3. Science Opportunities in Physics and X-ray Photonics

High intensity, ultrashort pulses of X-rays create new possibilities in physics and new potential in X-ray photonics that will find future application across the sciences. Here we consider new basic physics enabled by XFELs, and the exciting science opportunities provided by new X-ray based measurement methods.

3.1 Frontiers in ultrafast chemical physics
3.2 New concepts in scattering
3.3 Attosecond science and non-linear X-ray spectroscopy
3.4 Capturing conformational dynamics and rare thermodynamic states
3.5 Non-linear X-ray physics and physics beyond the Standard Model with XFELs
3.6 High brightness relativistic electron beam science

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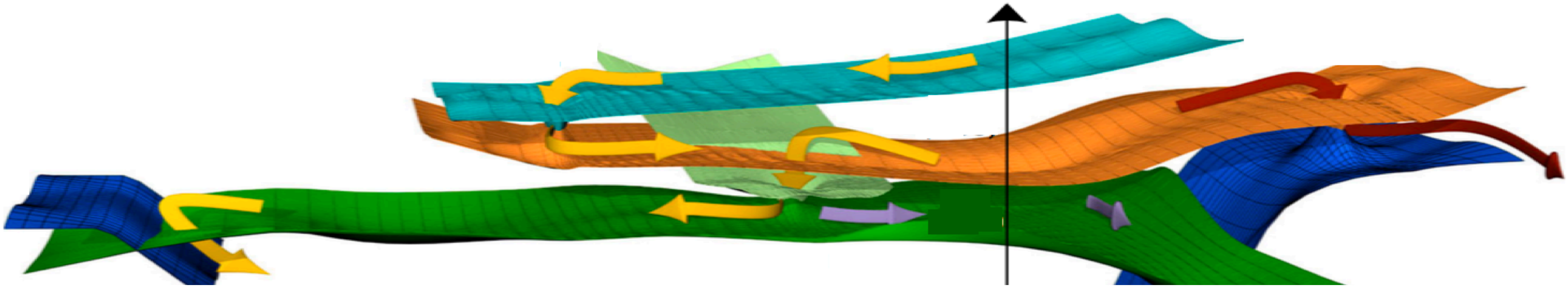
UK XFEL as a driver of new physics and photonics

- **Basic science**
- **New measurement methods**
- **Fundamental physics experiments and tests**

New discoveries and frontiers

Examples of science questions:

- Electronic *quantum coherence* in photo-excitation of matter?
- Electron-nuclear coupling and conical intersections in *chemical reactions*?
- Dynamical mechanisms for *radiation damage* in biomolecules?
- Conformational pathways that control the function of *molecular machines*?
- Use X-rays to detect *dark matter* and test fundamental physics?



Active UK research area

LETTERS
https://doi.org/10.1038/s41567-019-0610-9
nature physics

Generation and acceleration of electron bunches from a plasma photocathode

A. Deng[1,2,14], O. S. Karger[3,14], T. Heinemann[4,5,6], A. Knetsch[6], P. Scherkl[4,5], G. G. Manahan[4,5], A. Beaton[4,5], D. Ullmann[4,5], G. Wittig[3], A. F. Habib[4,5], Y. Xi[1], M. D. Litos[7], B. D. O'Shea[8], S. Gessner[8], C. I. Clarke[8], S. Z. Green[8], C. A. Lindstrøm[9], E. Adli[9], R. Zgadzaj[10], M. C. Downer[10], G. Andonian[1,11], A. Murokh[11], D. L. Bruhwiler[12], J. R. Cary[13], M. J. Hogan[8], V. Yakimenko[8], J. B. Rosenzweig[1] and B. Hidding[4,5*]

ARTICLES
https://doi.org/10.1038/s41566-019-0549-5
nature photonics

Tunable isolated attosecond X-ray pulses with gigawatt peak power from a free-electron laser

Joseph Duris[1,12], Siqi Li[1,2,12], Taran Driver[1,3,4], Elio G. Champenois[3], James P. MacArthur[1,2], Alberto A. Lutman[1], Zhen Zhang[1], Philipp Rosenberger[1,3,5,6], Jeff W. Aldrich[1], Ryan Coffee[1], Giacomo Coslovich[1], Franz-Josef Decker[1], James M. Glownia[1], Gregor Hartmann[7], Wolfram Helml[6,8,9], Andrei Kamalov[2,3], Jonas Knurr[3], Jacek Krzywinski[1], Ming-Fu Lin[1], Jon P. Marangos[4], Megan Nantel[1,2], Adi Natan[3], Jordan T. O'Neal[2,3], Niranjan Shivaram[1], Peter Walter[1], Anna Li Wang[3,10], James J. Welch[1], Thomas J. A. Wolf[3], Joseph Z. Xu[11], Matthias F. Kling[1,3,5,6], Philip H. Bucksbaum[1,2,3,10], Alexander Zholents[11], Zhirong Huang[1,10], James P. Cryan[1,3*] and Agostino Marinelli[1*]

nature COMMUNICATIONS

Observation of the molecular response to light upon photoexcitation

Haiwang Yong[1], Nikola Zotev[2], Jennifer M. Ruddock[1,3], Brian Stankus[1], Mats Simmermacher[2], Andrés Moreno Carrascosa[2], Wenpeng Du[1], Nathan Goff[1], Yu Chang[1], Darren Bellshaw[2], Mengning Liang[3], Sergio Carbajo[3], Jason E. Koglin[3], Joseph S. Robinson[3], Sébastien Boutet[3], Michael P. Minitti[3], Adam Kirrander[2✉] & Peter M. Weber[1✉]

SCIENTIFIC REPORTS
natureresearch

Characterisation of microbunching instability with 2D Fourier analysis

A. D. Brynes[1,2,3*], I. Akkermans[4], E. Allaria[5], L. Badano[5], S. Brussaard[4], G. De Ninno[5,6], D. Gauthier[5,7], G. Gaio[5], L. Giannessi[5], N. S. Mirian[5], G. Penco[5], G. Perosa[8], P. Rebernik[5], I. Setija[4], S. Spampinati[5], C. Spezzani[5], M. Trovò[5], M. Veronese[5], P. H. Williams[1,2], A. Wolski[2,3] & S. Di Mitri[5,8]

nature physics
ARTICLES
https://doi.org/10.1038/s41567-019-0665-7
Corrected: Author Correction

Femtosecond-resolved observation of the fragmentation of buckminsterfullerene following X-ray multiphoton ionization

N. Berrah[1*], A. Sanchez-Gonzalez[2], Z. Jurek[3], R. Obaid[1], H. Xiong[1], R. J. Squibb[4], T. Osipov[5], A. Lutman[5], L. Fang[6], T. Barillot[2], J. D. Bozek[7], J. Cryan[8], T. J. A. Wolf[8], D. Rolles[9], R. Coffee[5], K. Schnorr[10], S. Augustin[9], H. Fukuzawa[11], K. Motomura[11], N. Niebuhr[12], L. J. Frasinski[2], R. Feifel[4], C. P. Schulz[13], K. Toyota[3], S.-K. Son[3], K. Ueda[11], T. Pfeifer[10], J. P. Marangos[2] and R. Santra[3,14]

