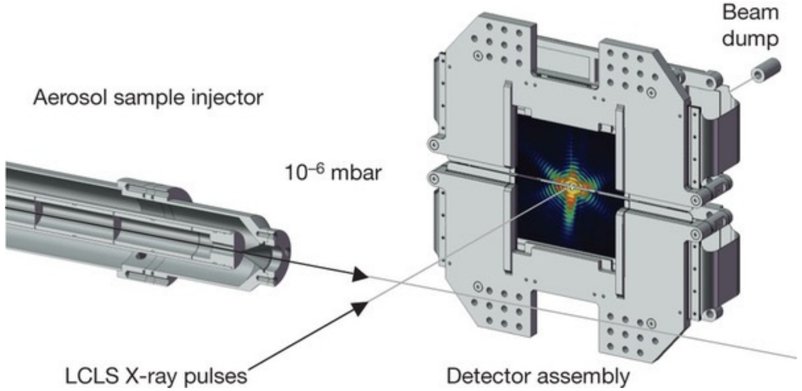
Destroy before Diffract

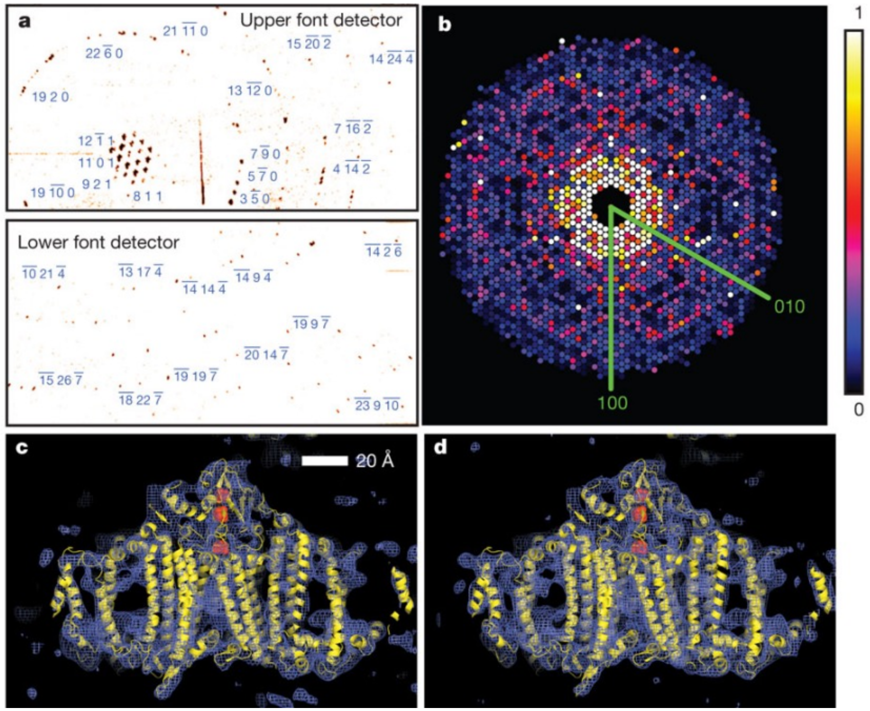
Conventional X-ray sources non-crystal samples destroyed before signal enough to determine structure.

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)*

UK XFEL Next Generation Definition

- **Near transform-limited operation across the x-ray range**
  - Photon energies from 0.05-20 keV
  - Pulse durations from 100 as to 100 fs
  - Non-transform-limited operation at 20-50 keV
- **High efficiency facility, with a step-change in the simultaneous operation of multiple end stations**
  - Minimum of six FELs, with upwards of ten end stations to be simultaneously operated
- **Evenly spaced, high repetition rate pulses to match samples, lasers, and detectors**
  - 100 kHz per FEL, with flexibility of repetition rate
- **Improved synchronization/timing data with external lasers to <1 fs**
- **Widely separated, multiple colour x-rays to at least one end station**
- **Full array of synchronized sources**
  - XUV-THz, e-beams, ion beams, high power & high energy lasers at high repetition rate
- **Minimal carbon footprint with minimal energy consumption for both operation and build**

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The Science Case

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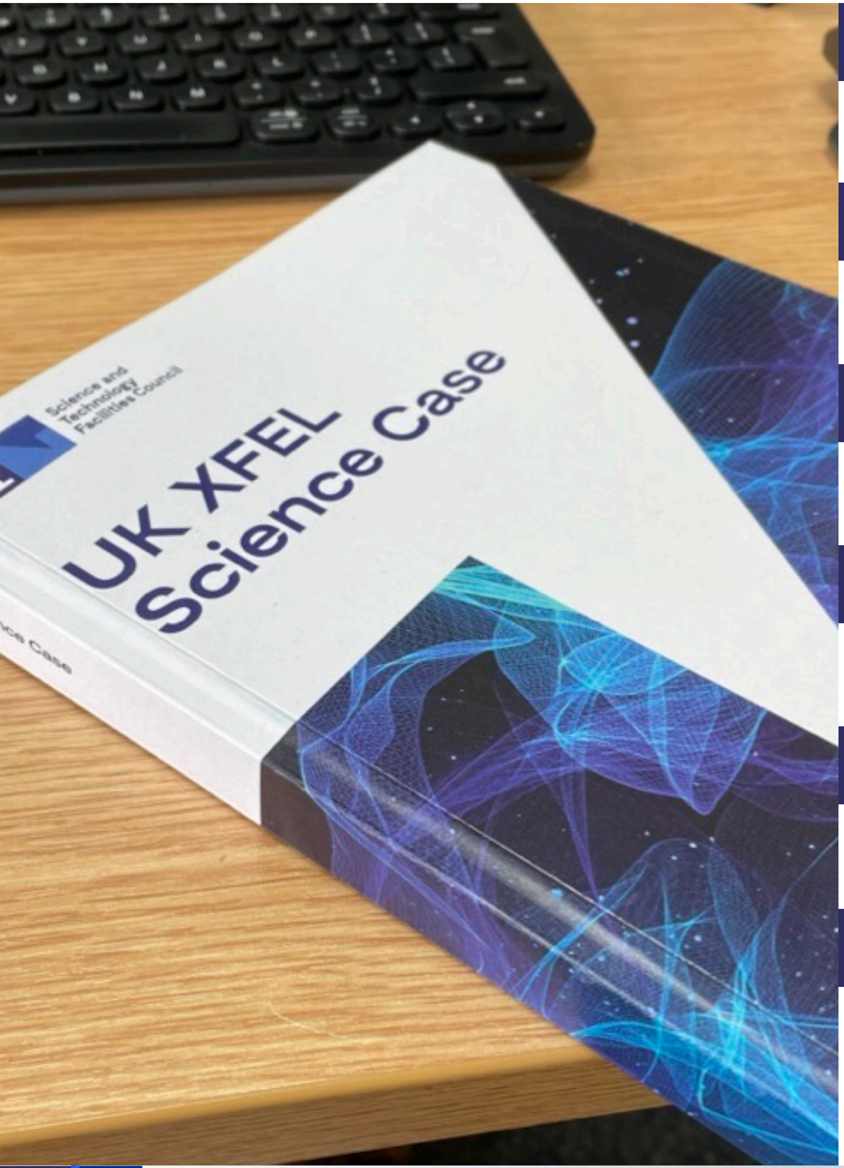
Expert Science Team



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

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

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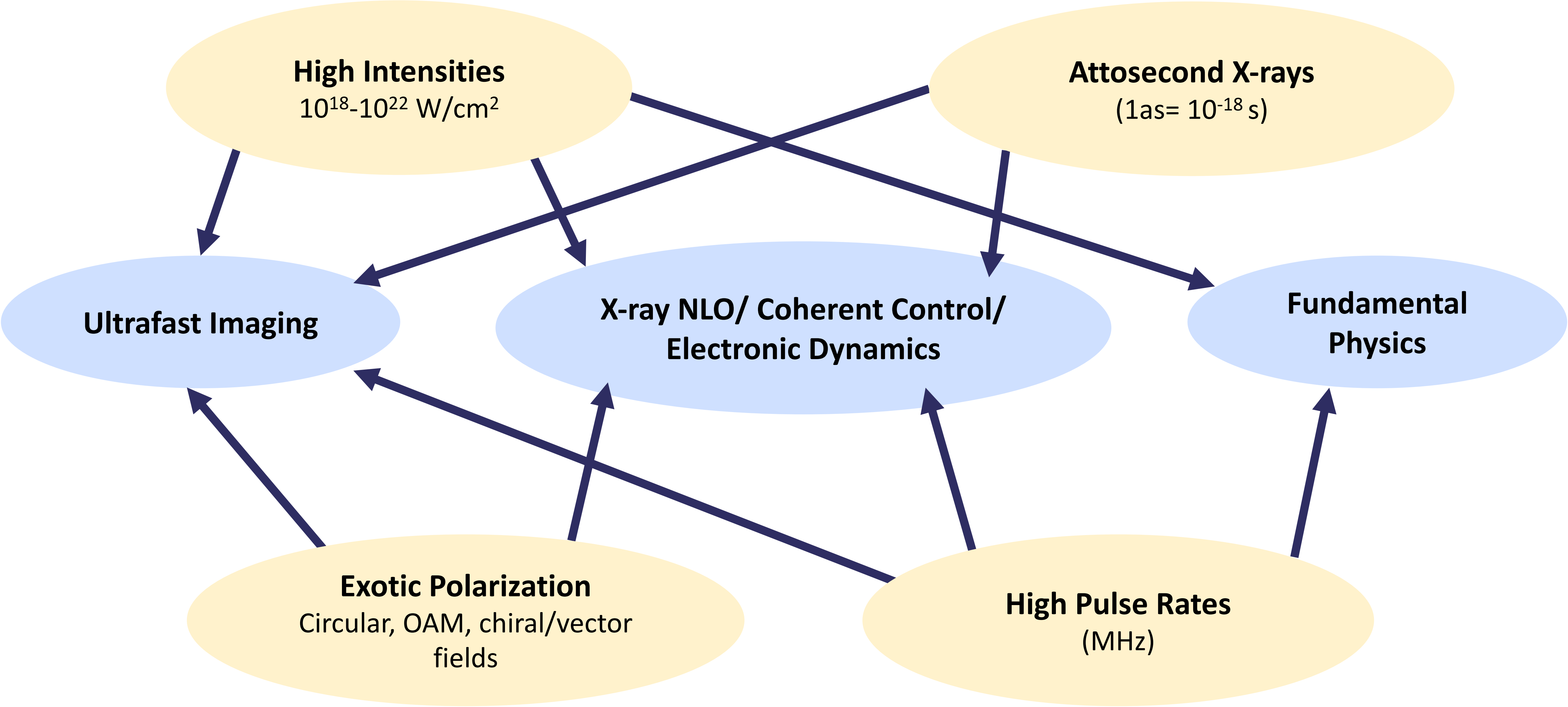
Physical Sciences

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

New Physics and X-ray Photonics



High Intensities
10^{18}-10^{22} W/cm^2

Attosecond X-rays
(1as= 10^{-18} s)

Ultrafast Imaging

X-ray NLO/ Coherent Control/ Electronic Dynamics

Fundamental Physics

Exotic Polarization
Circular, OAM, chiral/vector fields

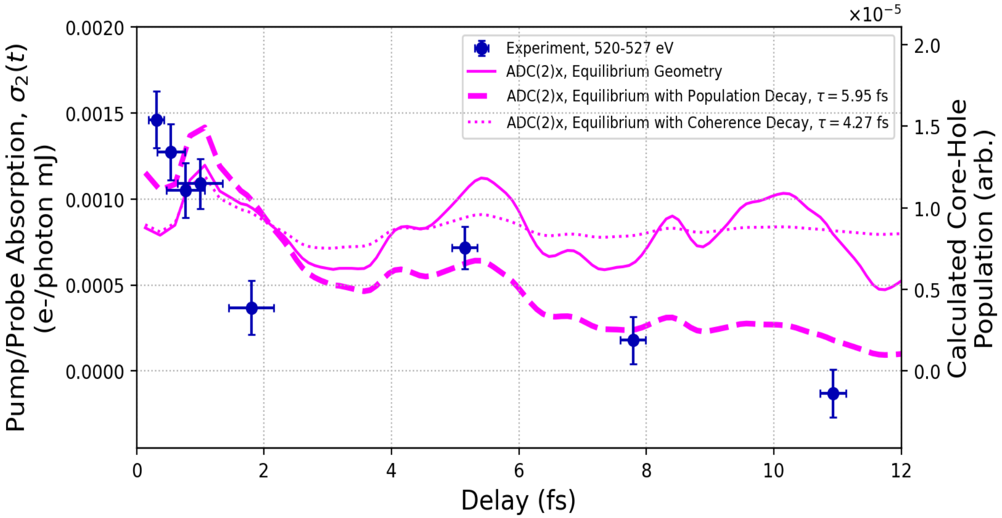
High Pulse Rates
(MHz)

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 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)

