

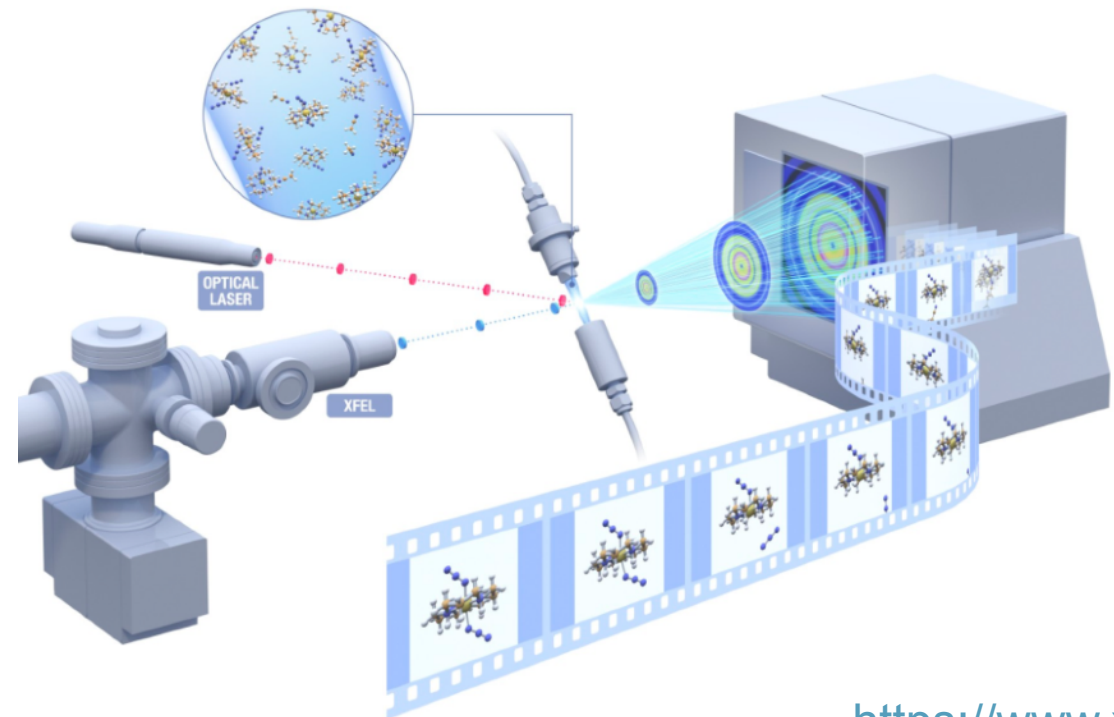
Run 10 @ Femtosecond X-ray Experiments



Chris Milne on behalf of FXE

European XFEL
FXE – Femtosecond X-ray Experiments

European XFEL Town Hall
10.11.2022



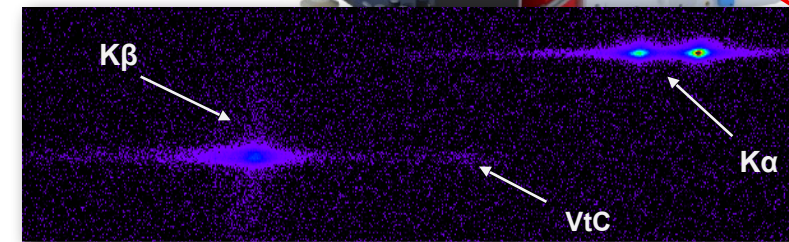