ARTICLES
https://doi.org/10.1038/s41557-019-0291-0
nature chemistry

Ultrafast X-ray scattering reveals vibrational coherence following Rydberg excitation

Brian Stankus[1,4], Haiwang Yong[1,4], Nikola Zotev[2], Jennifer M. Ruddock[1], Darren Bellshaw[2], Thomas J. Lane[3], Mengning Liang[3], Sébastien Boutet[3], Sergio Carbajo[3], Joseph S. Robinson[3], Wenpeng Du[1], Nathan Goff[1], Yu Chang[1], Jason E. Koglin[3], Michael P. Minitti[3], Adam Kirrander[2] and Peter M. Weber[1*]

PHYSICAL REVIEW LETTERS **121**, 194801 (2018)

Emittance Preservation in an Aberration-Free Active Plasma Lens

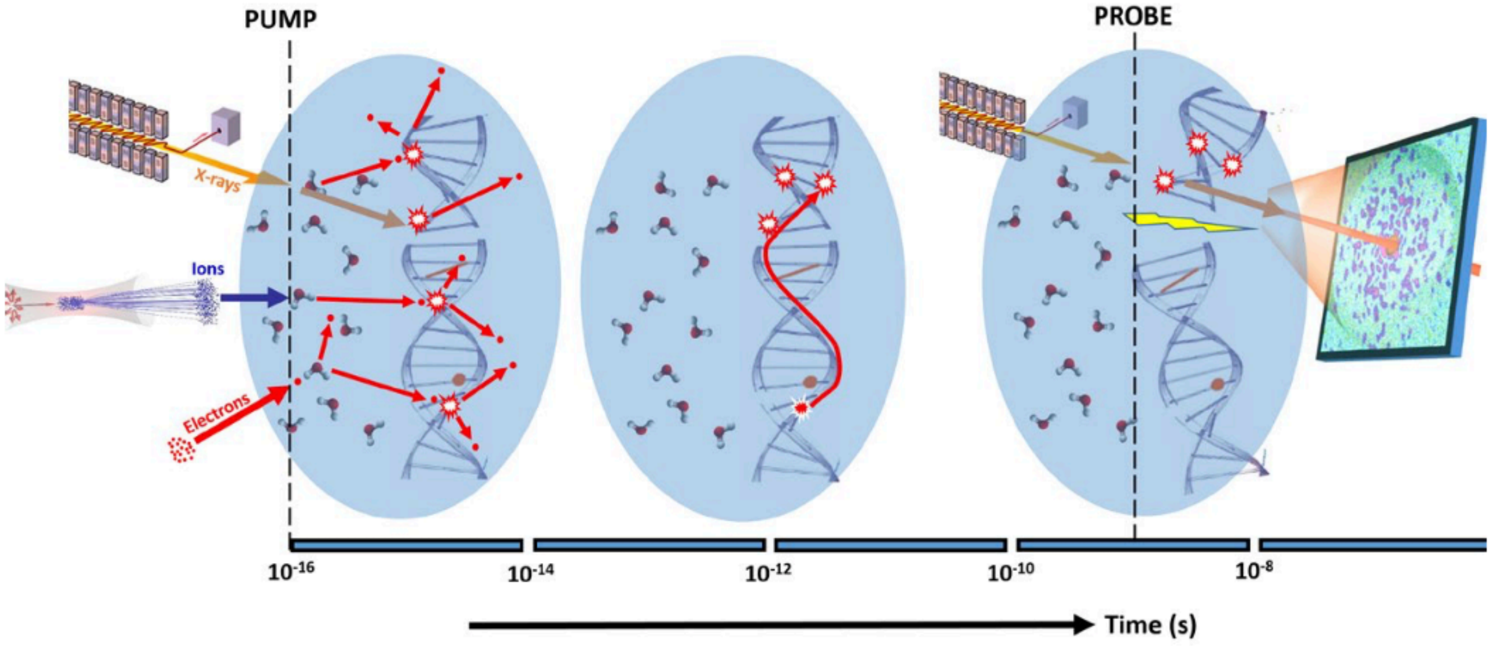
C. A. Lindstrøm,[1,*] E. Adli,[1] G. Boyle,[2] R. Corsini,[3] A. E. Dyson,[4] W. Farabolini,[3] S. M. Hooker,[4,5] M. Meisel,[2] J. Osterhoff,[2] J.-H. Röckemann,[2] L. Schaper,[2] and K. N. Sjobak[1]

3.1 Frontiers in ultrafast chemical physics

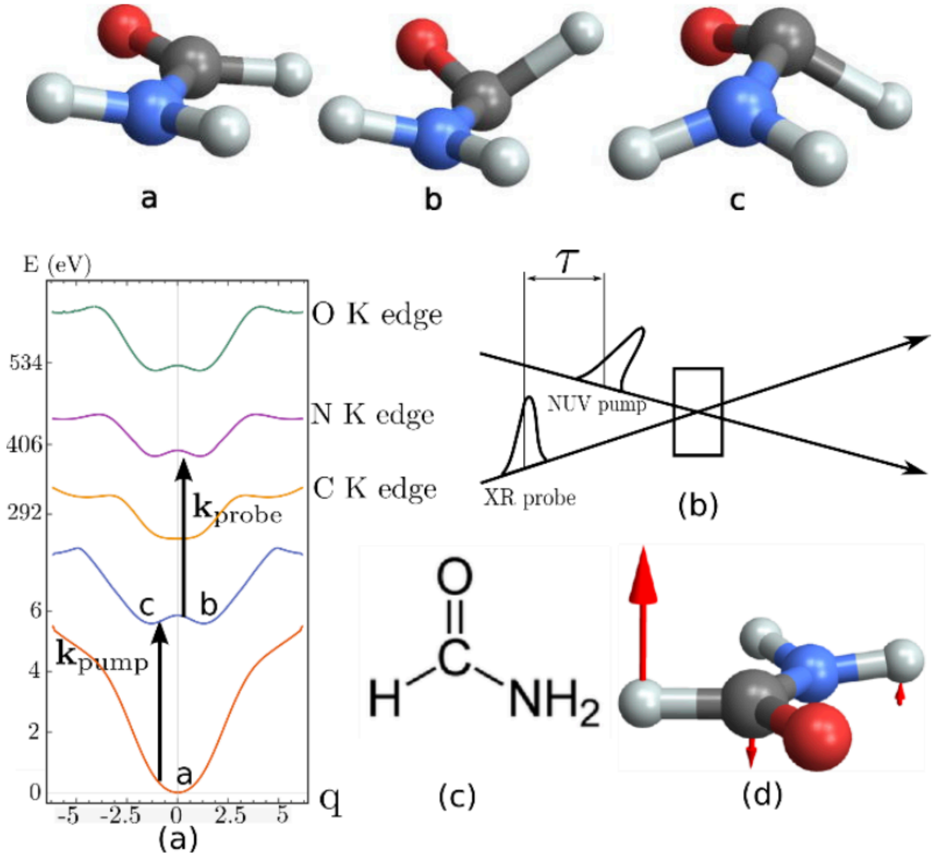
Powerful non-linear optical techniques implemented in the X-ray regime will enable dynamic probing of electronic properties and how they couple to molecular structure