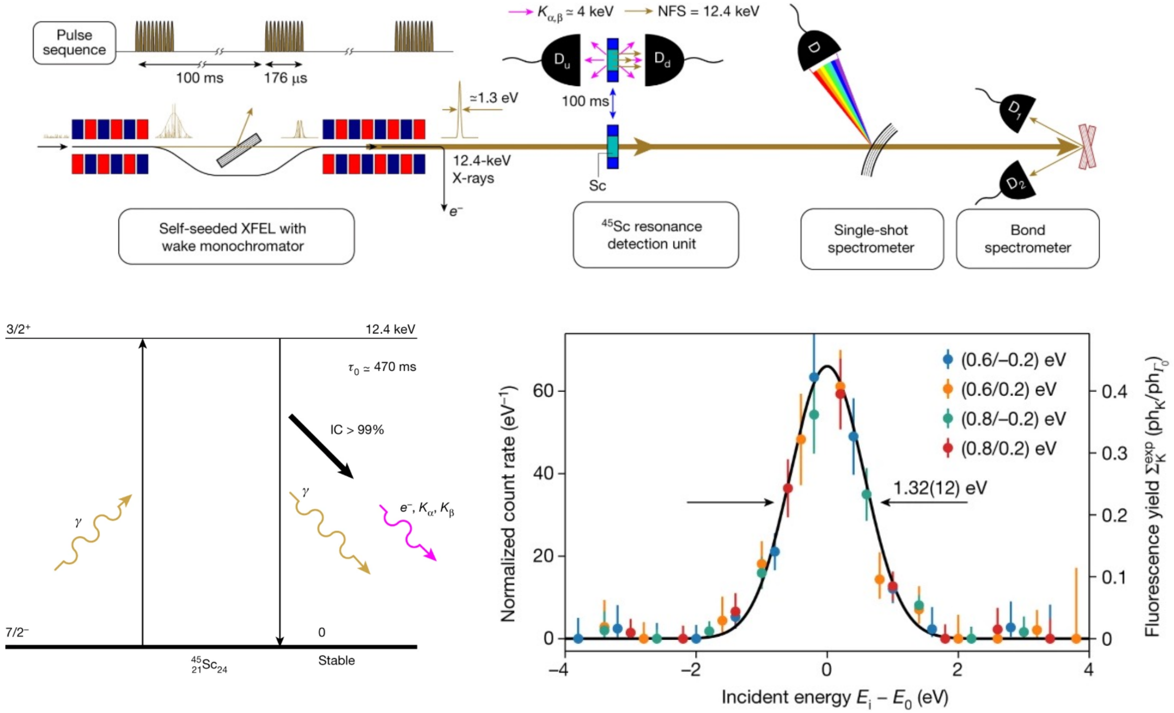
Ionisation physics of water *Science* eadn6059 (2024)

Attosecond pump-probe *Nature Photonics* (2024)

Explore fundamental physics

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

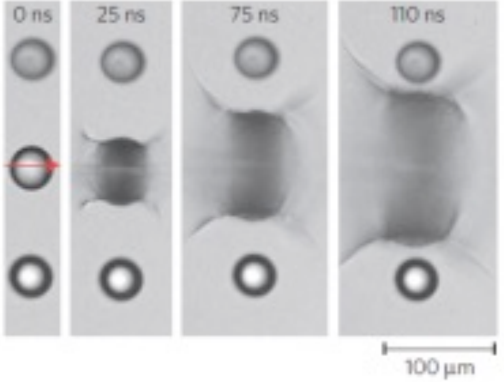
Resonant x-ray excitation of nuclear clock isomer ^{45} Sc



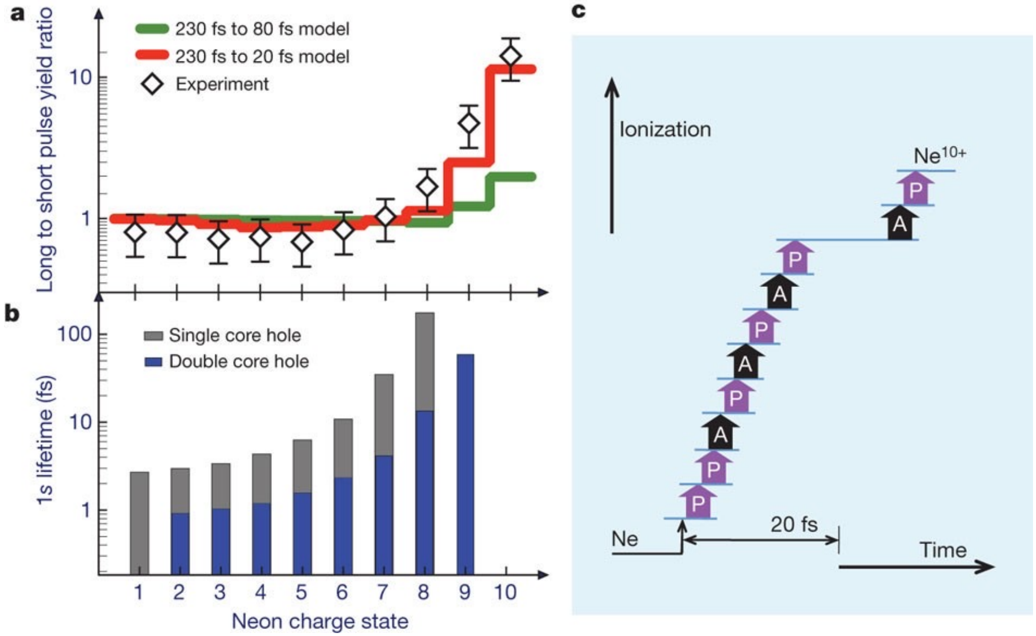
Resonant X-ray excitation of the nuclear clock isomer ^{45}Sc *Nature* 622 471 (2023)

New Physics and X-ray Photonics

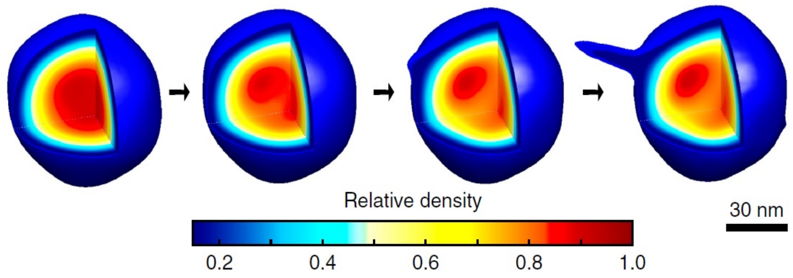
X-ray - matter interaction



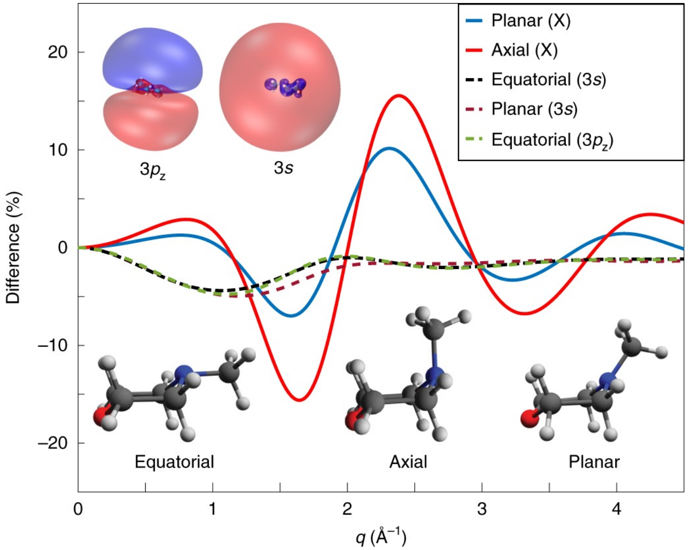
Response to ultra-intense X-rays *Nature* 466 56 (2010)
Interaction with liquids *Nature Physics* 12 966 (2016)
Nonlinear x-ray optics *Science* 369, 1630–1633 (2020)
Ultrafast radiolysis *Science* 367 179 (2020)



New directions in x-ray scattering



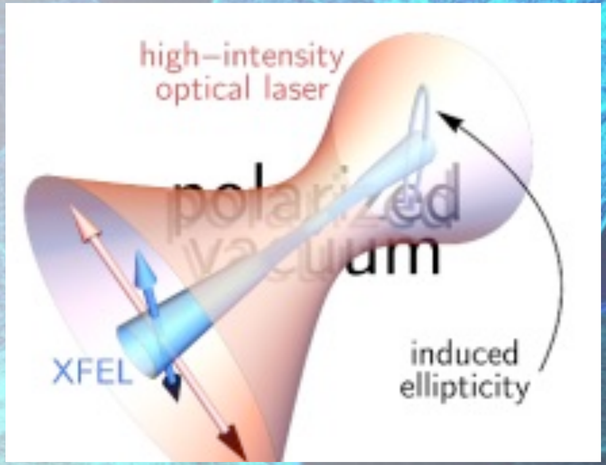
Conformational dynamics from data driven approaches *Nature Methods* 14 877 (2017)
Ultrafast coherent dynamics in isolated molecules *Nature Chemistry* 11 716 (2019)



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

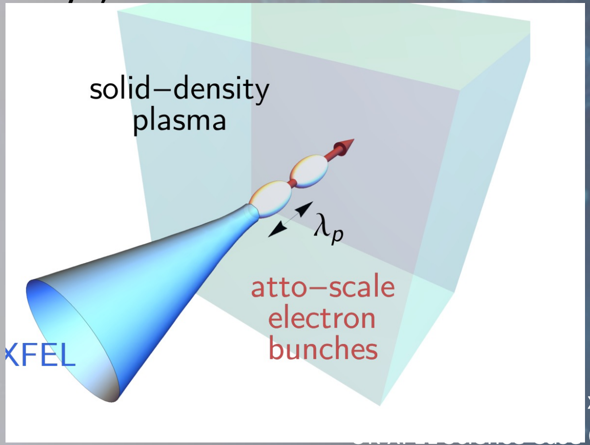
Conformational dynamics across wide spatial and temporal scales (high rep rate, hard x-rays)

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/specificity (nanofocusing, high rep-rate, short pulses)



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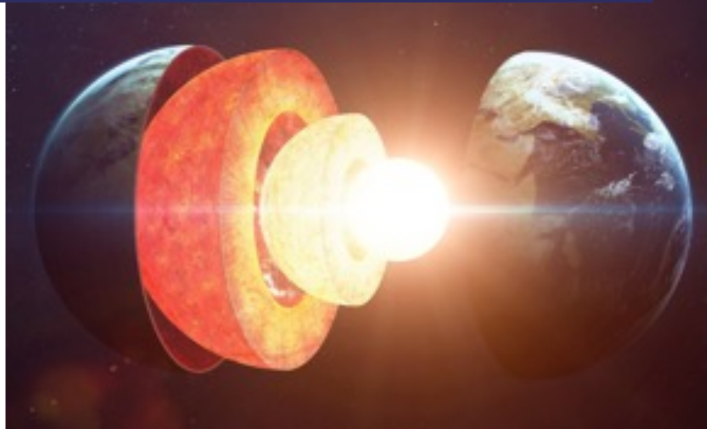
Matter at extreme conditions

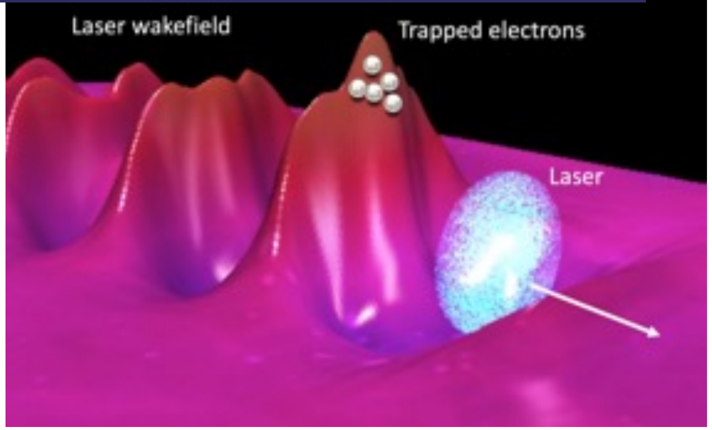
Andy Higginbotham (York), Andy Comley (AWE), Emma McBride (QUB), Sam Vinko (Ox), Marco Borghesi (QUB), Malcolm McMahon (Edinburgh), Justin Wark (Ox)

Matter at Extreme Conditions

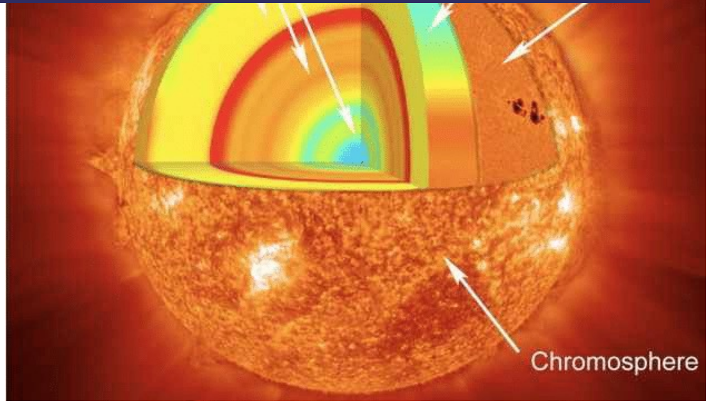
Shocked materials and matter at extremes



Interactions with energetic electron and ion beams



Quantum plasmas: warm and hot dense matter



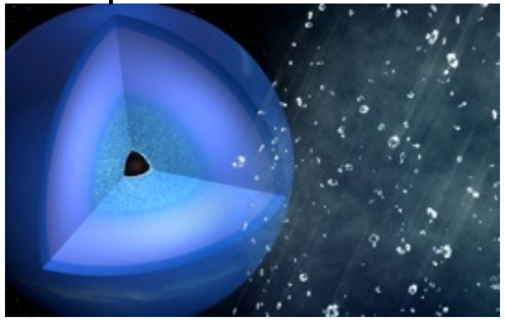
Probing physics of spherical compression

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

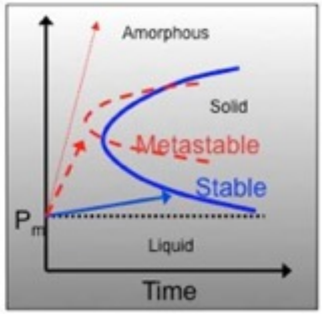
Partial dissociation of C-H and formation of diamond on Neptune



Kraus et al. *Nat. Ast. 1, 606 (2017)*
M.Frost et al. *Nat. Ast. 8, 174 (2024)*

Novel material synthesis

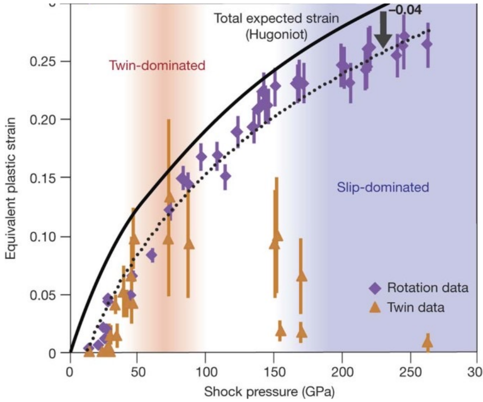
Observation of metastable phase in bismuth