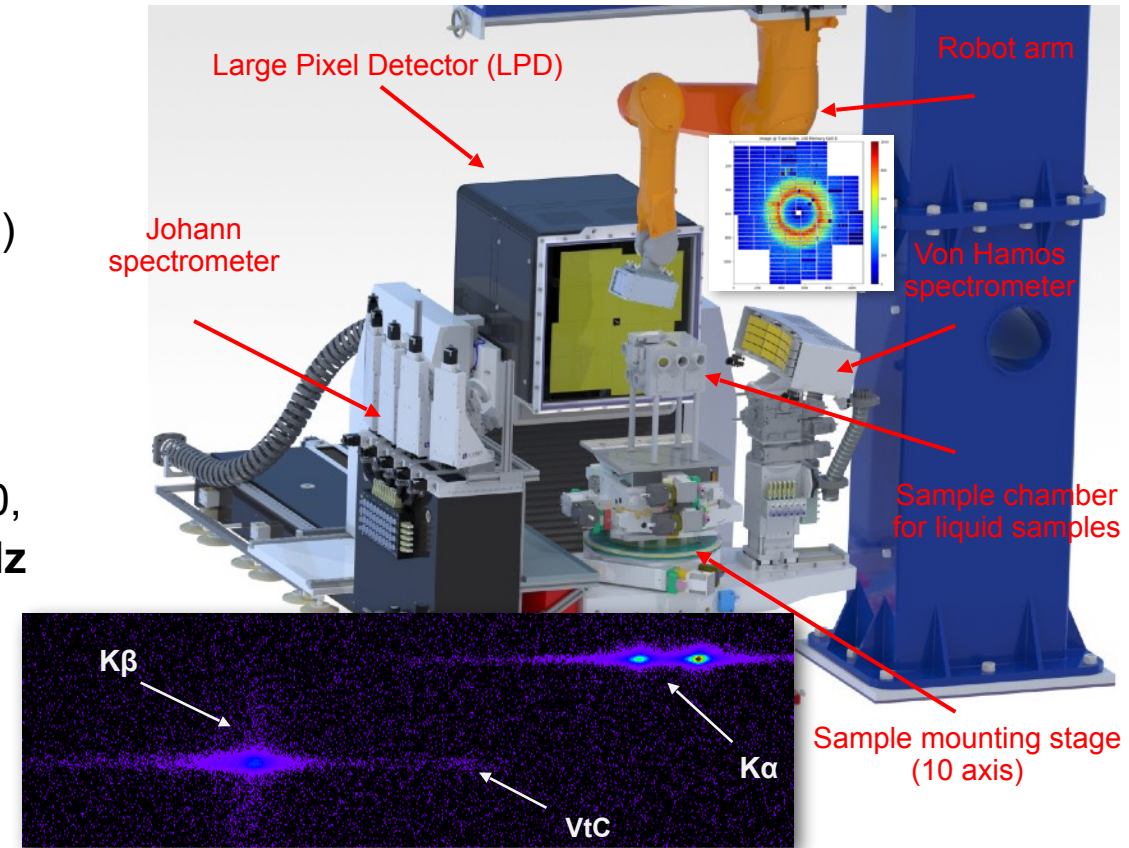
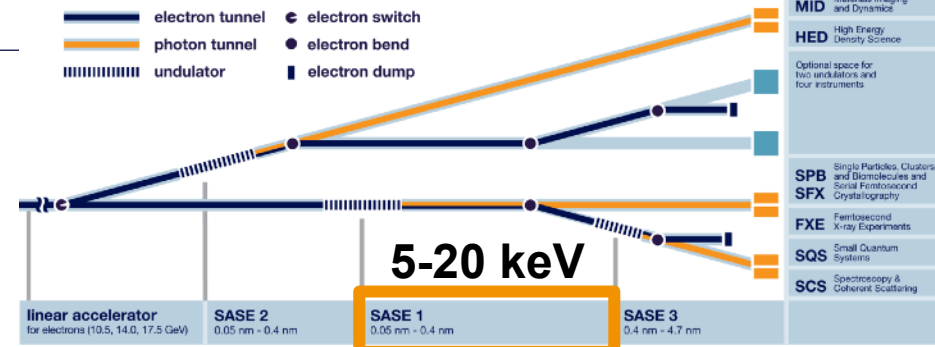
<https://www.xfel.eu/>

christopher.milne@xfel.eu

FXE: Femtosecond Hard X-ray Experiments

A Suite of **Simultaneous X-ray Tools** combined with flexible Laser Excitation Sources