Determine **flow of charge and energy across and between molecules** with sub-Ångström resolution and *atomic specificity*

DNA radiation damage



Chirality



XFEL requirements: high rep rate, high pulse energy, sub-fs duration, multipulse w/ configurable λ and polarisation state, commensurate detector technology

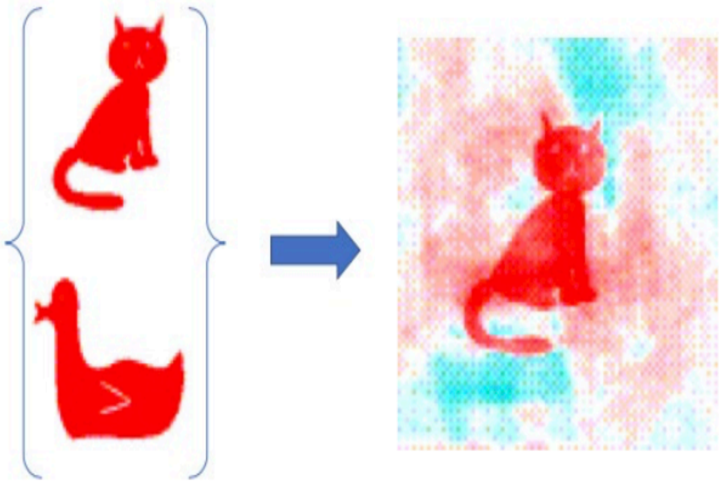
3.2 New concepts in scattering

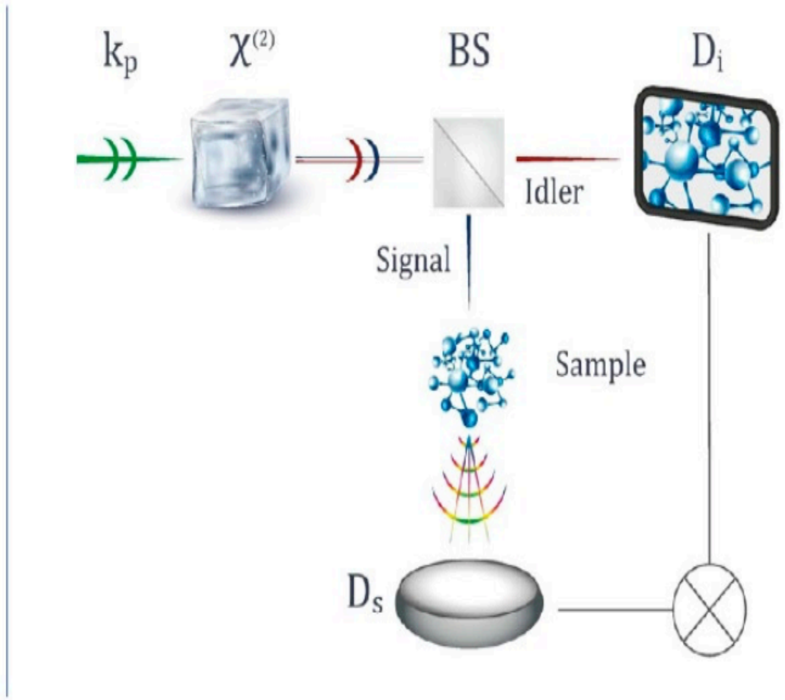
Concepts from quantum optics and new X-ray scattering physics will circumvent the phase problem and provide new tools to image dynamic processes

Capture **transient** structure, electron dynamics, and coherent transport phenomena, even in **disordered** or **fragile** samples

Structure is a key property of matter

Could XFELs solve the phase-problem in structure determination?





XFEL requirements: high rep rate, sub-fs duration, tunable energy, transform limited pulses, high shot-to-shot reproducibility, detectors and optical systems

3.2 New concepts in scattering

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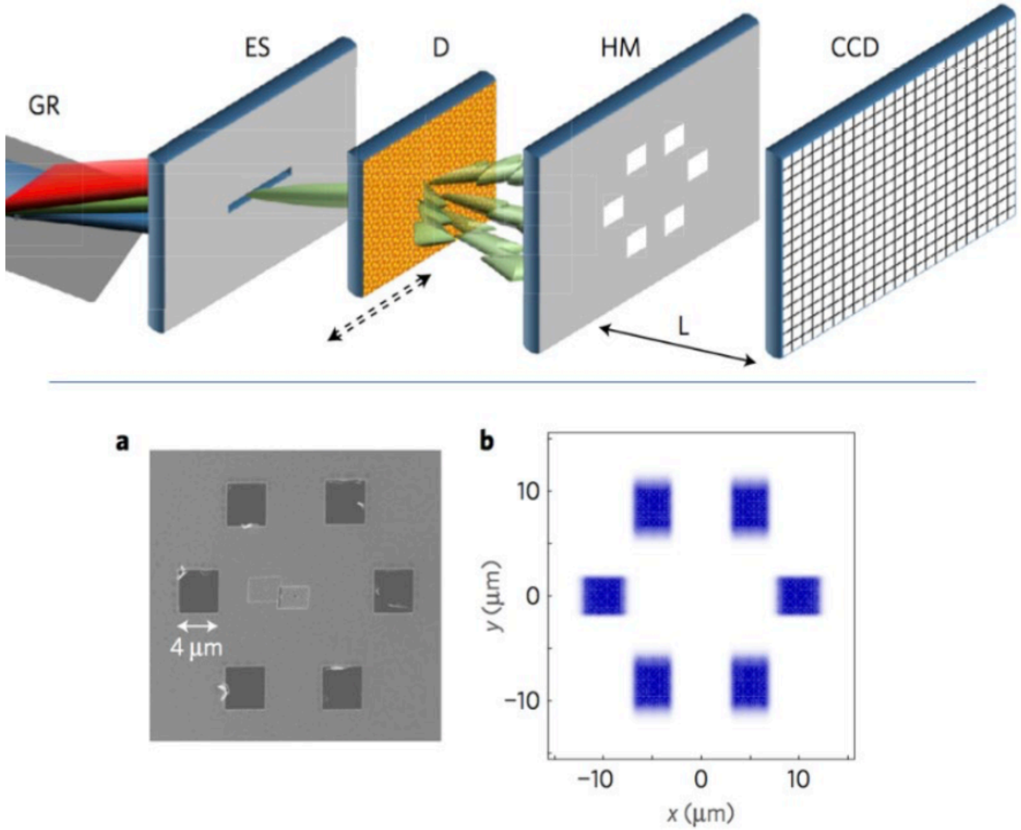
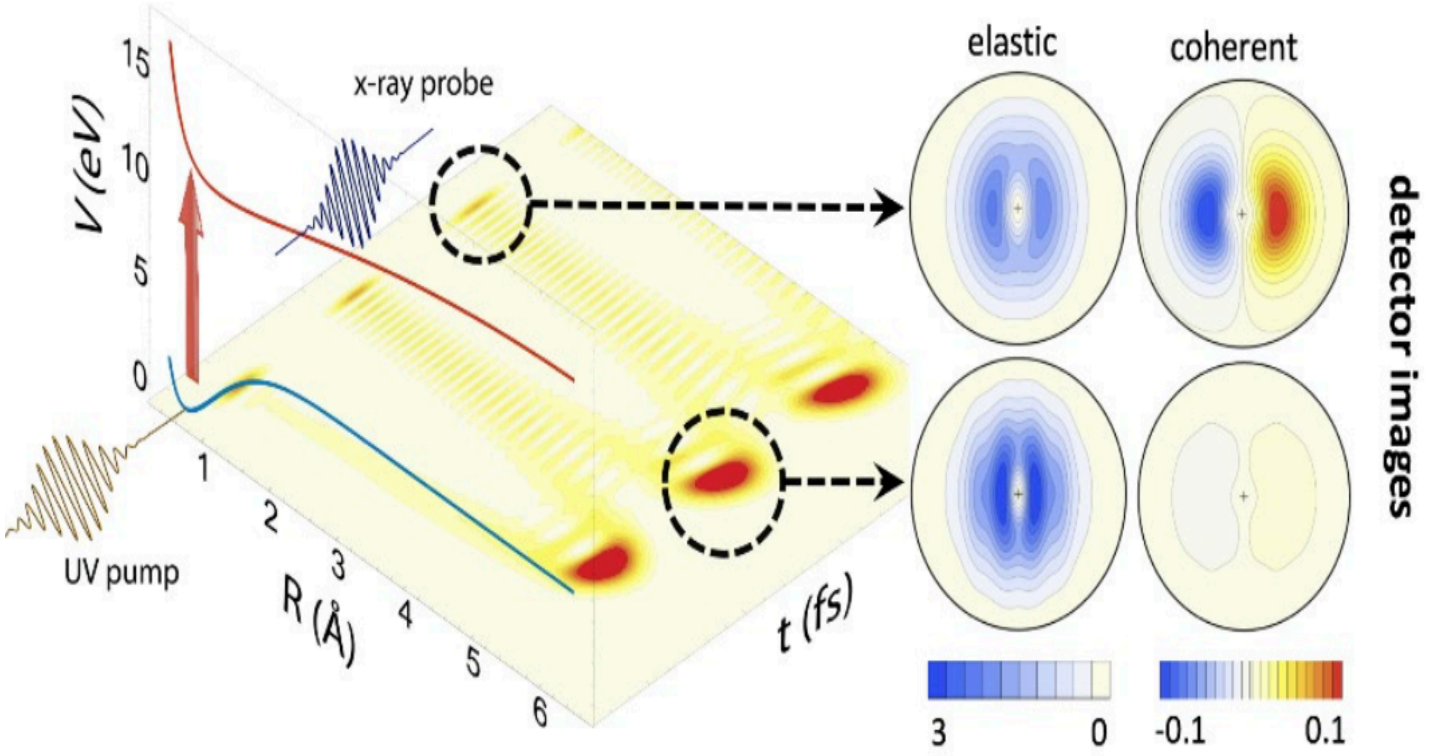
Incoherent diffraction with element specificity