Gorman et al. *APL 114 120601 (2019), J.App.Phys 135, 165902 (2024)*

Dynamic strength of materials

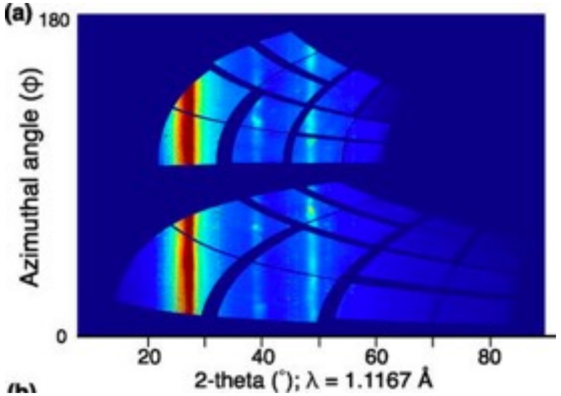
Twinning in dynamically compressed tantalum



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

Melting at extreme pressures

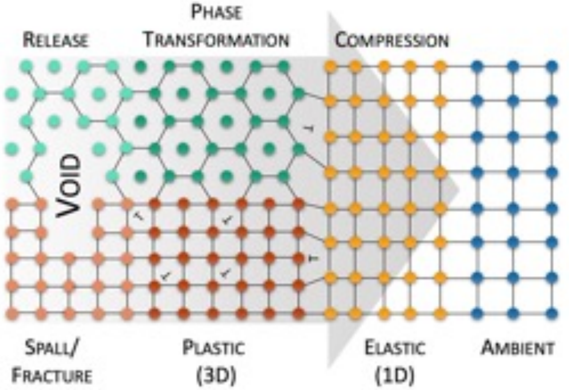
Shock-induced melting in tin



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

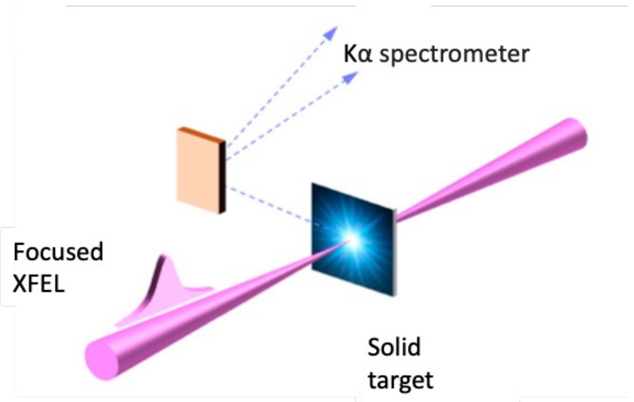
High strain rate phenomena

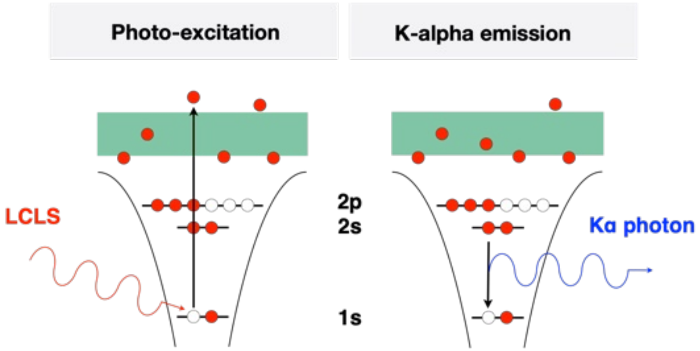
Response of silicon to uniaxial compression



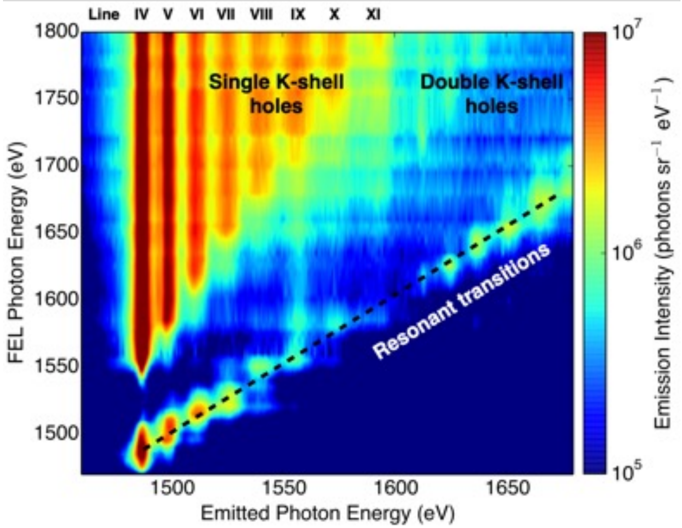
McBride et al. *Nat. Phys 15, 89 (2019)*

Quantum plasmas: warm and hot dense matter



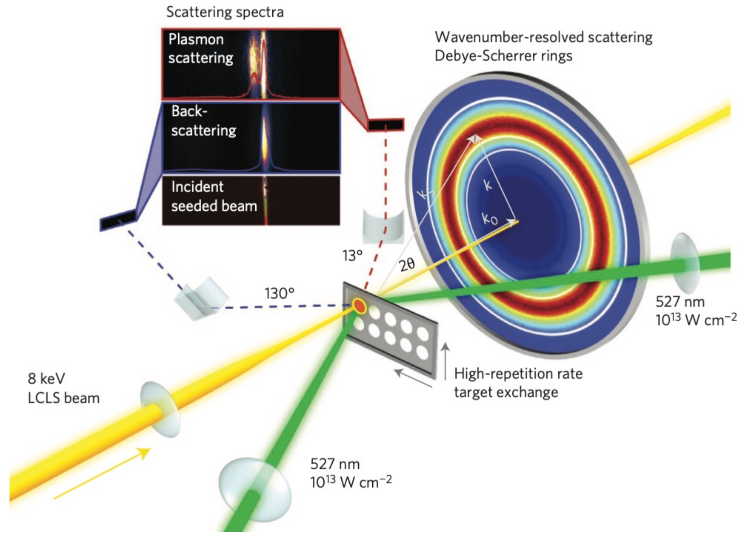


Al solid density plasma at 150eV



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

Inelastic X-ray scattering in warm dense matter



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

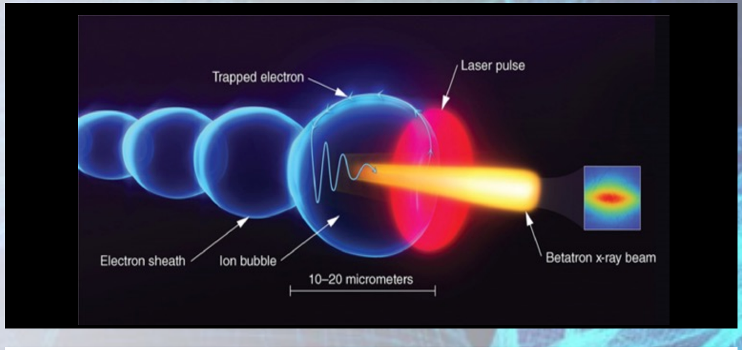
Higher X-ray pulse energies and nanofocusing will achieve even more extreme states

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

Future Opportunities

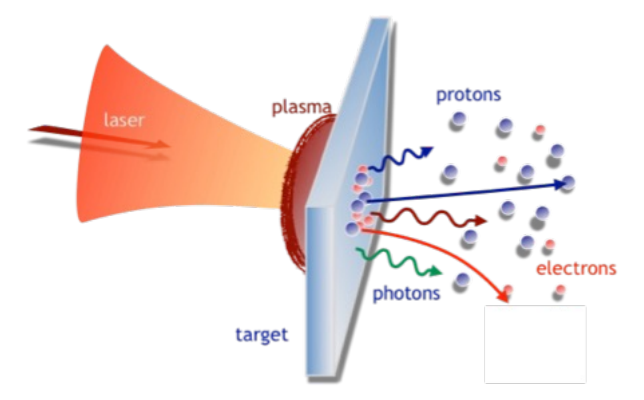
Interaction with laser accelerated electrons

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



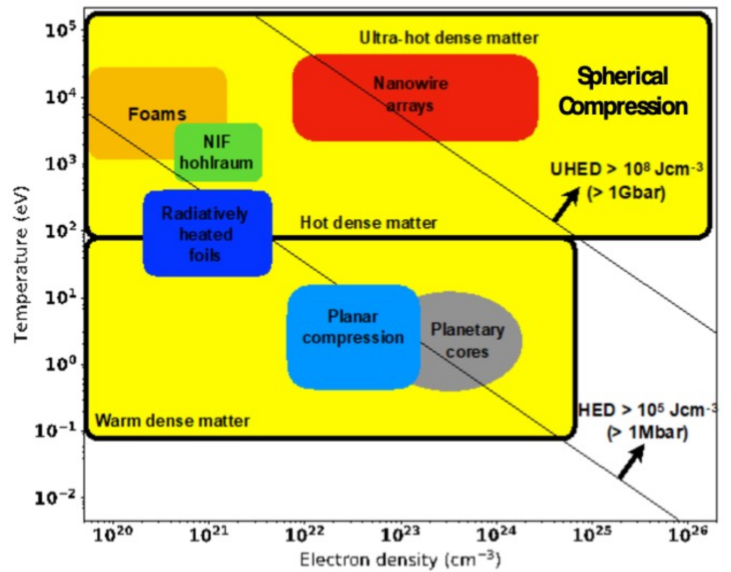
Even more extremes conditions

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.



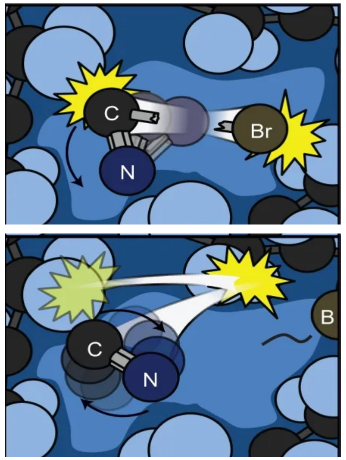
The UK has a wealth of expertise in creating diode pumped high rep. rate high intensity lasers and combining these drivers with hard X-rays to investigate matter at extremes

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

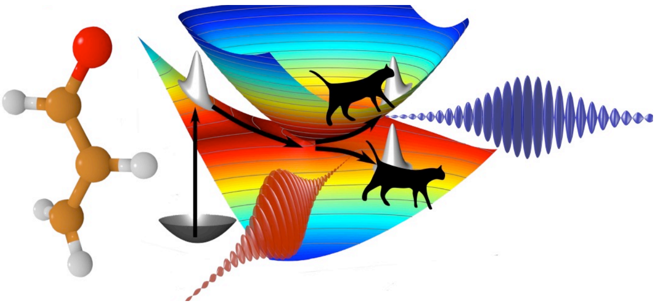
Solvation



Nature Chem, 242, (2016)

Transient electronic coherence

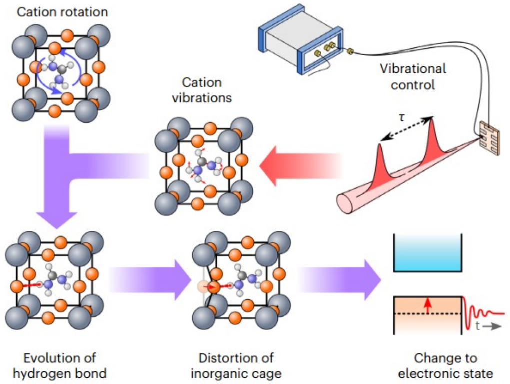
(attosecond X-Ray Raman)



Phys Rev Lett, 115, 19003 (2015)

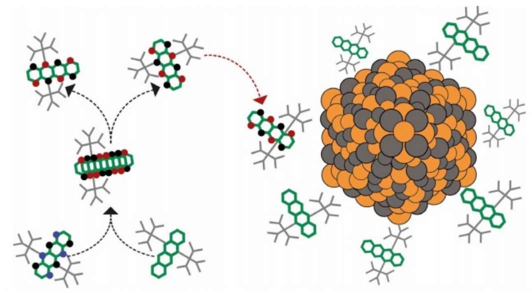
Energy Materials

Organohalide perovskite optoelectronic devices



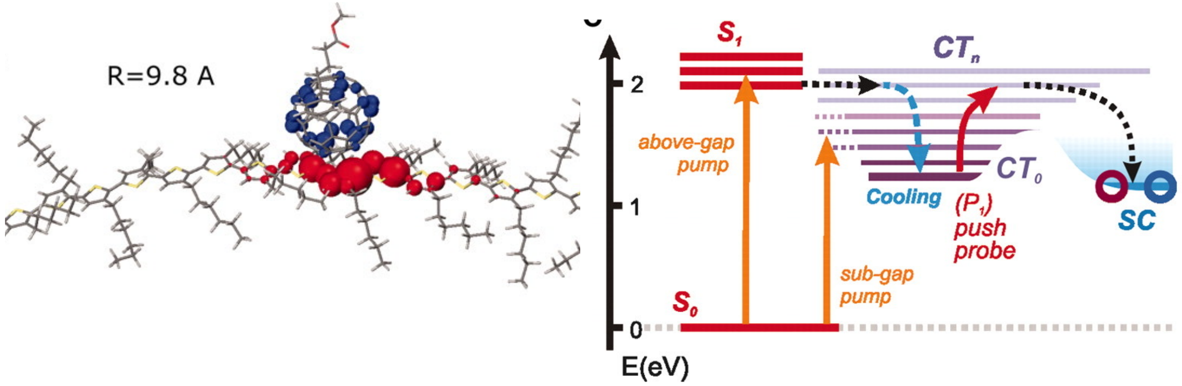
Nature Mat, 23 88–94 (2024)

Singlet fission



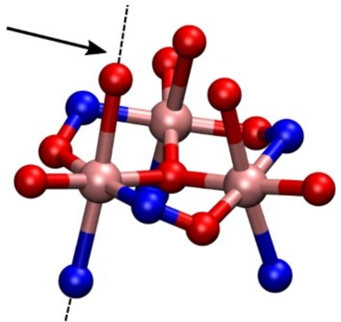
JACS 12907 (2019)