- Single-shot** dispersive resonant and non-resonant **XES**: von Hamos
- Wide(Small)-angle X-ray Scattering**: Large Pixel Detector (LPD) and Jungfrau
- Huber sample motion, goniometer for **single-crystal X-ray diffraction** with Jungfrau detector motion using the robot arm
- Tuneable laser excitation covering 1030, 515 nm (1 ps), 800, 400, 266 nm (15 or 50 fs) and an **OPA** (50 fs, 240 nm to 3 um) with **THz** in development (LiNbO₃, 0.2-0.3 THz)
- X-ray absorption spectroscopy** (5-20 keV): **scanning** (Si(111) 4-bounce mono) and **single-shot** (Spectrum analyzer)
- Scanning** resonant and non-resonant **XES** (RXES): Johann spectrometer



“Scientific instrument Femtosecond X-ray Experiments (FXE): instrumentation and baseline experimental capabilities” A. Galler, et al., *J. Synch. Rad.*, 26, 1432 (2019)
 “Ultrafast X-ray Photochemistry at European XFEL: Capabilities of the Femtosecond X-ray Experiments (FXE) Instrument” D. Khakhulin, et al., *Appl. Sci.*, 10, 995 (2020)

FXE group members

Engineering team



Martin Knoll



Paul Frankenberger



Siti Heder

Postdocs



Laser postdoc



Xinchao Huang



Doriana Vinci

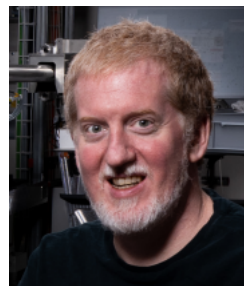


Hao Wang



Diana Bregenholt
Jakobsen

Leading Scientist



Chris Milne

PhD students



Sharmistha Paul Dutta

Administrative Support

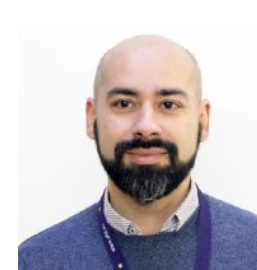


Maria Peter

Scientists



Dmitry Khakhulin



Frederico Alves Lima



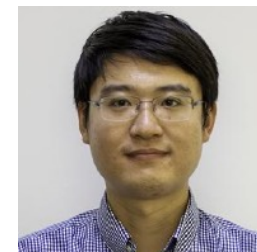
Mykola Biednov



Yohei Uemura



Peter Zalden



Yifeng Jiang



Fernando Ardana Lamas



Instrument
scientist

Detector Scientist



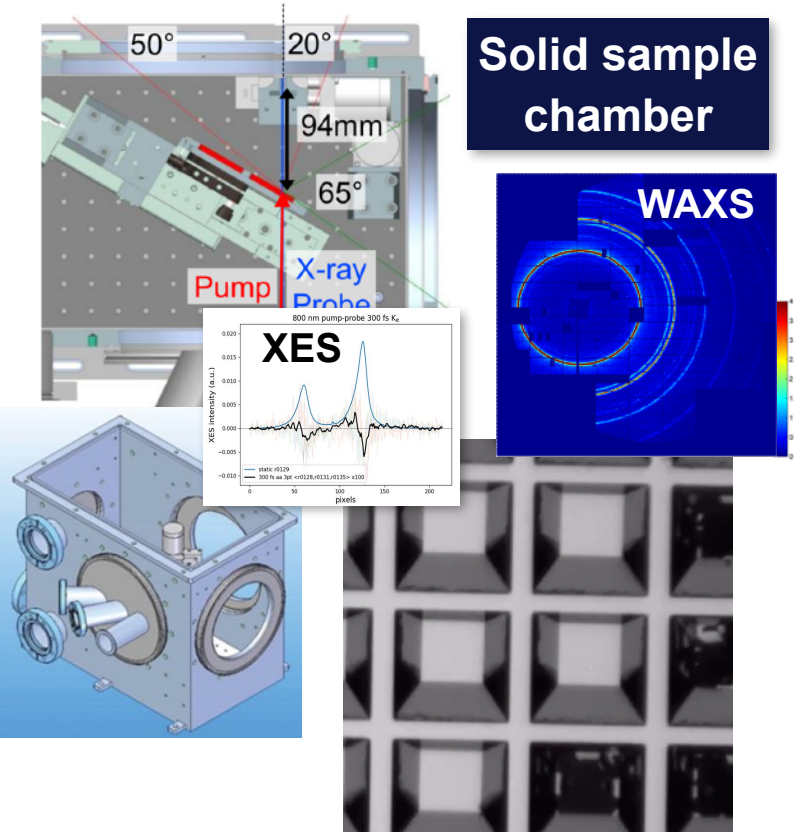
Hazem Yousef

XFEL Collaborators

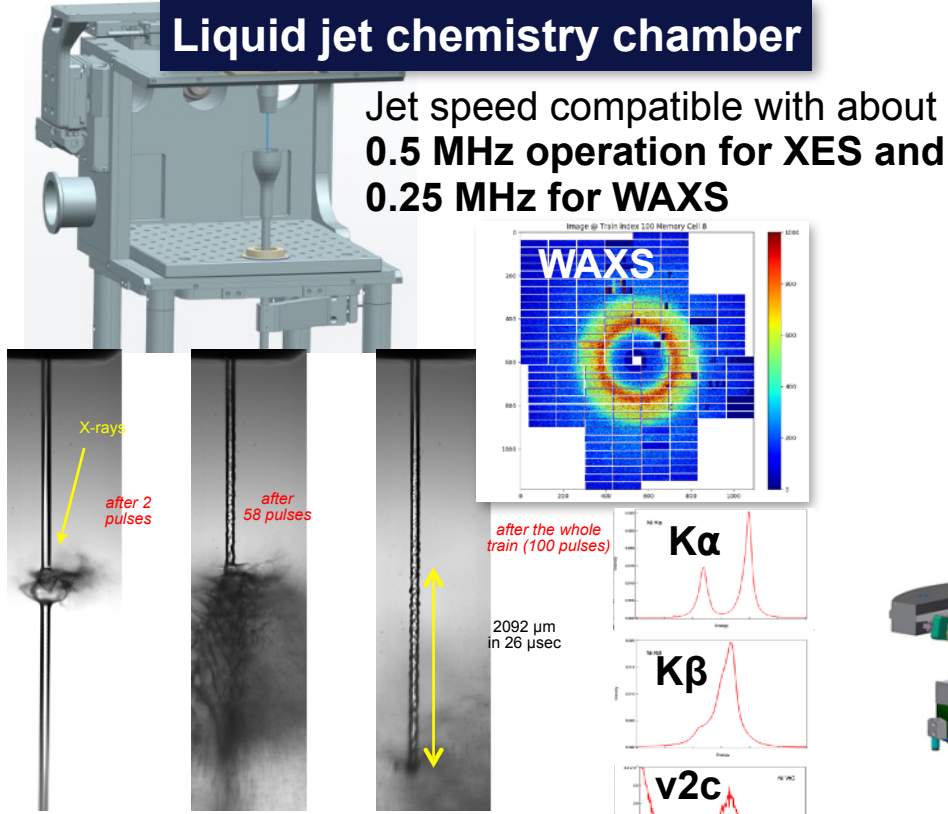
- Wajid Ehsan (Controls)
- Mohammed Vakili, Marco Kloos (SEC)
- Jia Liu, Theophilos Maltezopoulos, Jan Grünert, Wolfgang Freund (XPD)
- Marco Ramilli (Detectors)
- Kai Erik Ballak (EEE)
- Liuba Samoylova (XRO)
- Thomas Kluyver, James Wrigley (DA)