New scattering phenomena could detect coherences



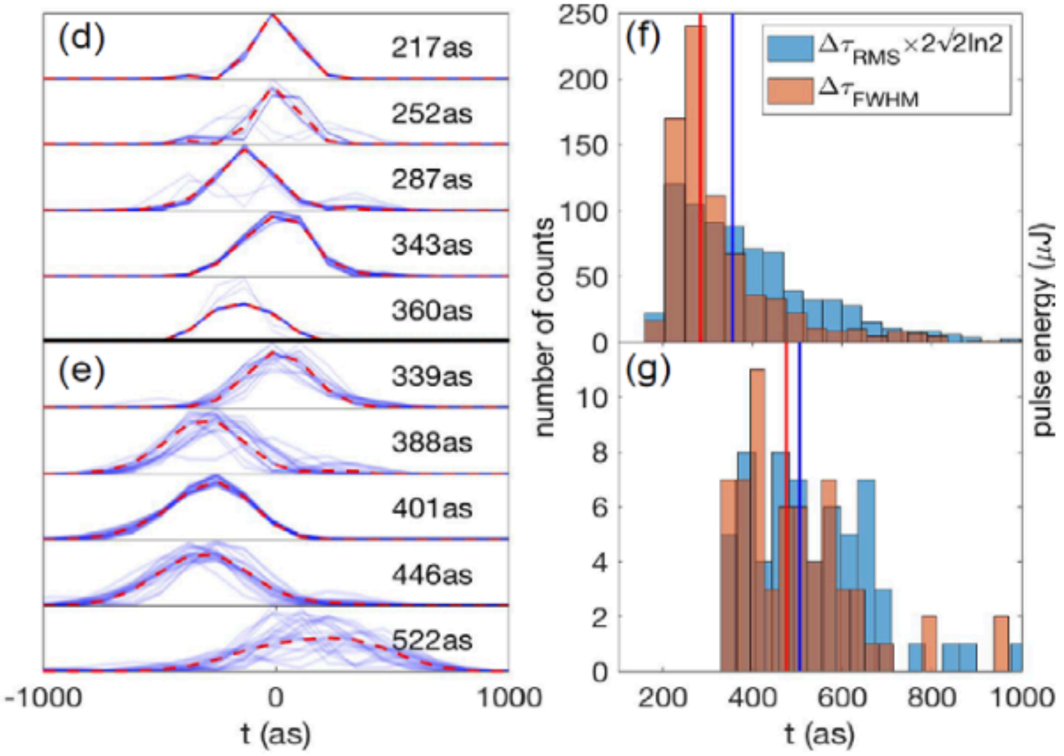
XFEL requirements: high rep rate, sub-fs duration, tunable energy, transform limited pulses, high shot-to-shot reproducibility, detectors and optical systems

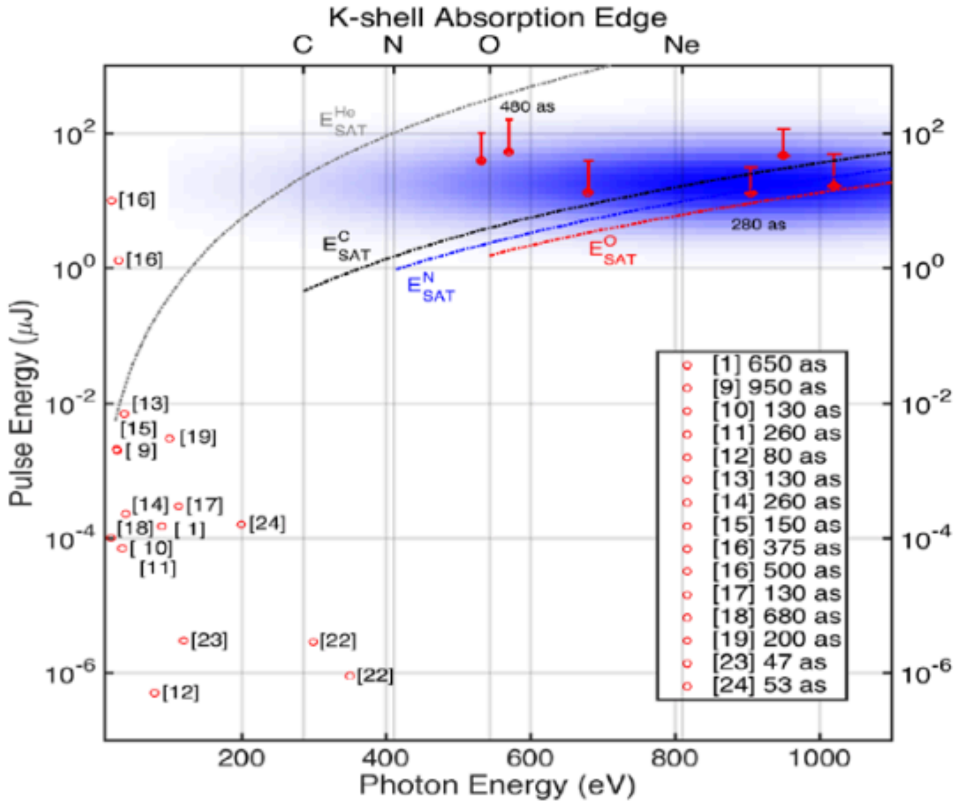
3.3 Attosecond science and non-linear X-ray spectroscopy