Exciton Dynamics



Science 2012, 335, 1340

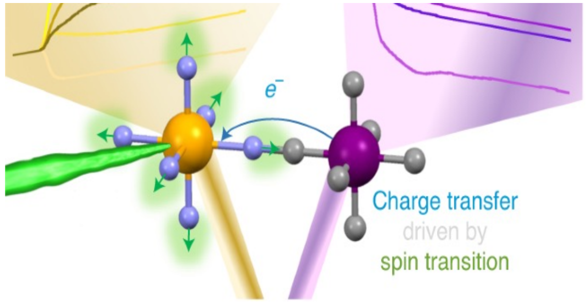
Spin dynamics



Vibrational coherence in single-molecule magnet

F. Liedy, *Nature Chem, 12, 452 (2020)*

Charge transfer dynamics



a CoFe Prussian blue analogue

Nature Chem 10 (2021)

Fundamentals of reaction dynamics

The Science Question

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

The Movie

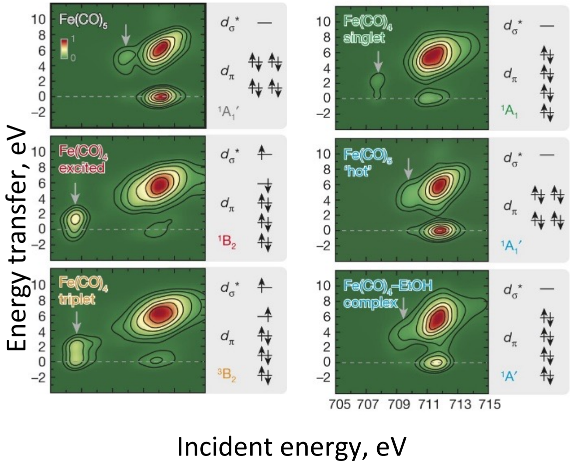
Ligand dissociation
Primary step in catalysis

The Applications

Magnetic materials, Information storage
Fundamentals of chemical reactivity

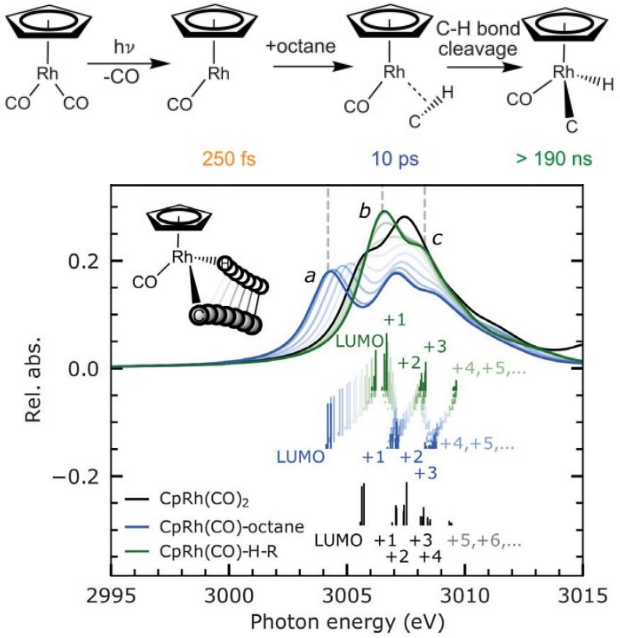
Element- and site-specific probing:

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



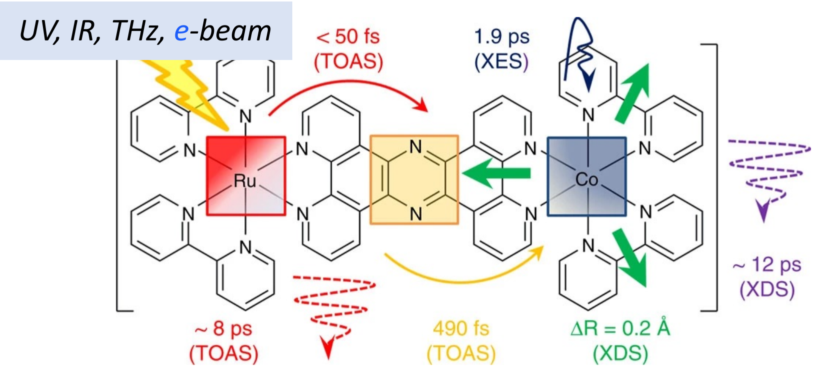
Orbital-specific mapping of the ligand exchange dynamics of $Fe(CO)_5$ in solution *Nature 520, 78 (2015)*

Photocatalysis, Enzyme catalysis

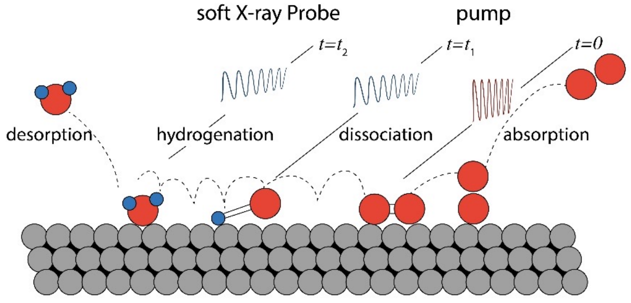


Tracking C–H activation with orbital resolution provides opportunities for manipulating C–H reactivity in transition metals *Science 380, 955 (2023)*

Homogeneous catalysis



Controlling catalytic reactions with THz excitation



Chem Phys Lett 675, 145 (2017)

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

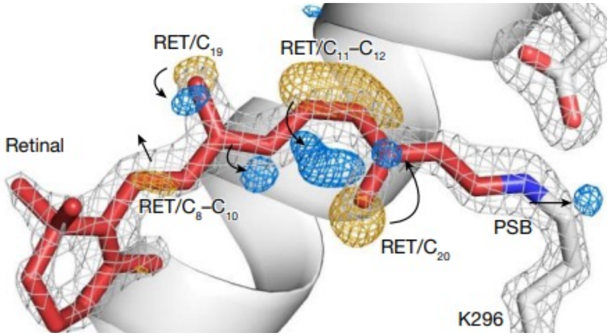
The Applications

Enzyme catalysis

Photoprotection

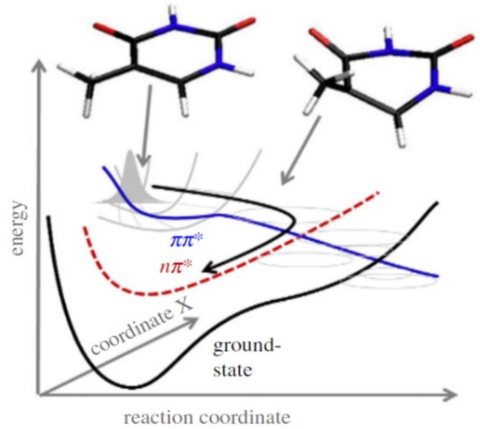
Drug-target interaction

Ultrafast structural changes direct the first molecular events of vision



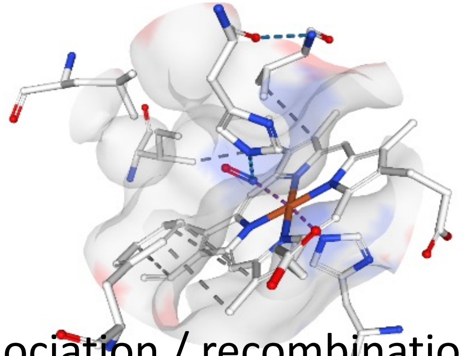
Nature, 615, 939 (2023)

Photochemistry of DNA



Nat. Comm. 8, 29, (2017)

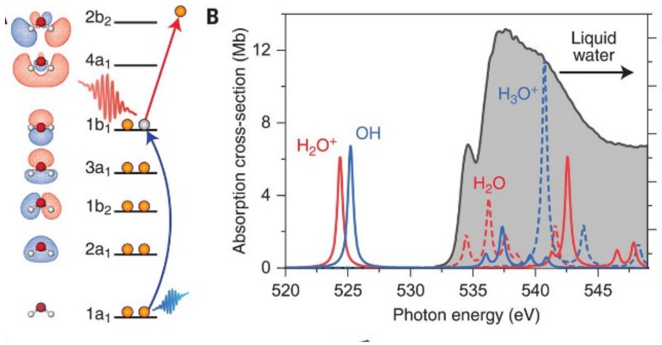
Correlated spin & structural dynamics



dissociation / recombination of NO to Fe-centre in Myoglobin

Nat. Comm. 11, 4145 (2020)

Observation of the fastest chemical processes in the radiolysis of water



Science, 367, 179 (2020)

Future Opportunities in Chemical Sciences and Energy

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

New linear and non-linear x-ray spectroscopies

Probe dynamics, charge, and energy transfer in matter

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

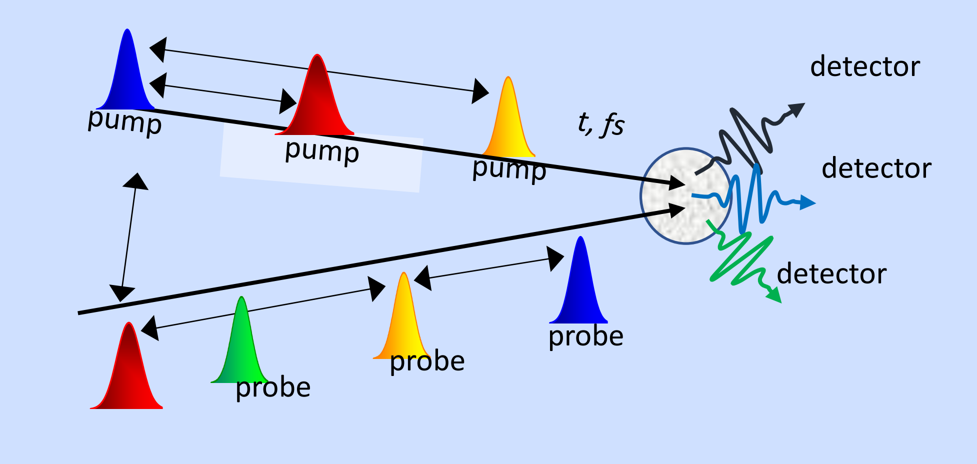
Understanding and development

- Fundamentals of reaction dynamics: nuclei, electrons and spin
- Energy materials and devices
- (Photo)(electro)catalysis *in operando*
- Environment: aerosols, space, combustion, corrosion
- Photodynamics in biomolecules, therapies, diagnostics

Control (photo)reatcivity of molecules, devices and materials

Game Changer

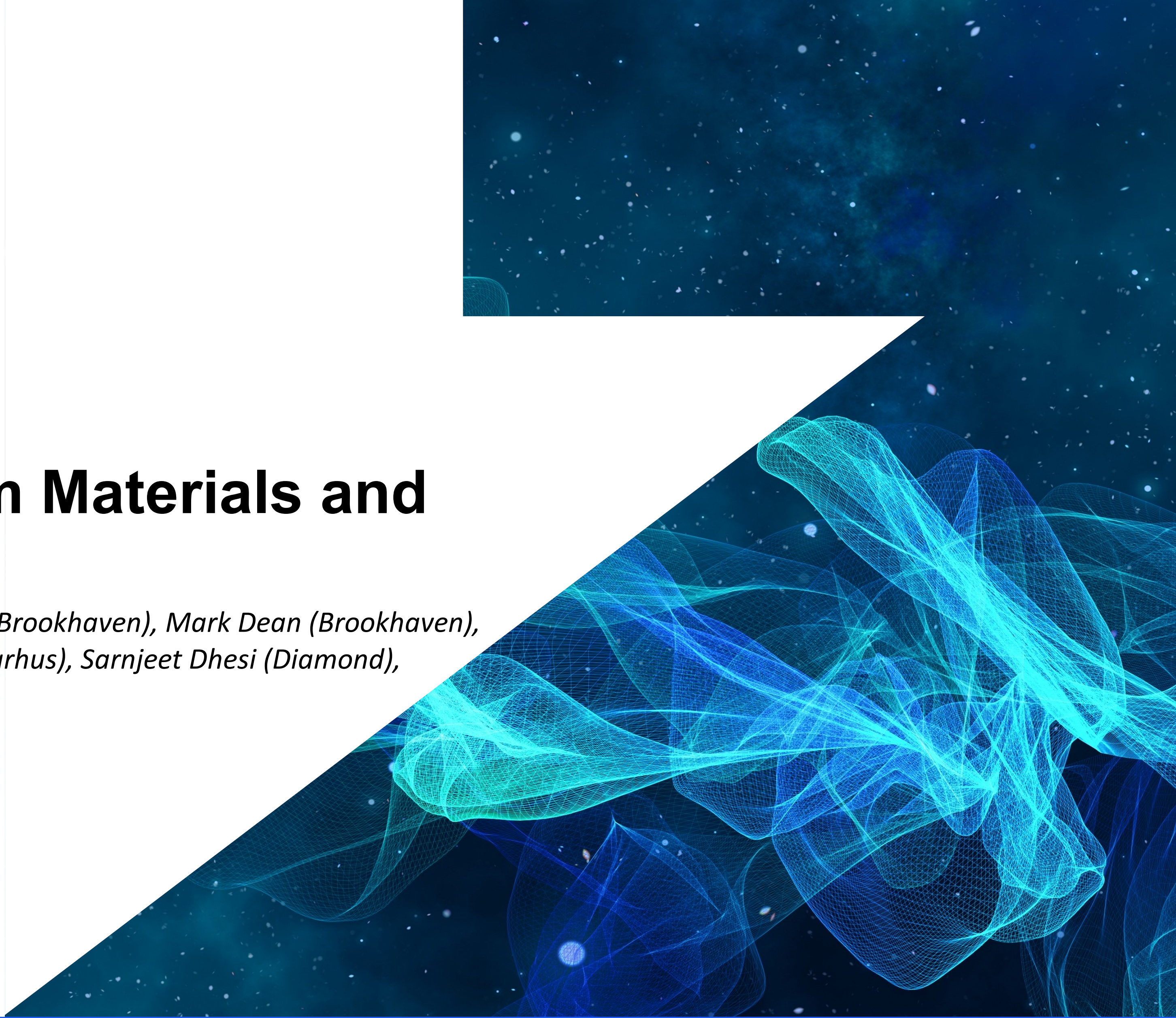
Combine X-rays with:
e-beam,
VUV, UV, Vis, IR, THz excitation and detections:
mix-and-match, multicolour, multi-parameter space,
multidimensional methods