Sample environment: Liquid & Solid state experiments

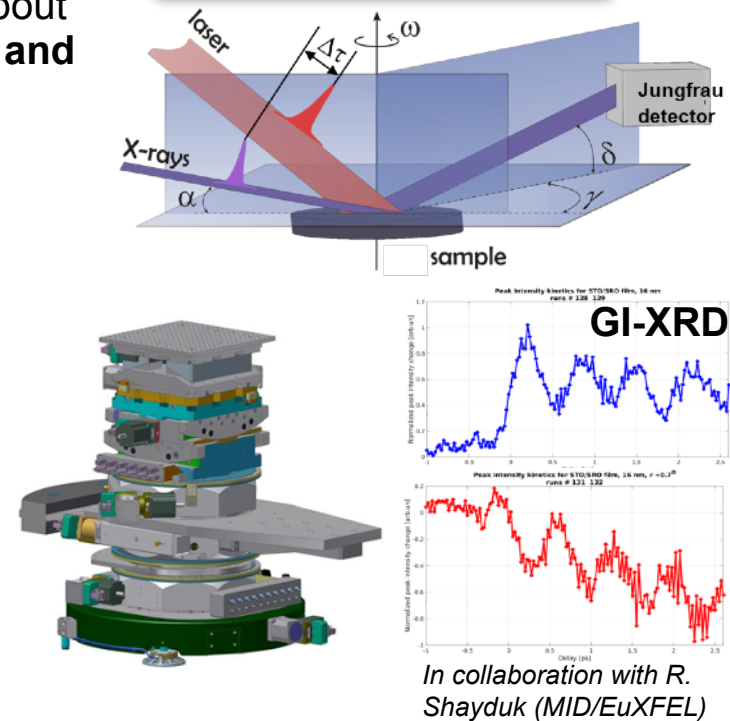
Solid sample chamber



Liquid jet chemistry chamber



Single-crystal grazing-incidence diffraction



- Vacuum environment (1e-5 mbar)
 - X-ray probe in transmission geometry
 - Up to 15k samples accessible per filling/evacuation
 - Parallel X-ray emission and scattering compatible
 - Diffraction up to 8.8 Å⁻¹ at 16.5 keV and 2 θ_{max} = 63°
- courtesy of P. Zalden (peter.zalden@xfel.eu)

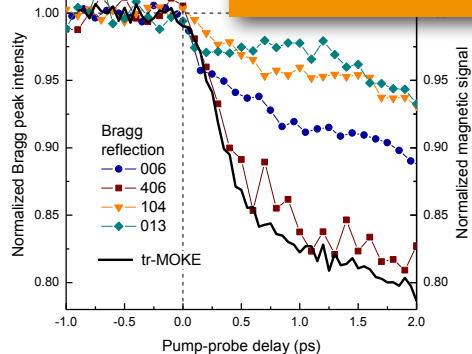
- He environment
 - Open on 3 sides (XES, XAS, WAXS compatible)
 - Parallel UV-Vis flow loop to monitor sample
 - Jet diameter 25-200 μm
 - Bragg angle range 67-83°
 - WAXS maximum Q up to 10 Å⁻¹
- courtesy of F. Lima (frederico.lima@xfel.eu)

- Vertical and horizontal geometry
 - Grazing and symmetric Bragg diffraction
 - Flexible tracking of Bragg peak with detector on Robot arm
 - Cooling and heating of samples supported
 - Compatible with von Hamos XES for vertical sample geometry
- courtesy of D. Khakhulin (dmitry.khakhulin@xfel.eu)

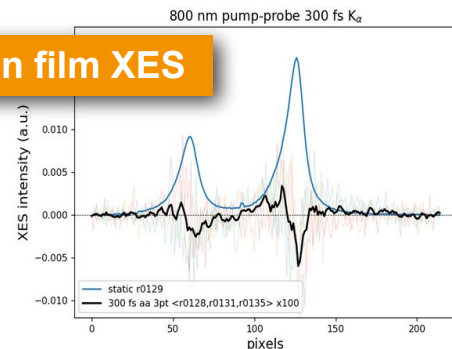
Scientific Scope of FXE: Measuring ultrafast dynamics with hard X-rays