XFELs surpass HHG as a source of attosecond pulses, opening opportunities for attosecond domain pump-probe measurements and non-linear X-ray spectroscopy

The sub-fs (10^{-16} s) time-scale is essential for **electron dynamics** that underpin light-harvesting and primary events in photocatalysis

Current XFELs can surpass peak power by 8 orders of magnitude in isolated attosecond pulses compared to HHG





XFEL requirements: ≥ 2 colours, high rep rate, ~10 eV coherent bandwidth across soft and hard X-rays. Synchronisation with external lasers systems

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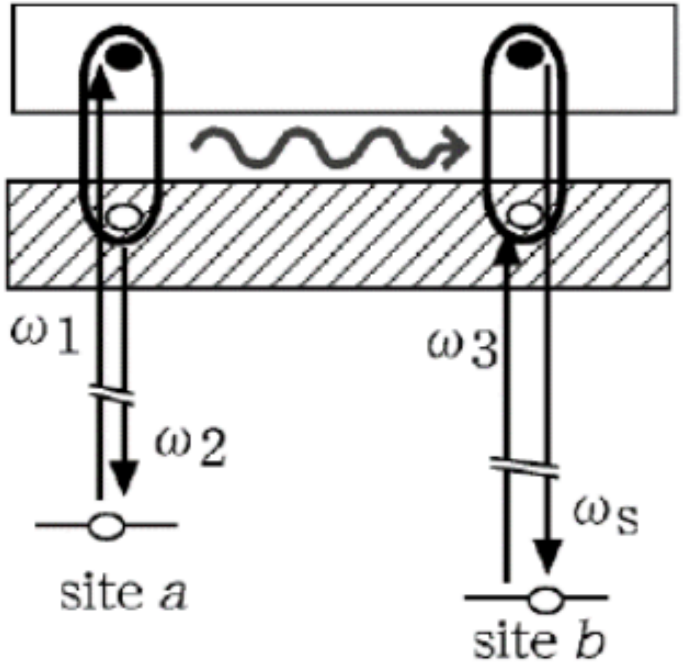
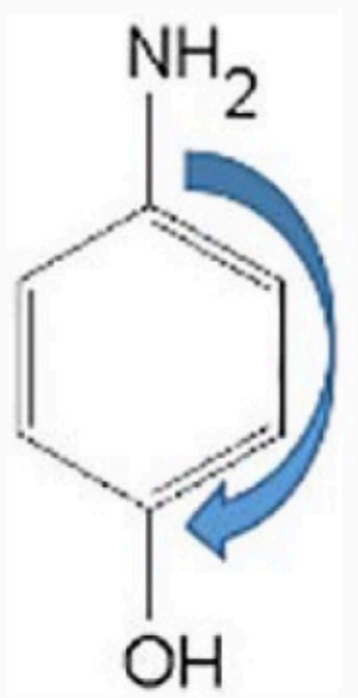
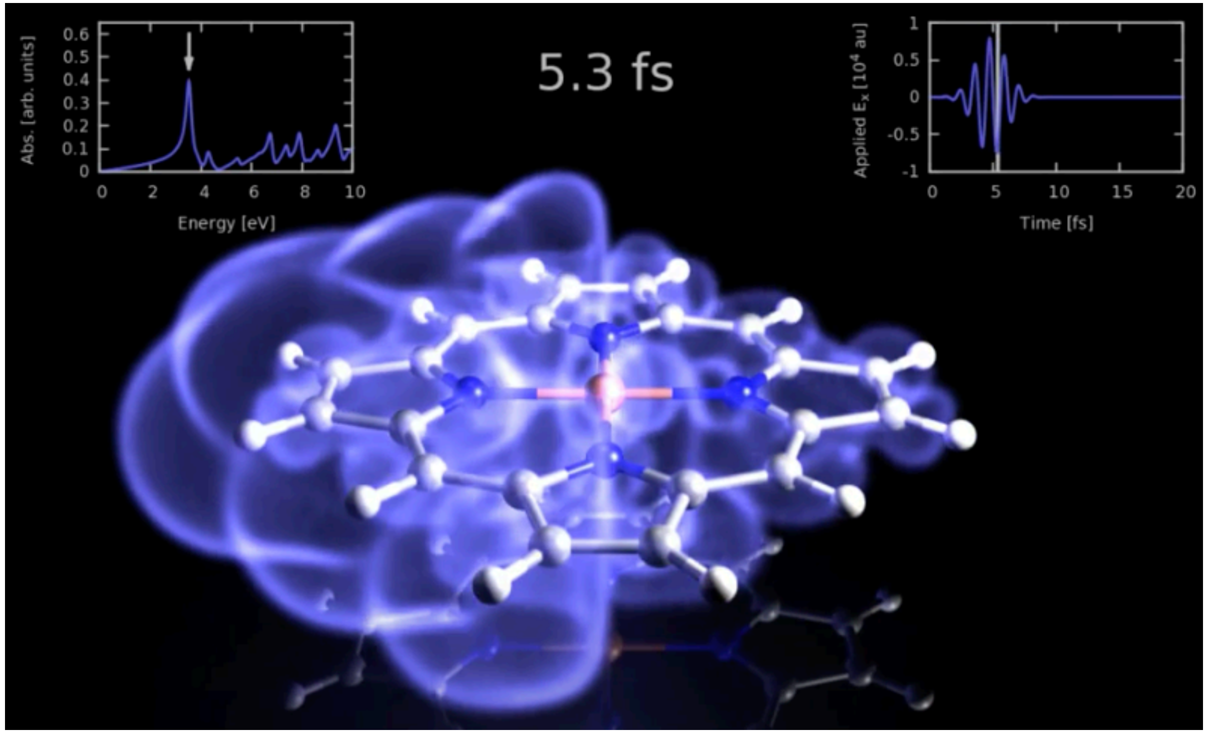
Space time localized measurement of electronic coupling