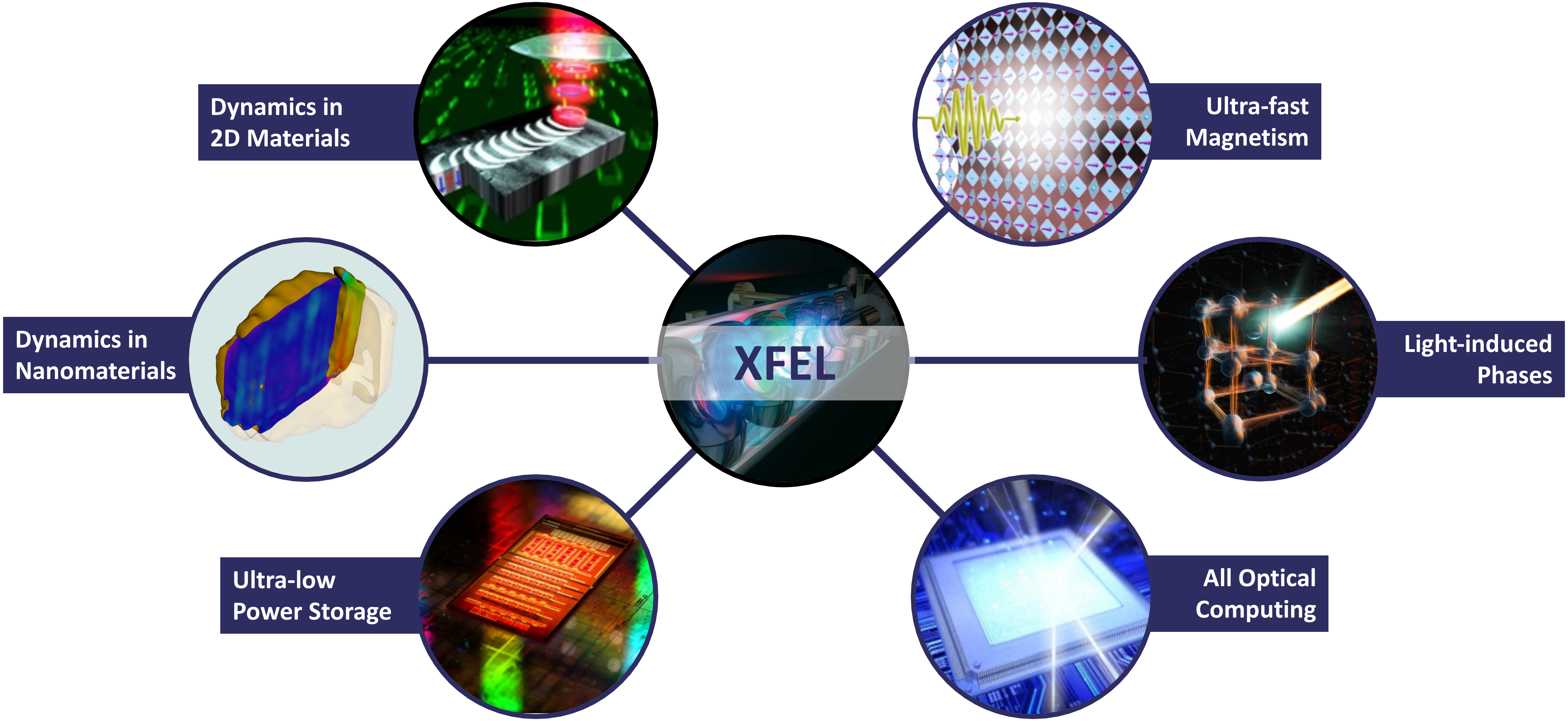
Science and
Technology
Facilities Council

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),*

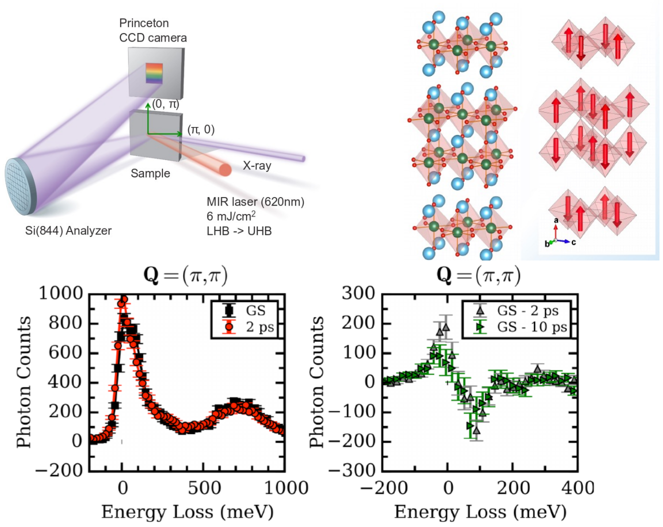


Condensed Phase, Quantum Materials and Nanotechnology



Recent work

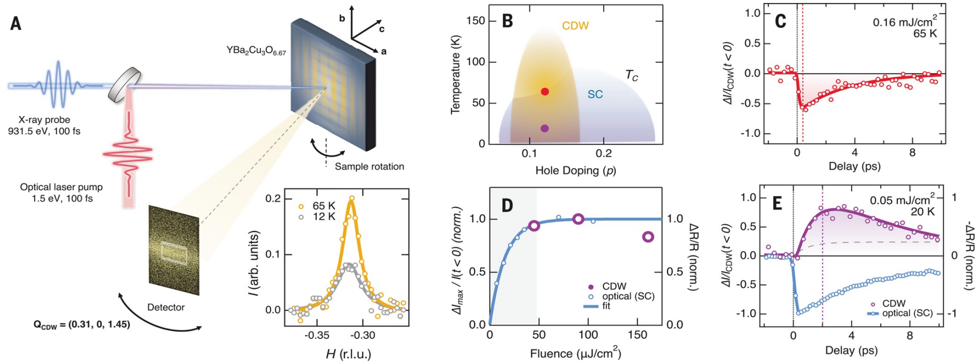
Time-resolved Resonant Inelastic X-ray Scattering (Tr-RIXS)



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)*

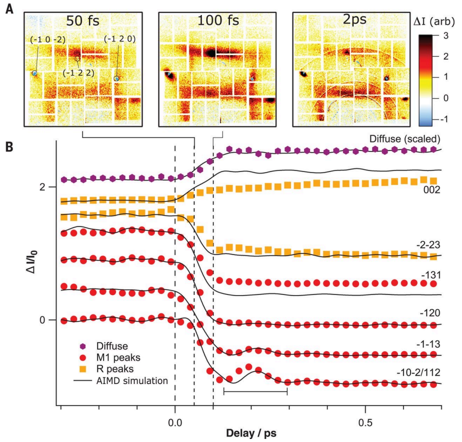
Laser pump, X-ray probe of Superconductivity and CDW Interactions



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)*

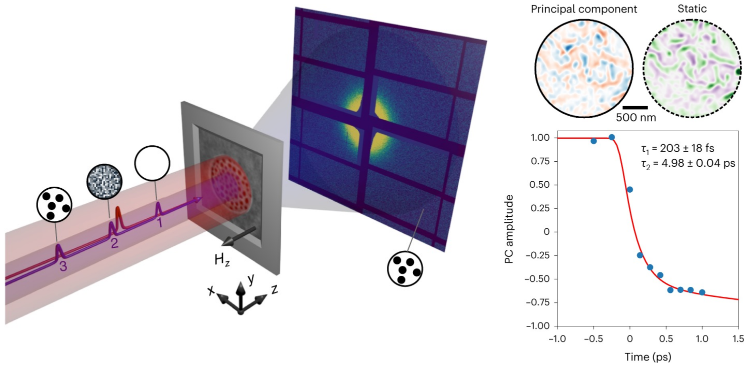
Time-Resolved thermal diffuse scattering



Measuring disorder in solids and manipulating it for energy-efficient control of phase transitions

Wall et al., *Science 362, 572–576 (2018)*
de la Peña Muñoz et al., *Nature Physics 19, 1489 (2023)*
Johnson et al., *Nature Physics – in press (2024)*

Imaging magnetic and quantum materials

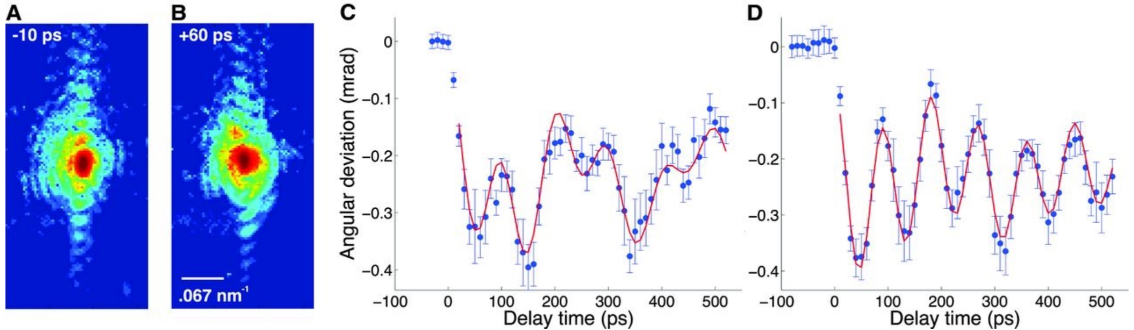


Coherent diffractive imaging of nanoscale dynamics on femtosecond timescale

Klose et al. *Nature 614, 256 (2023)*
Büttner et al. *Nature Materials 20, 30 (2021)*
Johnson et al. *Nature Physics 19, 215 (2023)*

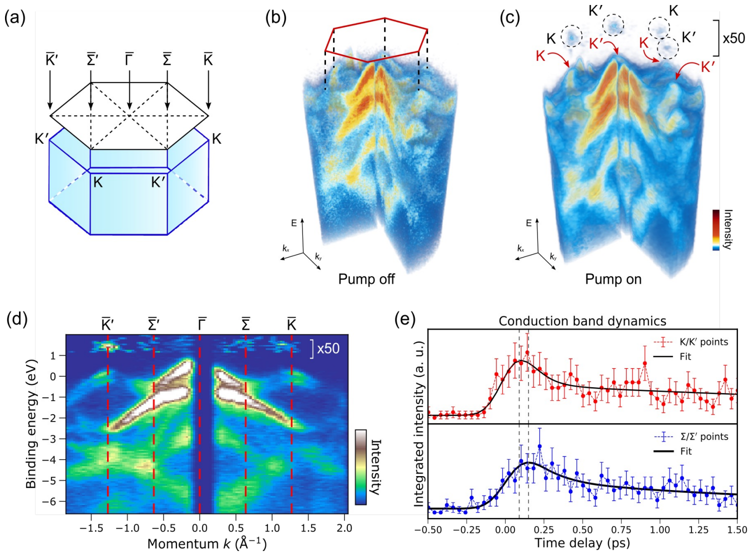
Recent work

Time-resolved Bragg Coherent Diffraction Imaging



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)*

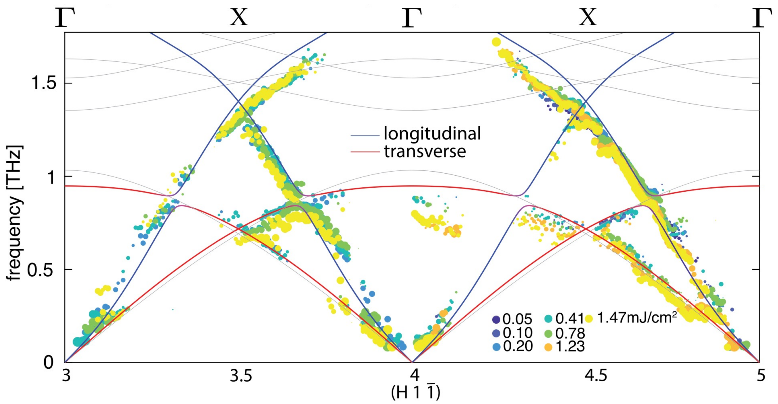
Photoelectron Momentum Microscopy of 2D Material



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)*

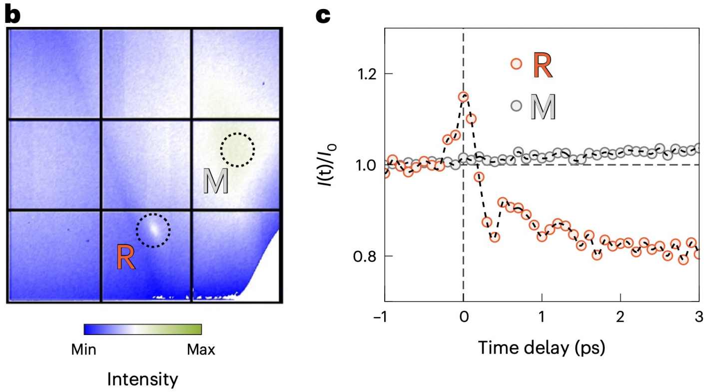
Phonon Dispersion softening of SnSe with pump fluence



Nonthermal Bonding Origin of a Novel Photoexcited Lattice Instability in SnSe [LCLS work by Trigo and Lindenberg]

Huang , Teitelbaum et al., *PRL 131, 156902 (2023)*

Short-time response of ferroelectric response in $SrTiO_3$ coupled to the antiferrodistortive instability



Quenched lattice fluctuations in optically driven $SrTiO_3$ [SwissFEL work by Trigo and Cavalleri]

Fechner et al. *Nature Materials 23 363–368 (2024)*
Orenstein et al. *arXiv:2403.17203v1 (2024)*

Future Opportunities

Ultrafast Magnetism

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

Imaging Dynamics in Nanomaterials

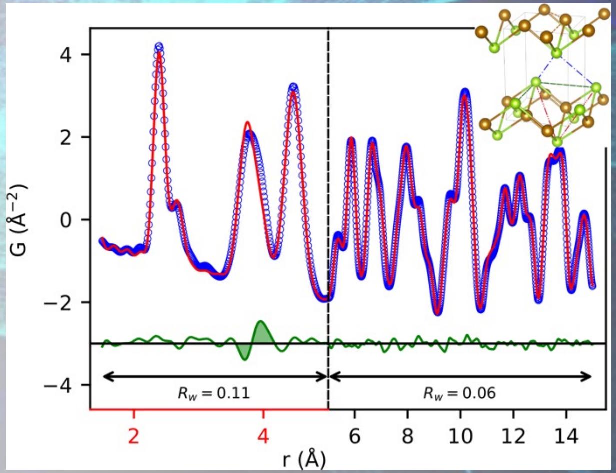
Femto/atto second time-resolution to unambiguously probe each stage during a structural phase transition in three-dimensions

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.