Ultrafast solid-state dynamics

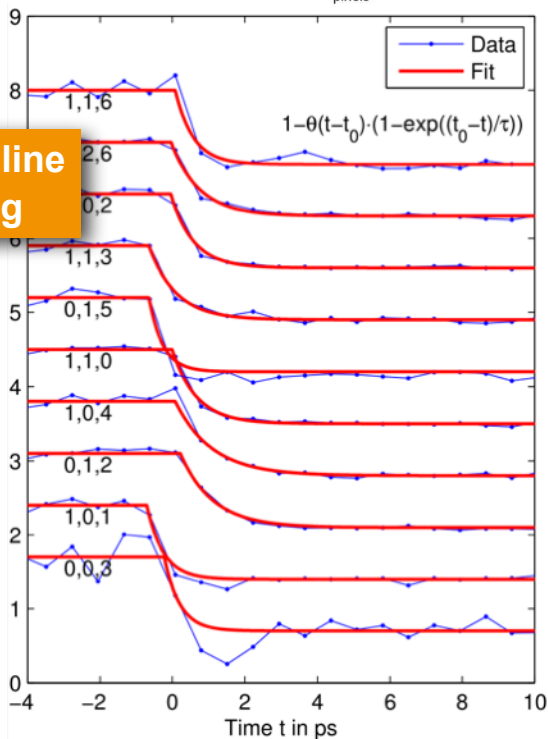
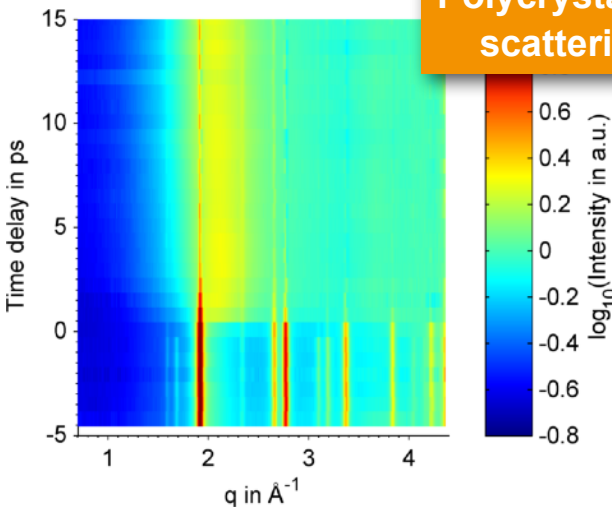
Single-crystal XRD



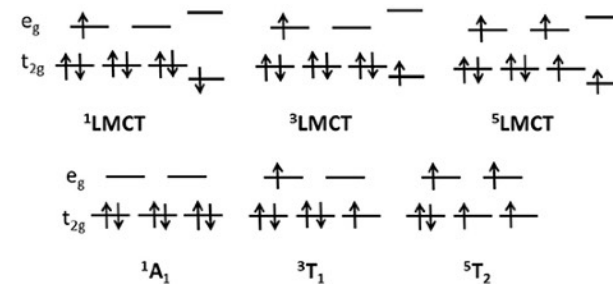
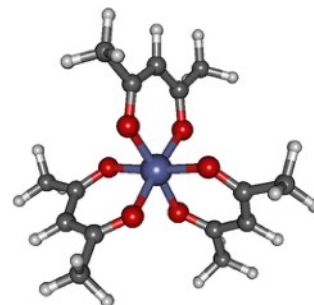
Thin film XES