Charge migration



XFEL requirements: ≥ 2 colours, high rep rate, ~10 eV coherent bandwidth across soft and hard X-rays. Synchronisation with external lasers systems

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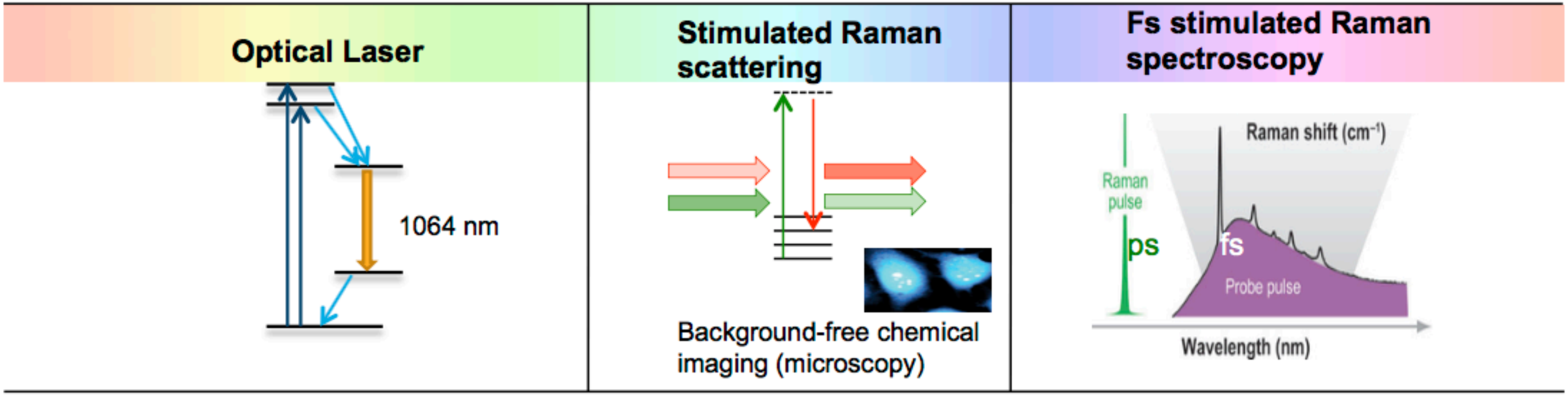
Transfer of non-linear optical spectroscopies to the X-ray spectral domain



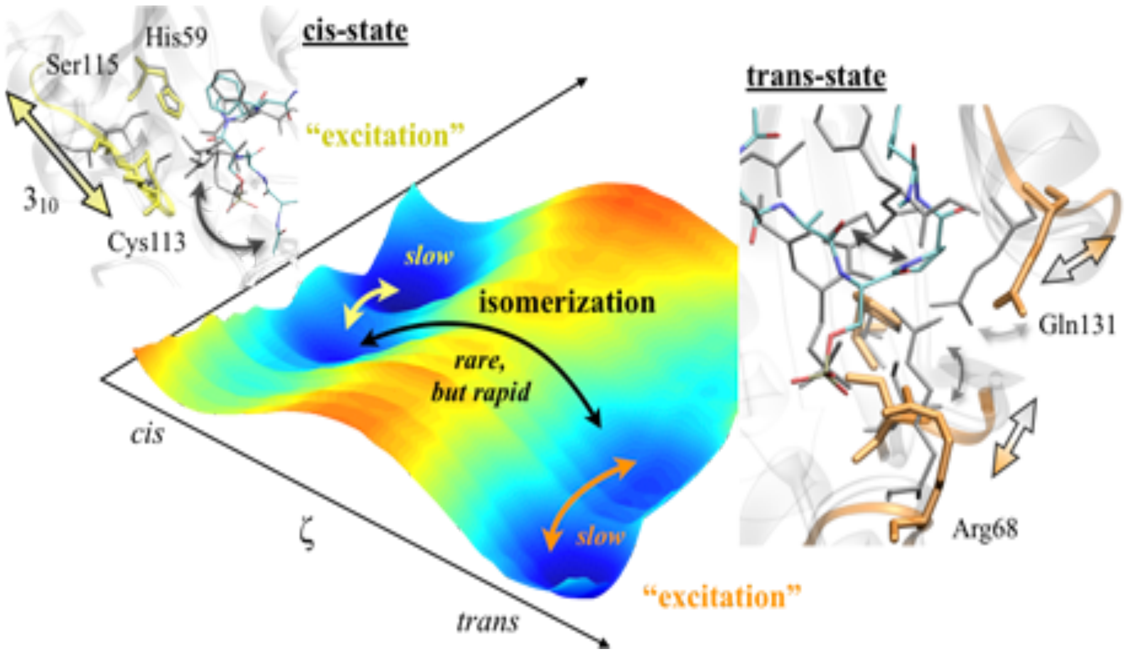
XFEL requirements: ≥ 2 colours, high rep rate, ~10 eV coherent bandwidth across soft and hard X-rays. Synchronisation with external lasers systems

3.4 Capturing conformational dynamics and rare states

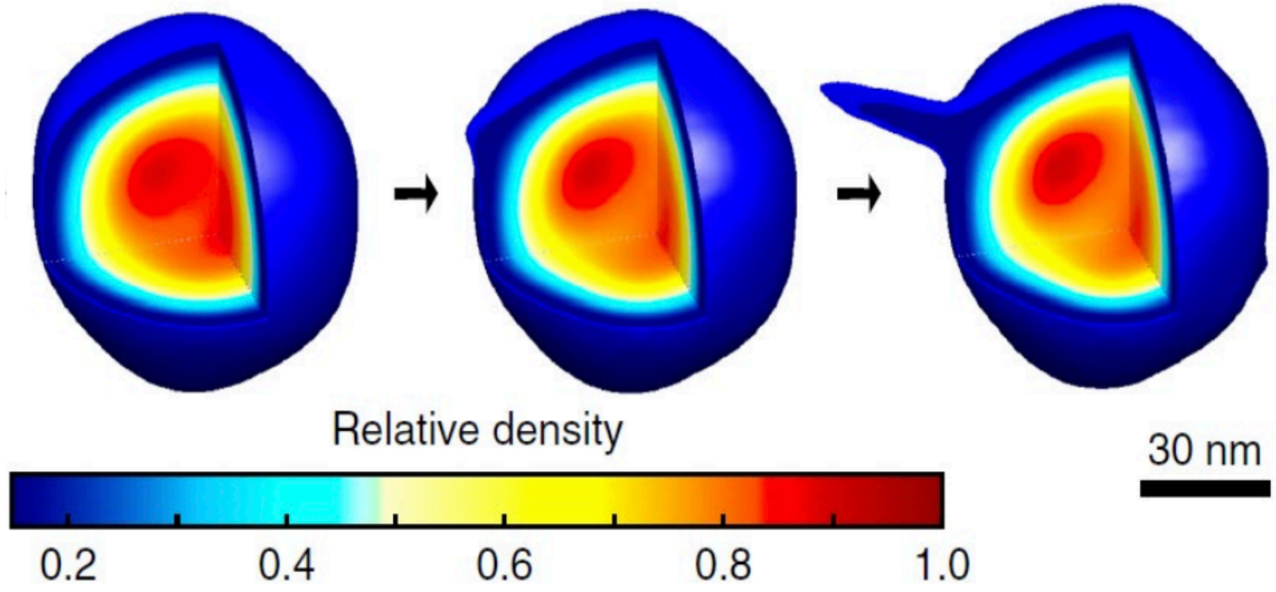
Single-shot structure determination will capture transient intermediates, dynamic and thermodynamic fluctuations, mapping the **full conformational space of macromolecules**