Science and
Technology
Facilities Council

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 artefacts 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

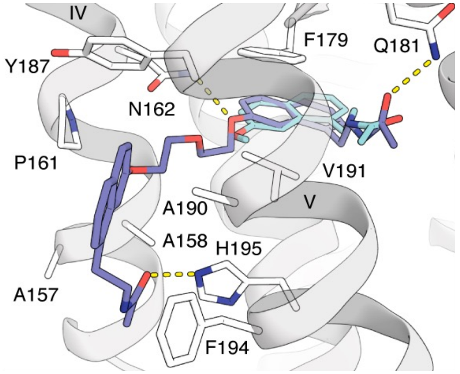
- High rep. rate detectors → more time points / Rxn
- Spatially Resolved Anomalous Dispersion → status of intermediates
- SASE *-vs-* Seeded → tr-SFX ± tr-XES ± ΔE across metal(s) absorption edge(s)

IMPACT

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

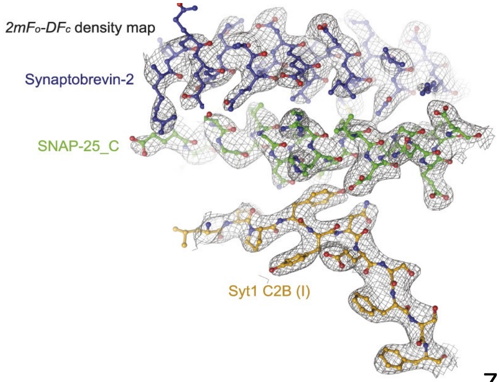
Atomic resolution structures without artefacts

Structural basis of ligand recognition at the human MT1 melatonin receptor



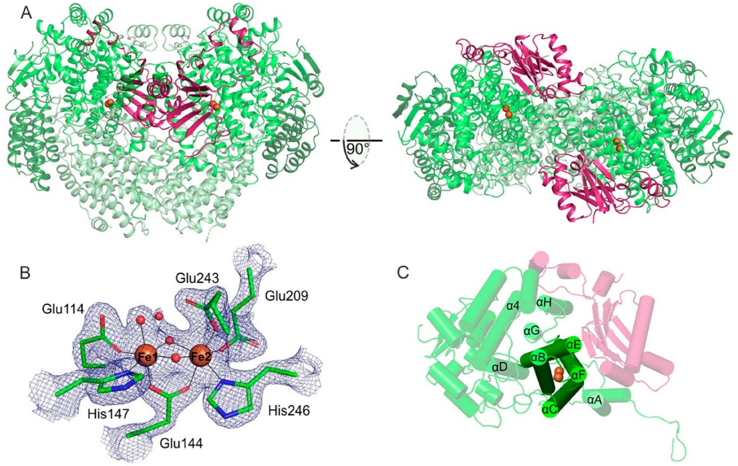
Stauch et al *Nature 569, 284-288 (2019)*

Architecture of the synaptotagnmin- SNARE machinery for neuronal exocytosis



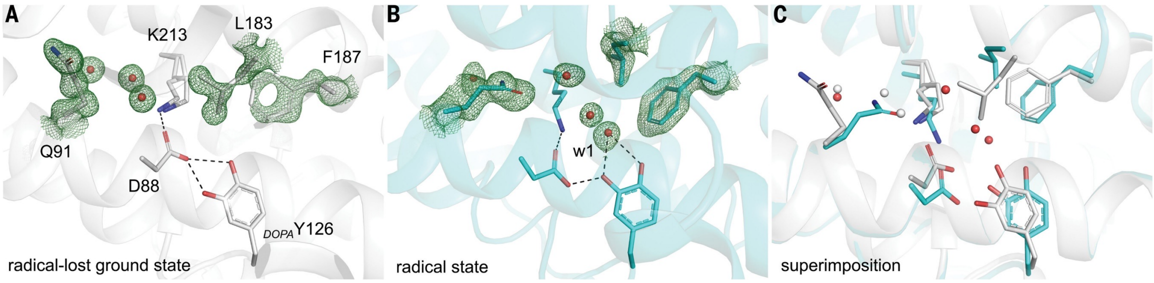
Zhou *et al* *Nature* 525, 62-67 *(2015)*

Structure of methane monooxygenase



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

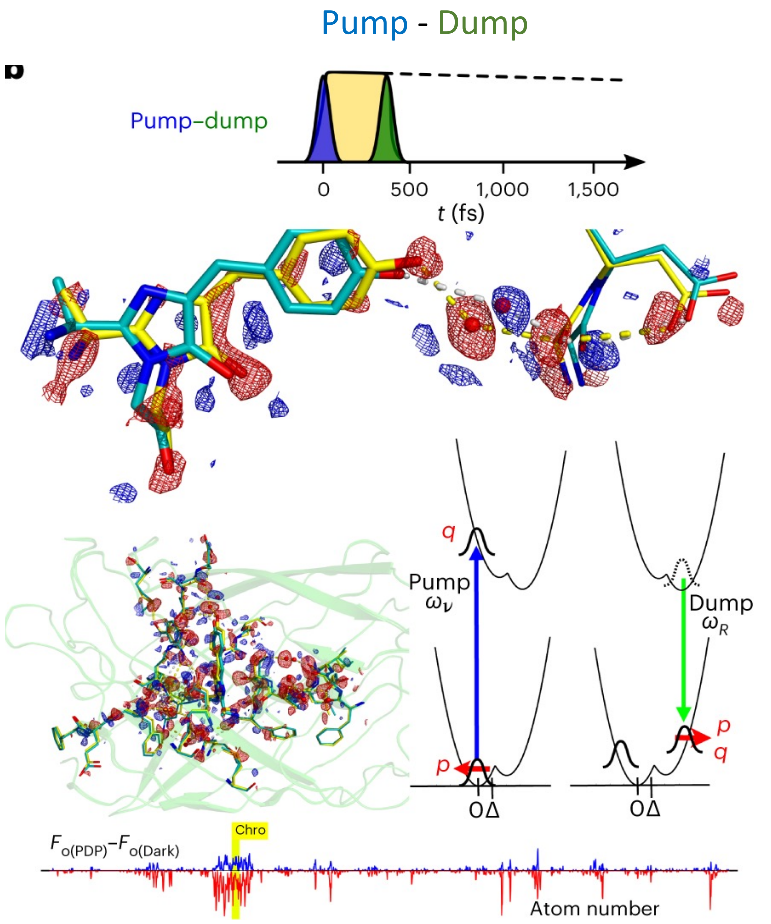
Structure of a ribonucleotide reductase R2 protein radical



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

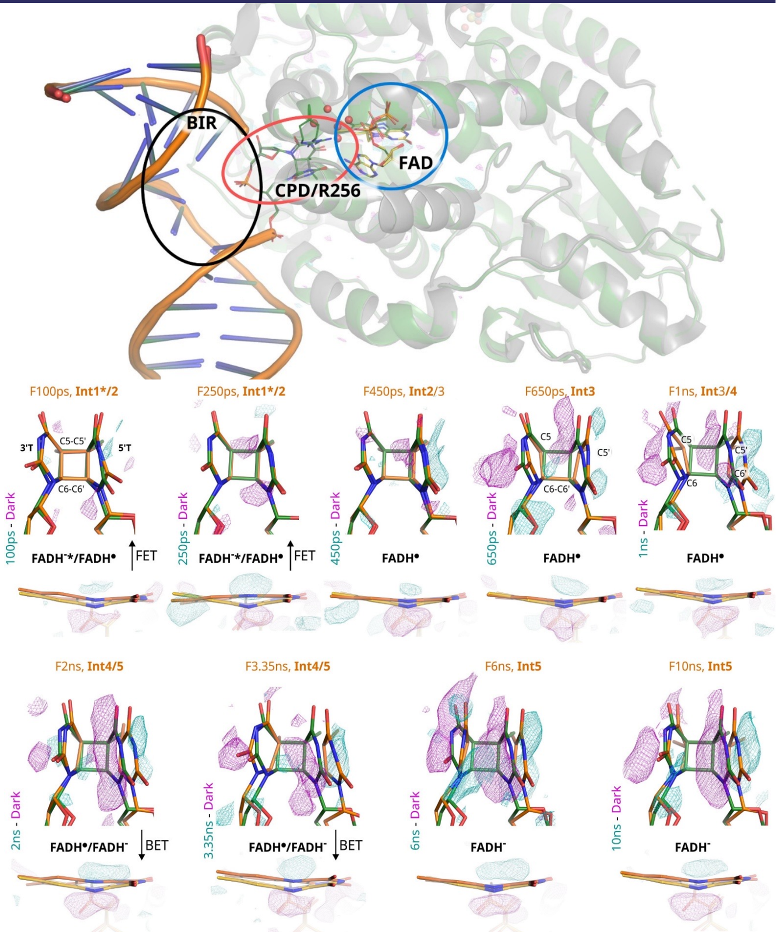
Dynamic structural biology

Optical control of ultrafast structural dynamics in a fluorescent protein.



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

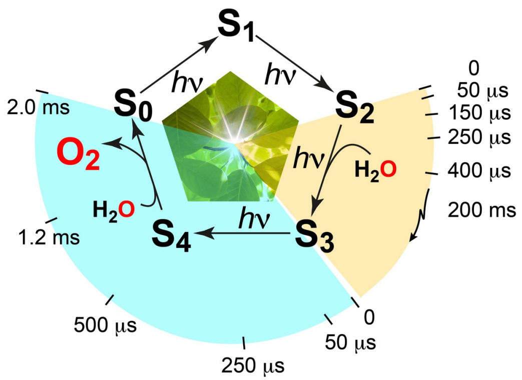
Visualizing the DNA repair process at atomic resolution

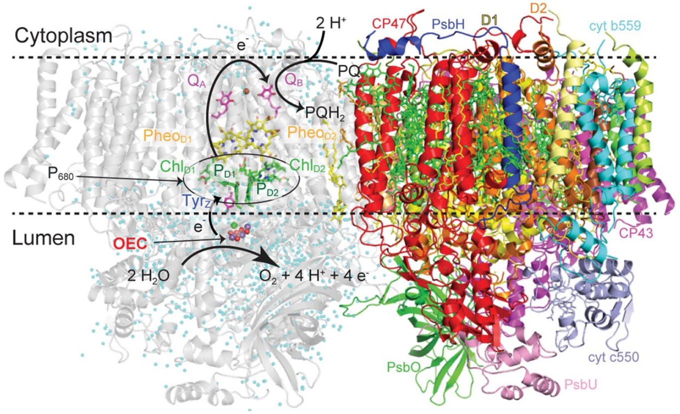


Christou et al *Science 382, 1015 (2023)*

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 delivery

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

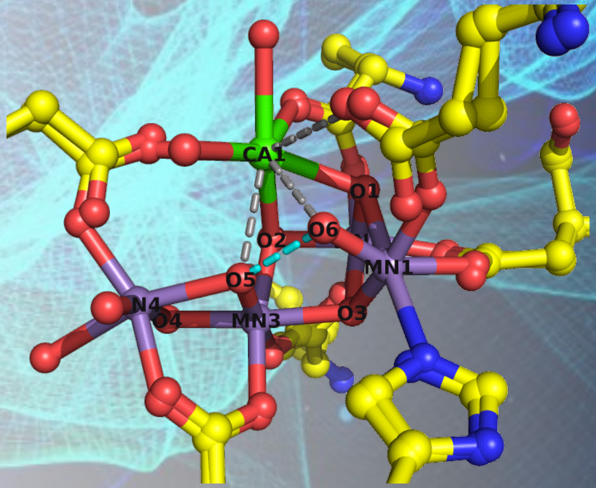
(high rep-rate/high intensity/hard x-rays)

Dynamic structural biology capturing dynamics across many timescales

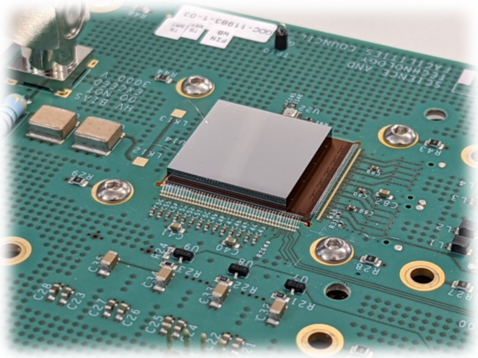
(high rep-rate x-rays, samples and detectors, synchronised laser and activation sources)

Radiation biology and medicine

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



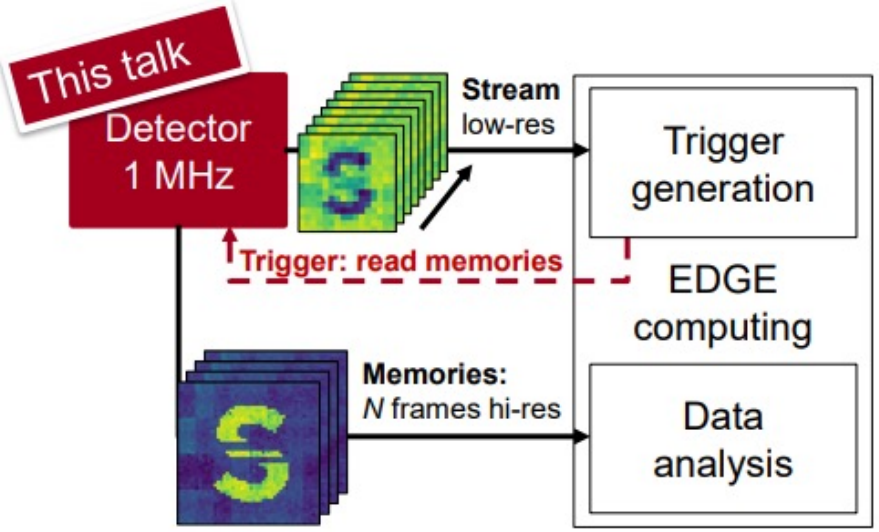
MHz continuous frame rate, Megapixel x-ray detector technology exists