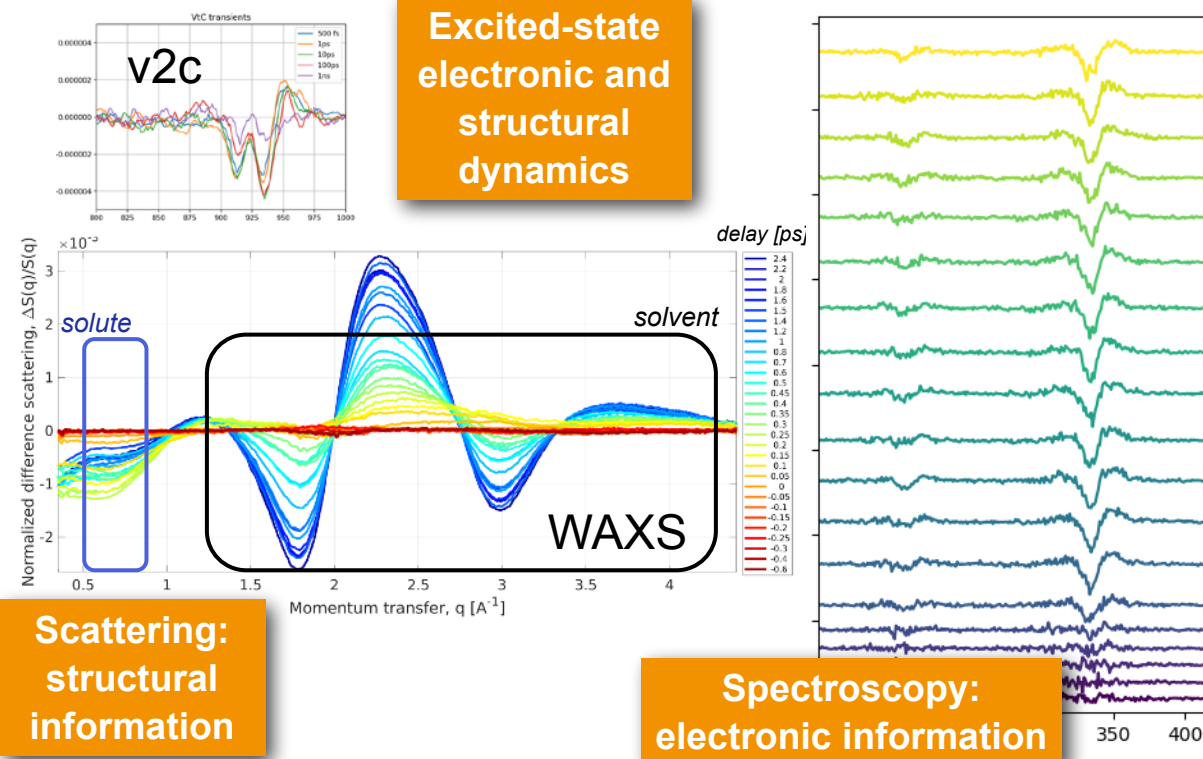
Polycrystalline scattering



Ultrafast (bio)chemical dynamics



Excited-state electronic and structural dynamics



Scattering: structural information

Spectroscopy: electronic information

FXE new developments: Ultrafast serial crystallography



3073: PI James N Hohman, University of Connecticut, United States

Data Analysis: Aaron Brewster, Berkeley Lab

MOCHAs: metal organic chalcogenide assemblies

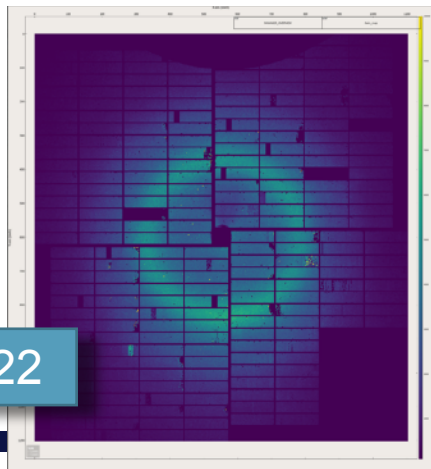
June 2022

Schriber, E.A. et al. Chemical crystallography by serial femtosecond X-ray diffraction. *Nature* **601**, 360 (2022)