Target function of enzymes, **molecular machines**, **solvent network** dynamics, **phase transitions**, and fluctuations/heterogeneity in **functional materials**

Transitions between thermodynamic states



Rare structures (here tubular structure in virus PR772)



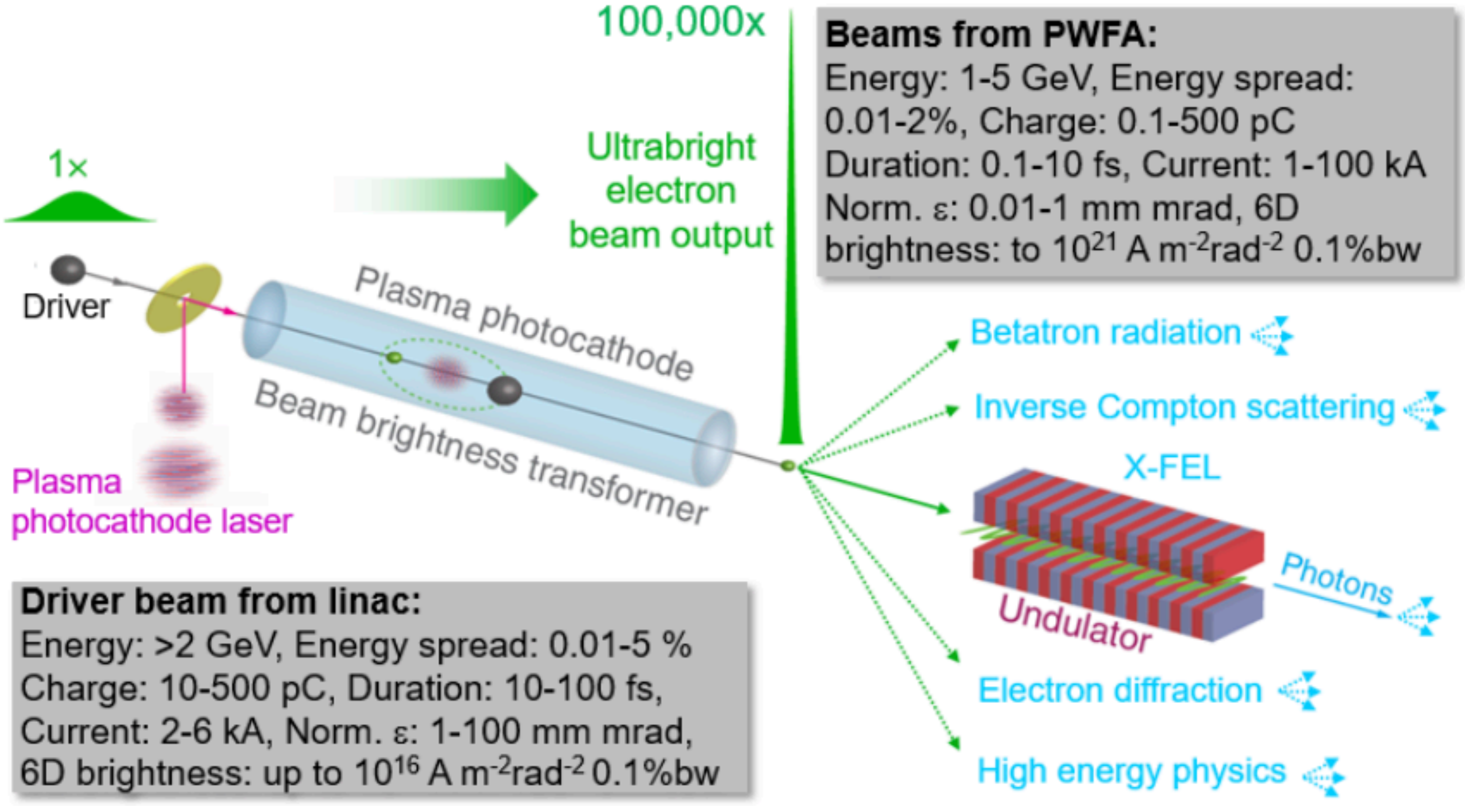
XFEL requirements: high rep rate, seeded at ~1 keV with high flux harmonics up to 3 keV. Hard X-rays with shot-to-shot stability transformative. Sample delivery

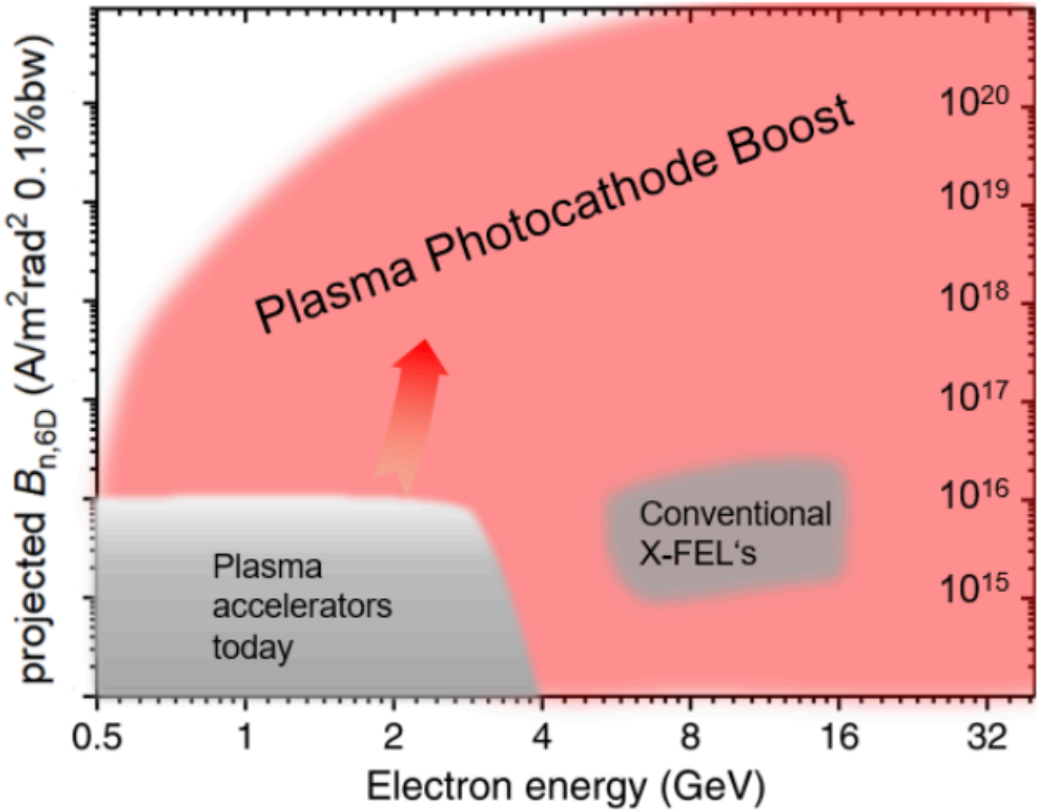
3.6 High brightness relativistic electron beam science