HEXITEC MHz

- *Built by STFC to test in pixel digitiser and high speed serialisers*
- *80x80 pixels on 0.25mm pitch for CZT*
- *Works but made to measure X-ray energy not big signals*
- *But shows you can get to MHz frame rates*

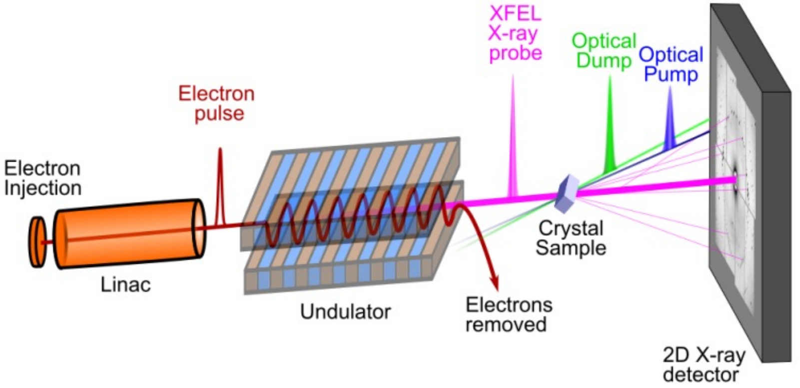
SparkPix → LCLS-II readout sparse area to decide to keep and readout

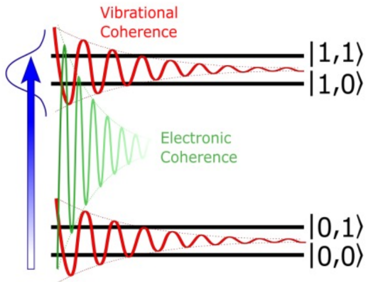


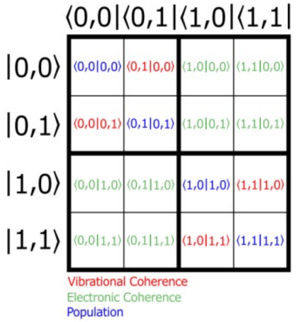
Data rate is the bottleneck: 1 Megapixel at 1 MHz is 2 TB per second
Data reduction strategies:
-SparkPix, ADC and save only rare events in high resolution
-FPGA pre-processing, either record only rare events, or full crystallographic integration and indexing

STFC detector team, Matt Wilson, Chris Armstrong, Sion Richards , Matthew Hart , Marcus French & Matthew Veale

High repetition rate enables new ultrafast science

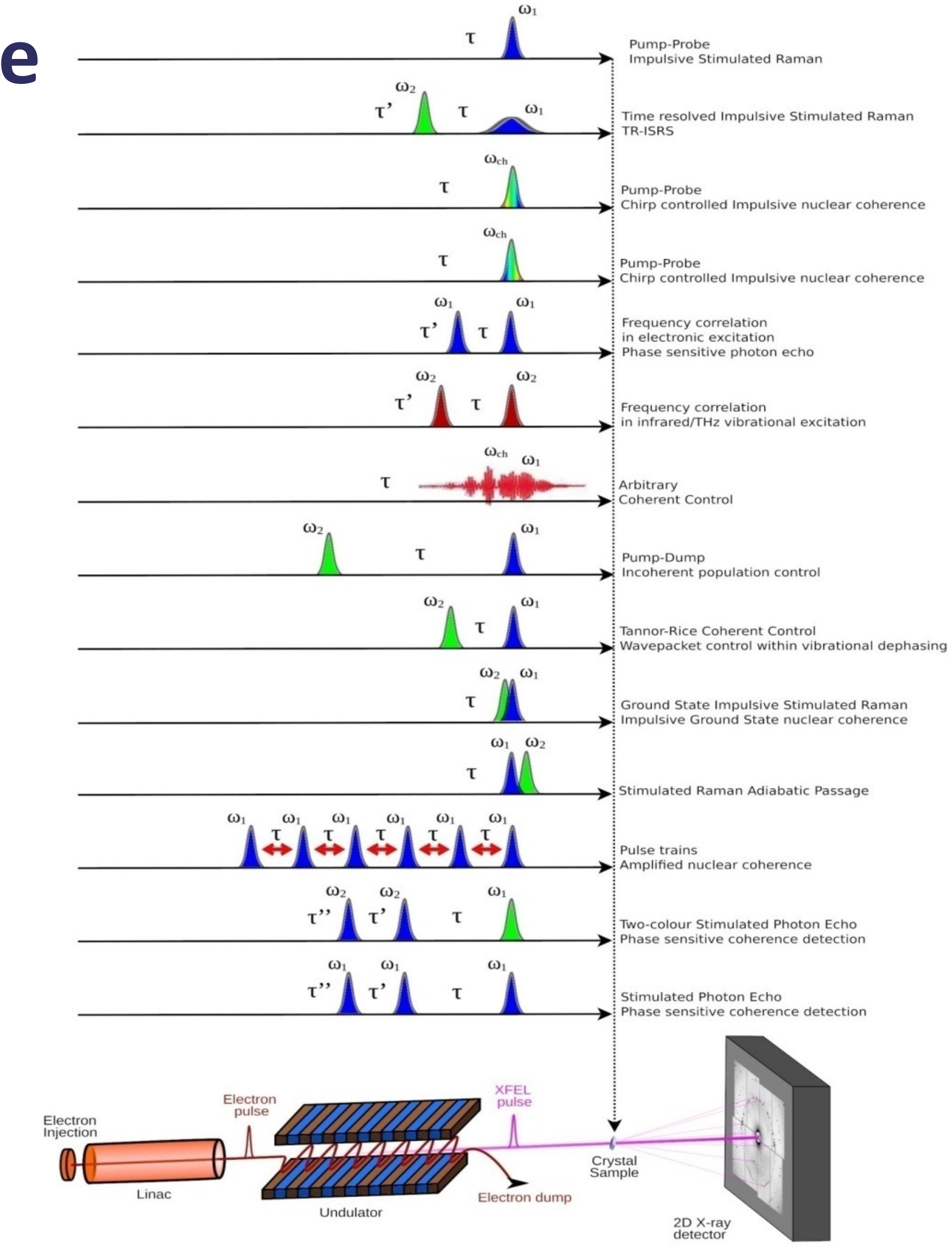






	⟨0,0|	⟨0,1|	⟨1,0|	⟨1,1|
|0,0⟩	⟨0,0|0,0⟩	⟨0,1|0,0⟩	⟨1,0|0,0⟩	⟨1,1|0,0⟩
|0,1⟩	⟨0,0|0,1⟩	⟨0,1|0,1⟩	⟨1,0|0,1⟩	⟨1,1|0,1⟩
|1,0⟩	⟨0,0|1,0⟩	⟨0,1|1,0⟩	⟨1,0|1,0⟩	⟨1,1|1,0⟩
|1,1⟩	⟨0,0|1,1⟩	⟨0,1|1,1⟩	⟨1,0|1,1⟩	⟨1,1|1,1⟩

Vibrational Coherence
Electronic Coherence
Population



Multi-pulse excitation is necessary to separate the coherences and populations, intrinsically present in ultrafast experimental conditions

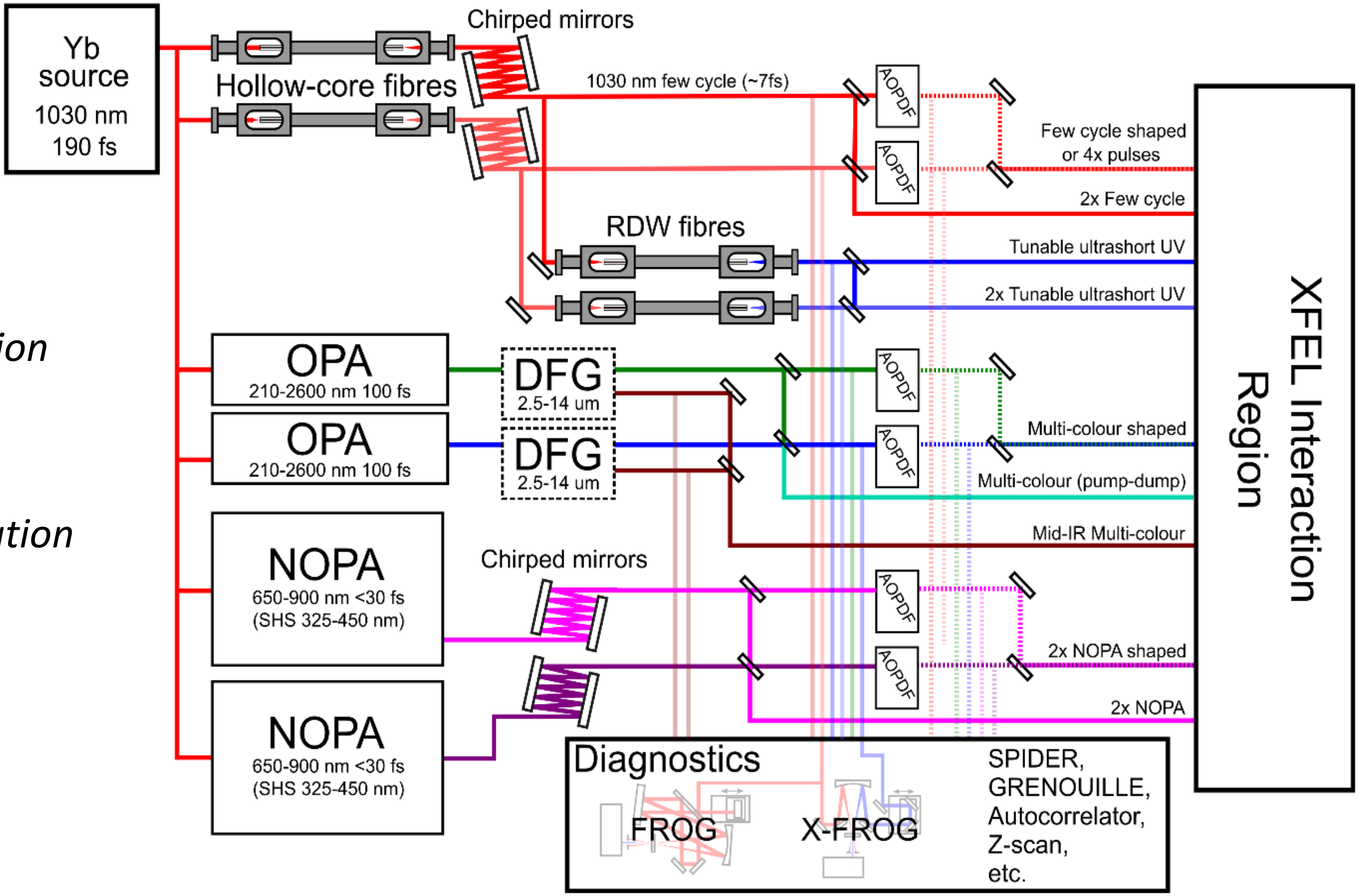
Hutchison, Perrett and van Thor. *J Phys Chem B. (2024)*
XFEL Beamline Optical Instrumentation for Ultrafast Science
https://doi.org/10.1021/acs.jpcb.4c01492

> KW Laser technology and frequency conversion a challenge for MHz work

Possible routes to MHz optical instrumentation

-Non-linear compression of Yb laser

- Optical Parametric Chirped-Pulse Amplification (OPCPA) technology



Hutchison, Perrett and van Thor. *J Phys Chem B. (2024)*
XFEL Beamline Optical Instrumentation for Ultrafast Science
https://doi.org/10.1021/acs.jpcb.4c01492

Proposed optical instrumentation for multi-pulse non-linear science at XFELs

Science and
Technology
Facilities Council

Applied and Industrial Research

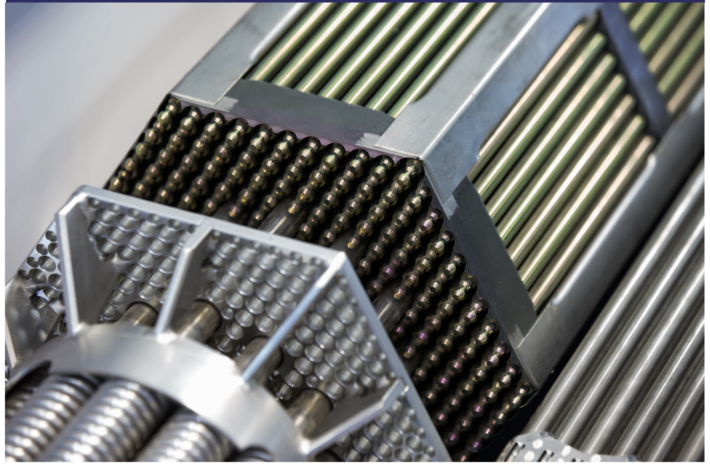
Initial Science Drivers for Applied and Industrial Research