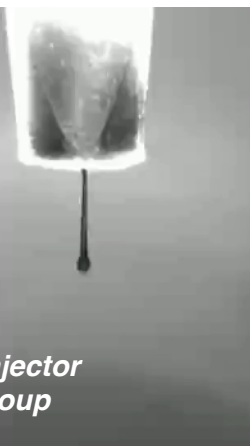
Joint with SEC, SPB-SFX and DA

Imperial College London 2808: PI Jasper van Thor, Imperial College London

Two-colour laser excitation on a photoactive protein sample



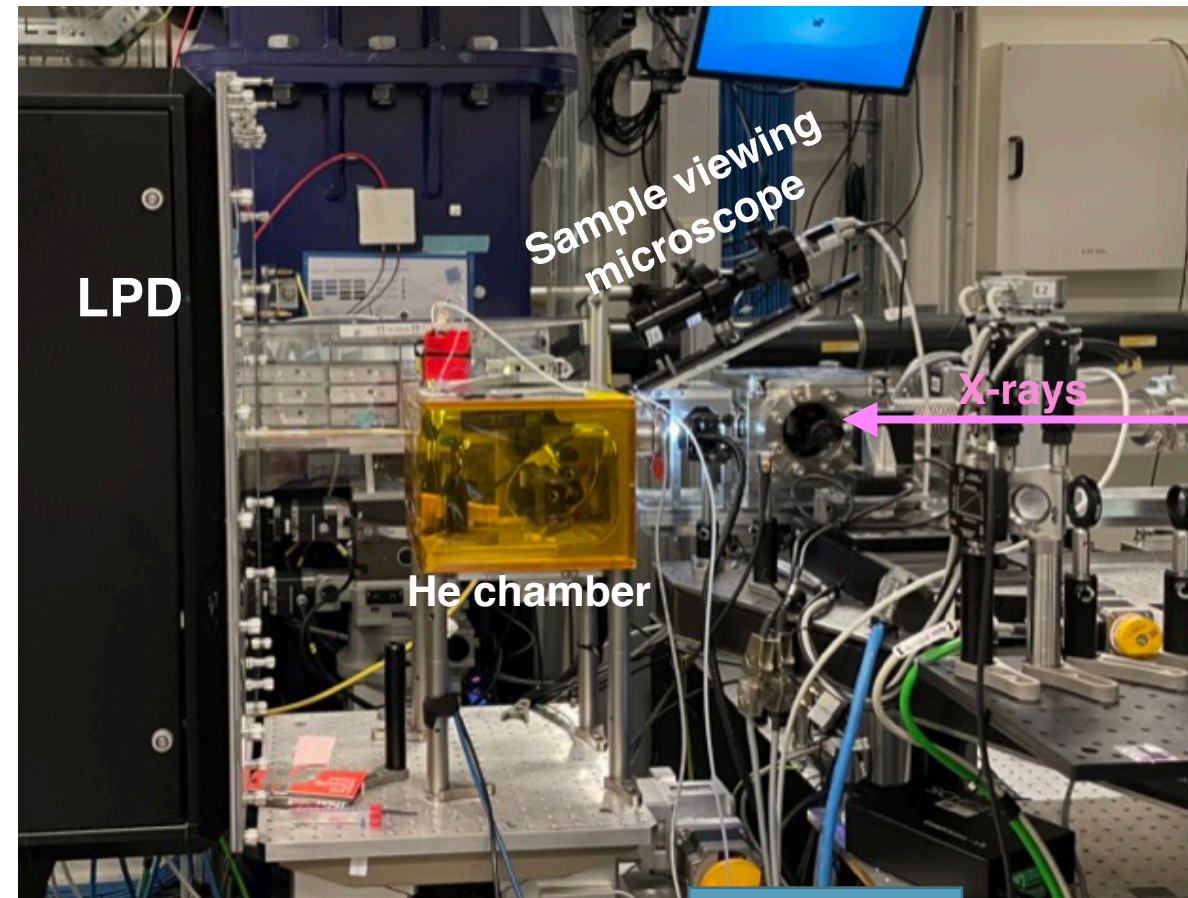
8 pulses/burst (80 Hz)



Droplet-on-demand injector supplied by user group

Nov 2022

Local Contact: Dmitry Khakhulin



3409: PI Yifeng Jiang, European XFEL

June 2023

Strongly-correlated materials

- Small unit cell
- Fixed orientation
- Few diffraction peaks (modeling required)

Molecular crystals

- Medium unit cell
- Rapid-scanning rotation method

Protein crystals

- Large unit cell
- Single-shot random orientation (SFX)
- Many diffraction peaks
- 3D charge density

Call 10: Contact us with any questions or for more details

<https://www.xfel.eu/facility/instruments/fxe/>



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