The monoenergetic relativistic electron beams with low emittance power XFELs and can be exploited directly for new research

Plasma wakefield acceleration (PWFA) could boost the future capacity of an UK XFEL and provide a valuable gamma source for nuclear science / industry

Plasma photocathode based PWFA and potential beam brightness boost





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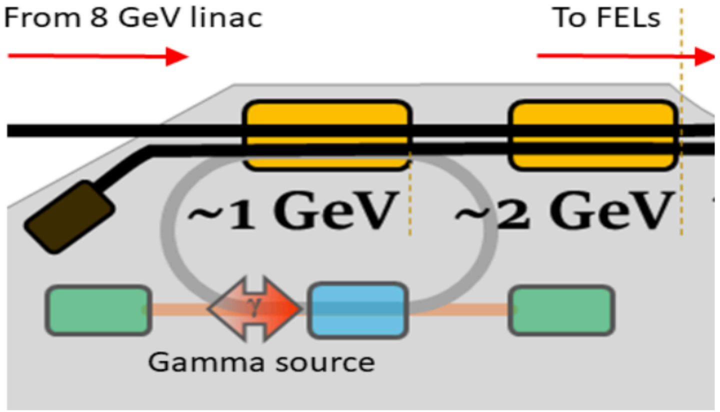
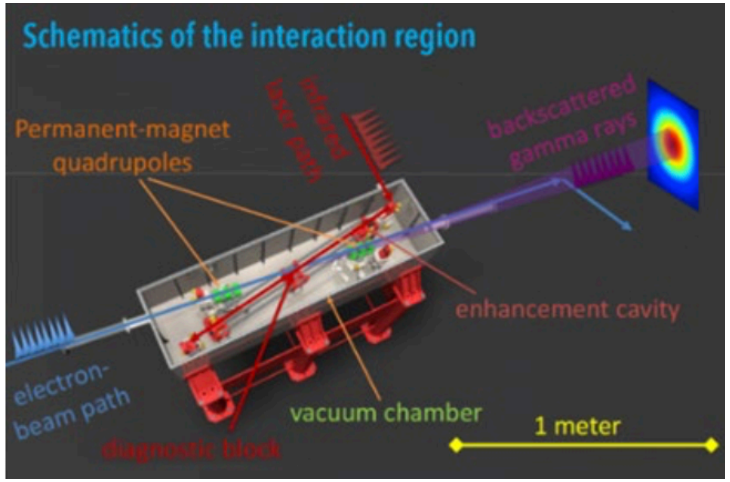
The monoenergetic relativistic electron beams with low emittance power XFELs and can be exploited directly for new research

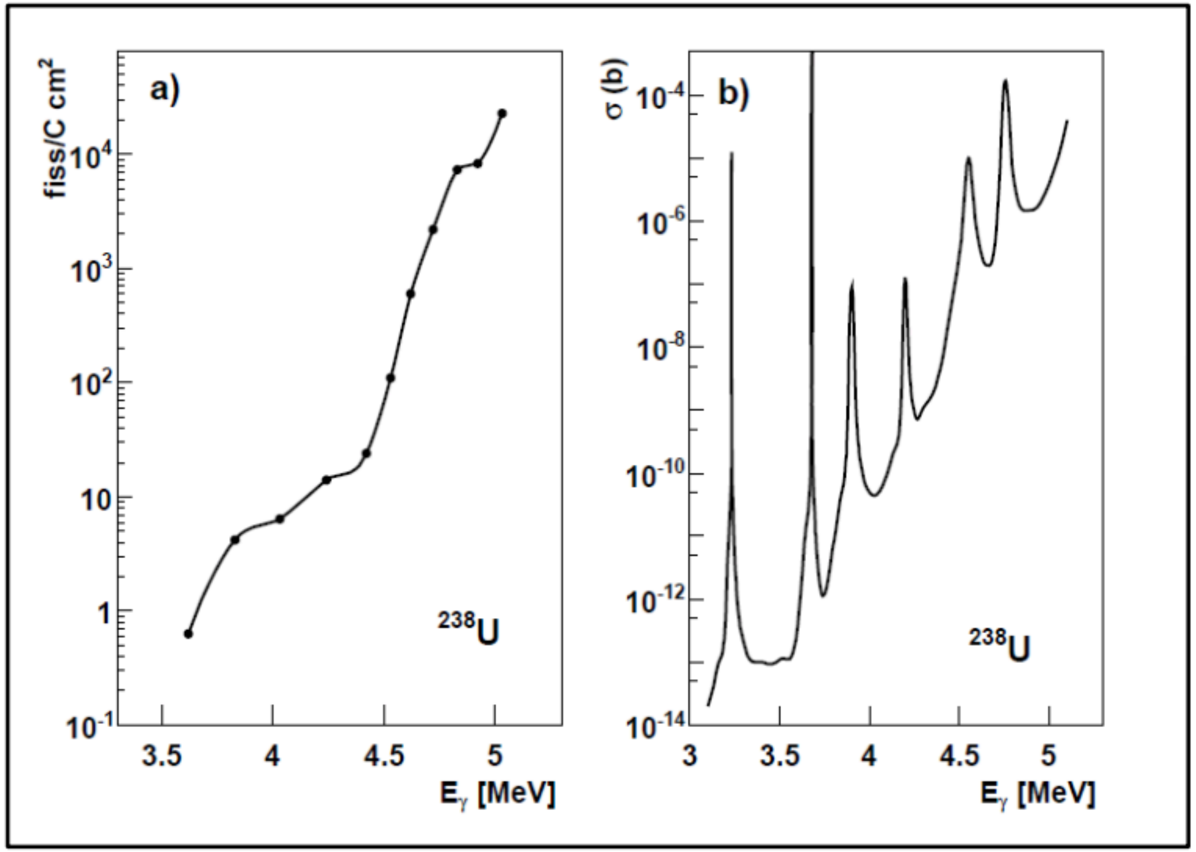
Plasma wakefield acceleration (PWFA) could boost the future capacity of an UK XFEL and provide a valuable gamma source for nuclear science / industry

Inverse Compton scattering Gamma source





Nuclear photonics: Giant Dipole Resonance in ^{238}U



3. Science Opportunities in Physics and X-ray Photonics

Summary

1. Molecular science: temporal, spatial and energetic resolution (see ‘everything’)
2. Thermodynamic processes: no averaging, rare states, and transitions between states
3. Powerful new methods for determining structure
4. New physics (nuclear photonics, nonlinear spectroscopy, scattering phenomena)

3.1 Frontiers in ultrafast chemical physics
3.2 New concepts in scattering
3.3 Attosecond science and non-linear X-ray spectroscopy
3.4 Capturing conformational dynamics and rare thermodynamic states
3.5 Non-linear X-ray physics and physics beyond the Standard Model with XFELs
3.6 High brightness relativistic electron beam science