Additive Manufacturing

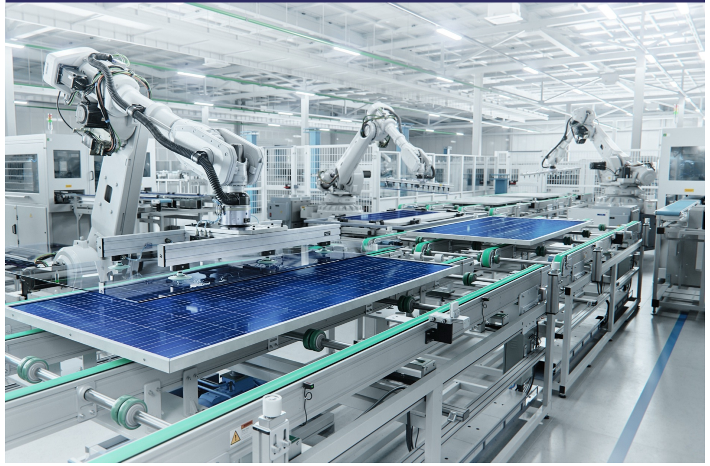
Drug Interactions & Formulation

Shocked Materials

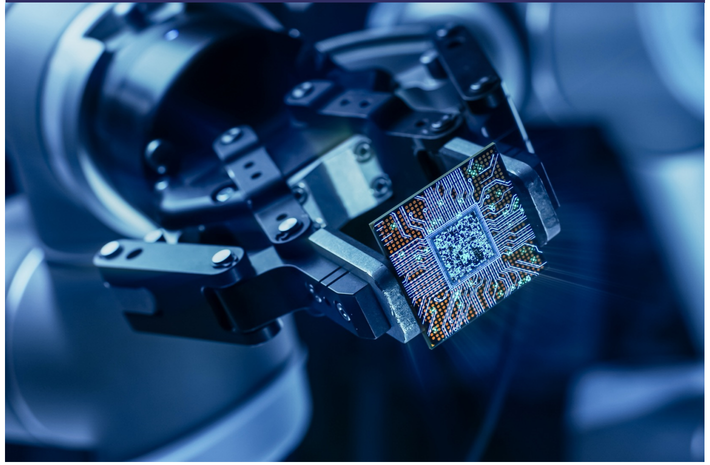
Nucleation



Catalysis

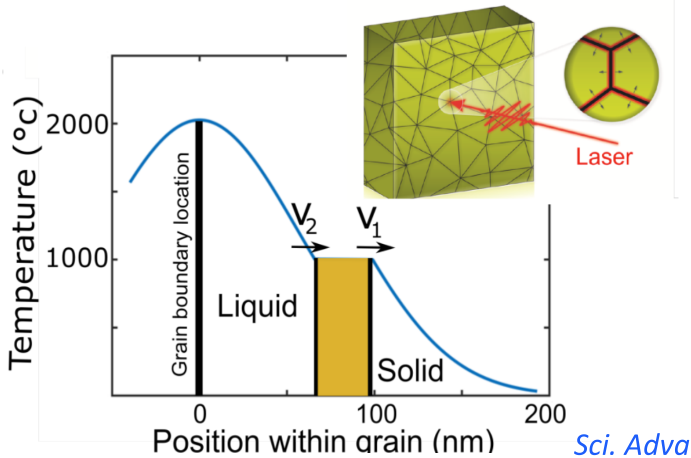


Quantum Tech & Data

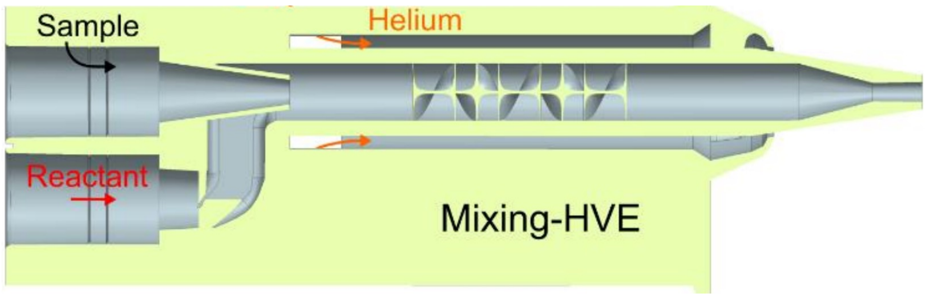


Applications to Laser Processing, Energy Materials, Manufacturing

In-Situ x-ray imaging of additive manufacturing

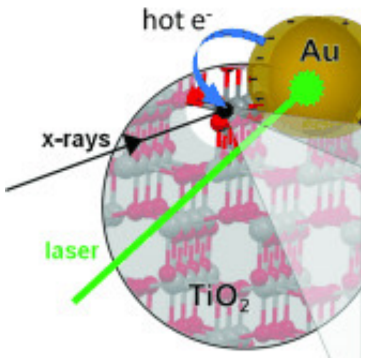


Sci. Advances 6, eaax2445 (2020)
Nat. Comm. 9, 1533 (2018)



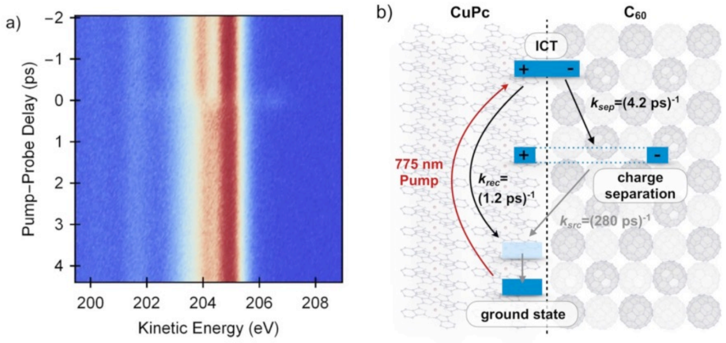
Mix-and-extrude crystallisation dynamics with 3D printed nozzles
J. Appl Cryst 56, 1038 (2023)

Plasmonic Photoctalysis



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

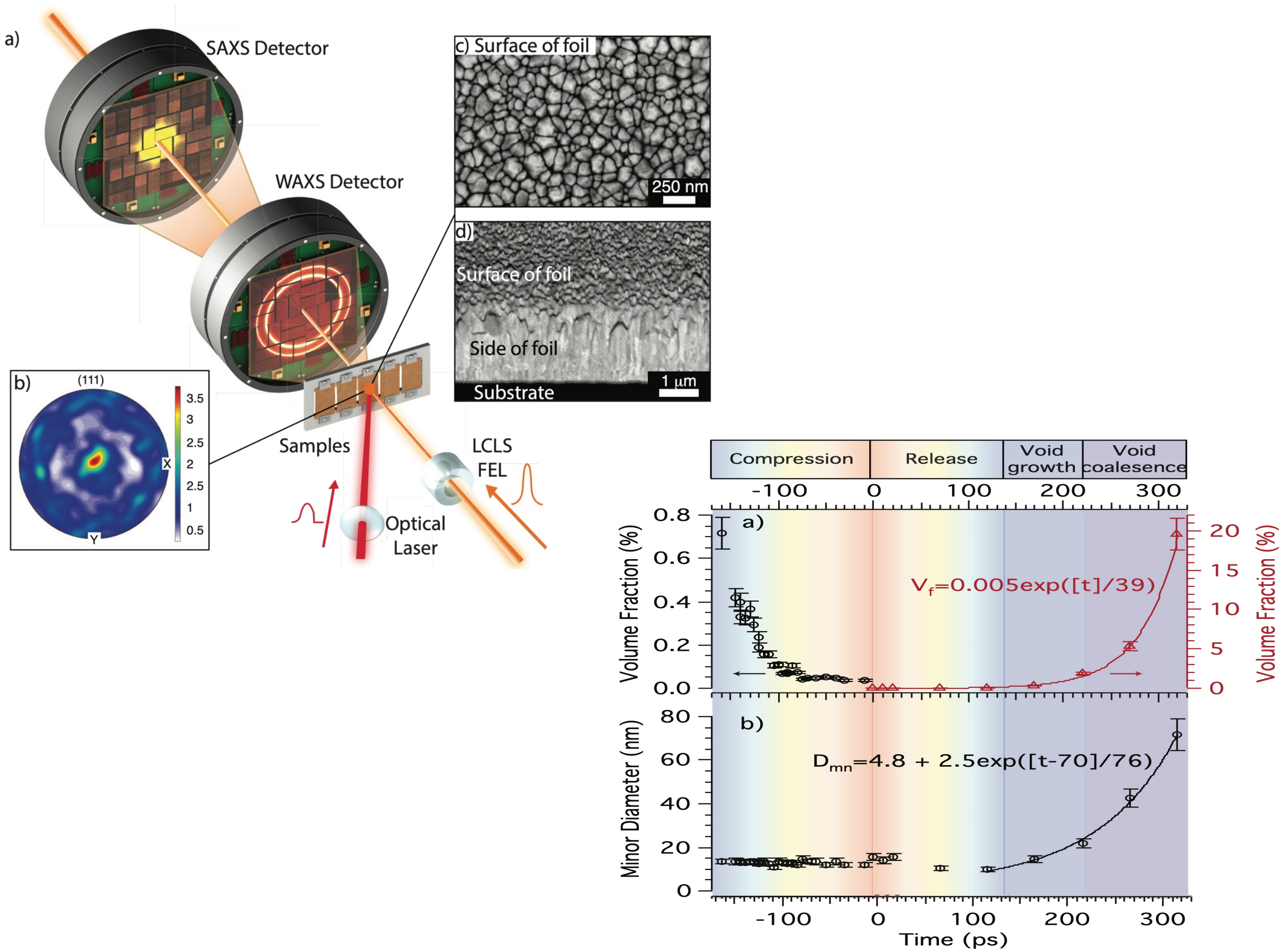
Organic Photovoltaics

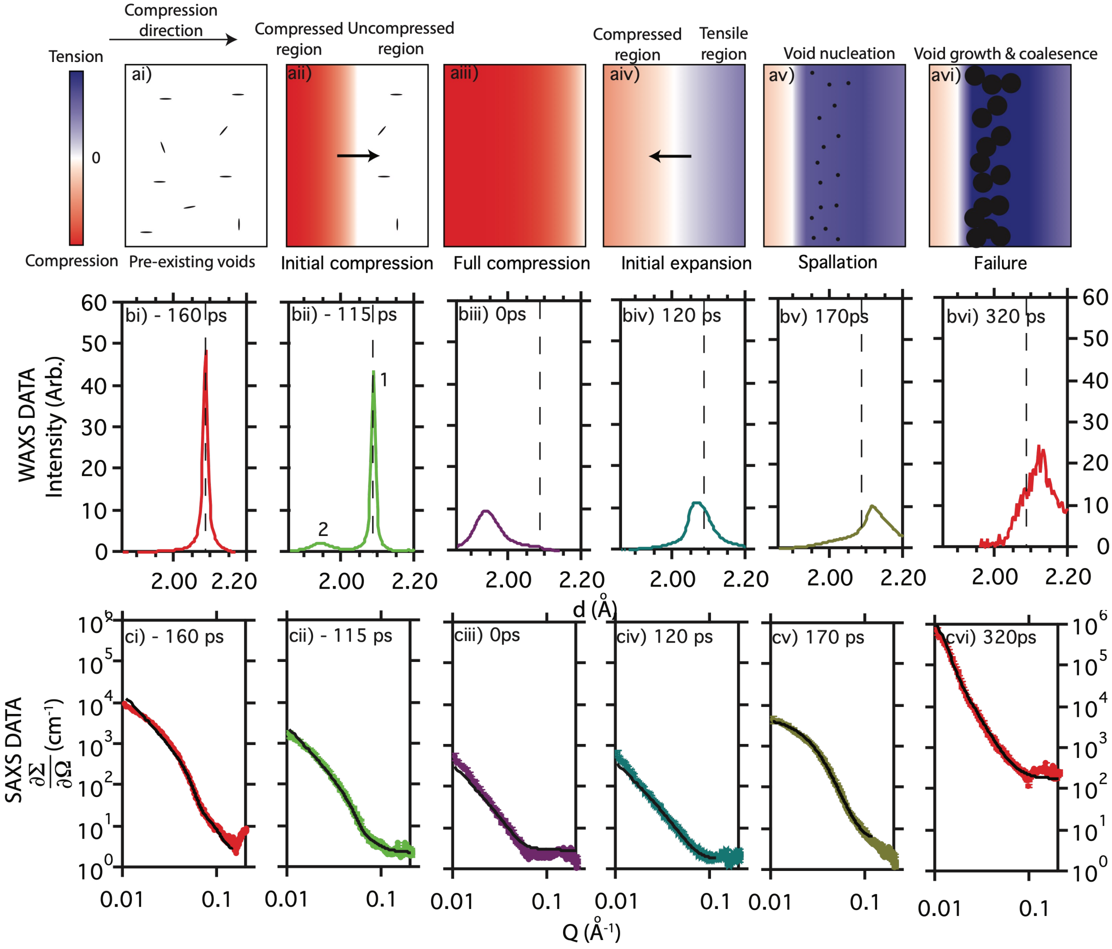


Organic photovoltaics *Nat.Comm. 12, 1196 (2021), Nat.Comm. 13, 3414, (2022)*

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

Powerful insights into the multi-timescale mechanisms crucial for understanding and mitigation
(High rep-rate x-rays, synchronised to ultrafast lasers, electron, proton and ion beams)

Potential for crucial contributions to five critical technologies

Artificial Intelligence

Informing nanoscale engineering of new materials and concepts for energy efficient data processing

Engineering biology

Advancing dynamical structural biology and accompanying insight into the crucial nanoscopic mechanisms

Future Telecommunications

Proving new materials at the ultrafast and nano-scale for future concepts and classes of device

Semiconductors

Through probing ultrafast mechanisms in operation and fabrication for optimisation and sustainability

Quantum Technology

Quantum scale understanding of mechanisms and dynamics in materials and operando-devices

Science and
Technology
Facilities Council

Satisfying Future National Research Needs

UK is Establishing Advanced Capabilities for Ultrafast Dynamics

Capability	RUEDI	UK XFEL
Time Resolution	~20 fs	~0.2 fs
Rep-rate	~1 kHz	100 kHz (x 10 end stations in parallel)
Sub-nm imaging	Dedicated End Station (10 ps res)	NA
CDI (including spectral resolved)	NA	Partial image retrieval (20fs res/sub nm)
Gas phase diffraction	Excellent (sensitive to protons)	Excellent
Thin film diffraction	Excellent	Excellent (including nanocrystals)
Liquid phase scattering	Excellent	Excellent
Bulk materials/buried structures	Limited	Excellent
Field dressed states	Limited	Excellent
Crystallographic structure solution	Limited	Excellent
Resonant elastic & inelastic scattering	NA	Excellent
Electronic state spectroscopy	NA	Excellent
Photoelectron momentum	NA	Excellent
Core level spectroscopy	NA	Excellent
Multi-dimensional spectroscopy	NA	Developing/Excellent prospects

Imaging Structural dynamics Electronic and quantum dynamics

Future Opportunities Unlocked With:

Transform limited operation across entire X-ray range

Fully resolving dynamics at the combined limits of temporal and energy resolution

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

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

Science and
Technology
Facilities Council

Thank You

Slides and References available at

xfel.ac.uk