

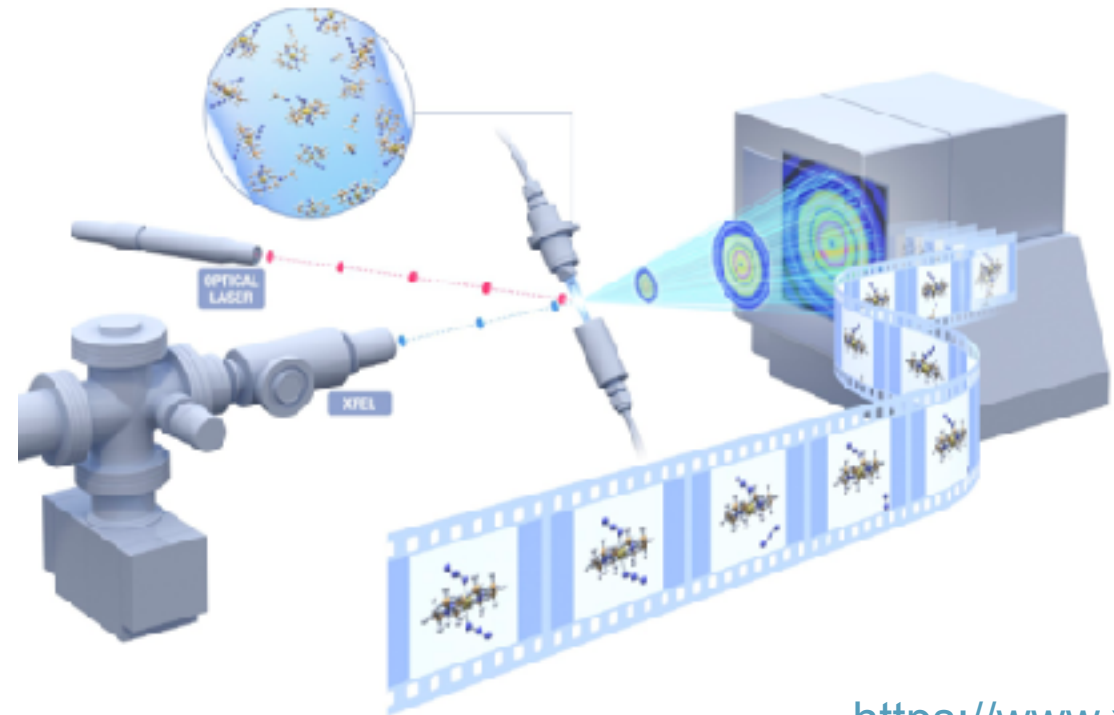
# Run 8 @ Femtosecond X-ray Experiments



Chris Milne on behalf of FXE

European XFEL  
FXE – Femtosecond X-ray Experiments

European XFEL Town Hall  
3.11.2021



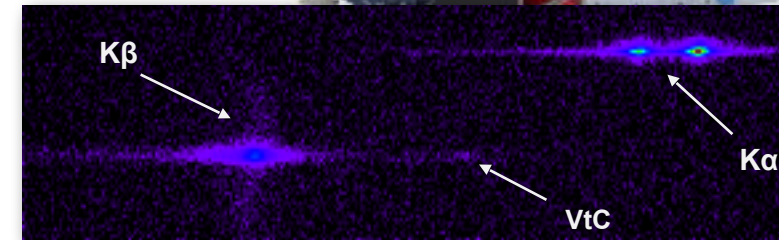
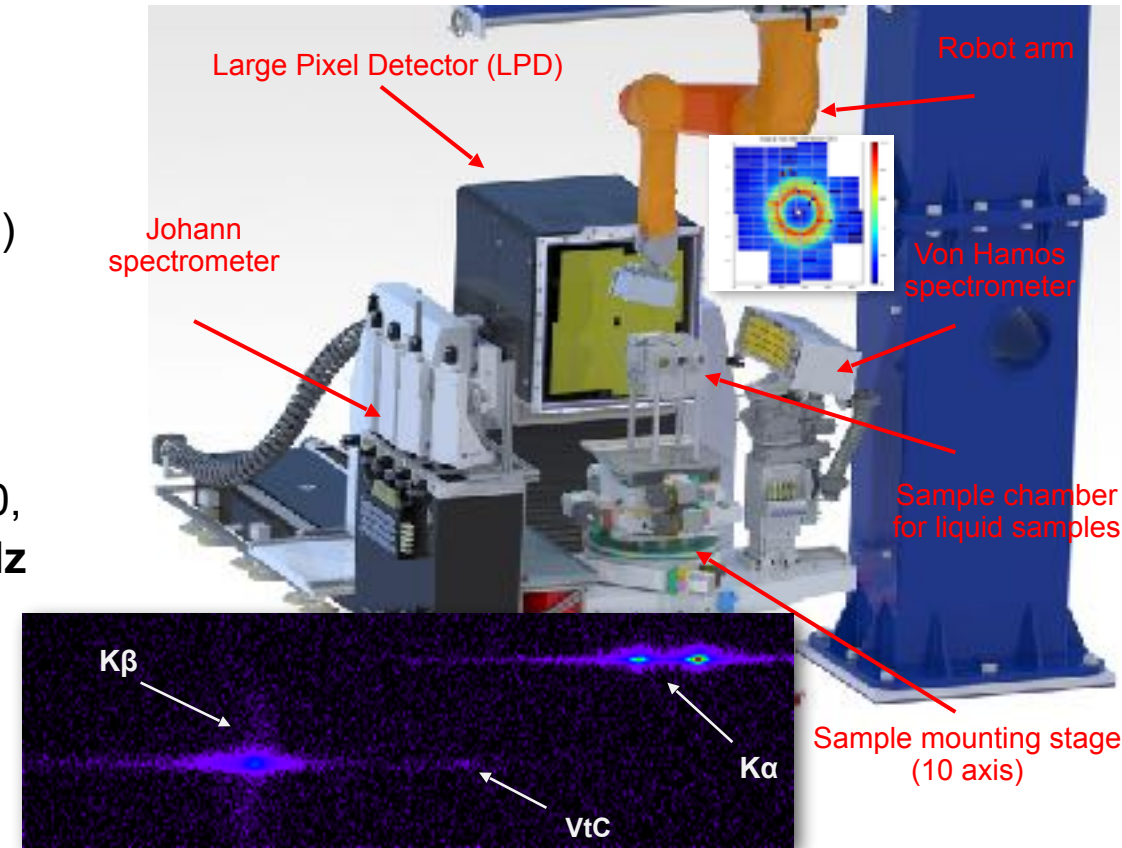
<https://www.xfel.eu/>

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# 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 (LiNbO<sub>3</sub>, 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*

## Postdocs



*Vandana Tiwari*



*Xinchao Huang*



*Hao Wang*



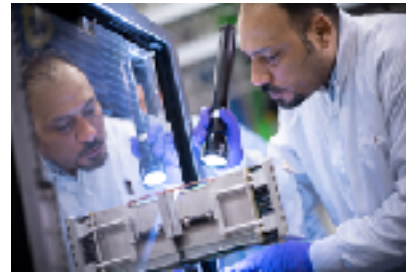
*Diana Bregenholt  
Jakobsen*

## Leading Scientist



*Chris Milne*

## Detector Scientist



*Hazem Yousef*

## PhD students



*Tae Kyu Choi  
Graduated 10.2021*

## Scientists



*Dmitry Khakhulin*



*Frederico Alves Lima*



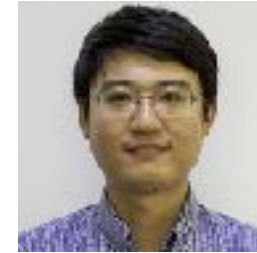
*Mykola Biednov*



*Yohei Uemura*



*Peter Zalden*



*Yifeng Jiang*



*Fernando Ardana Lamas*

## XFEL Collaborators

David Doblas Jimenez (DA)

Wajid Ehsan (Controls)

Mohammed Vakili (SEC)

Jia Liu (XPD)

Theophilos Maltezopoulos (XPD)

Marco Ramilli (Detectors)

Kai Erik Ballak (EEE)



*Florian Otte*

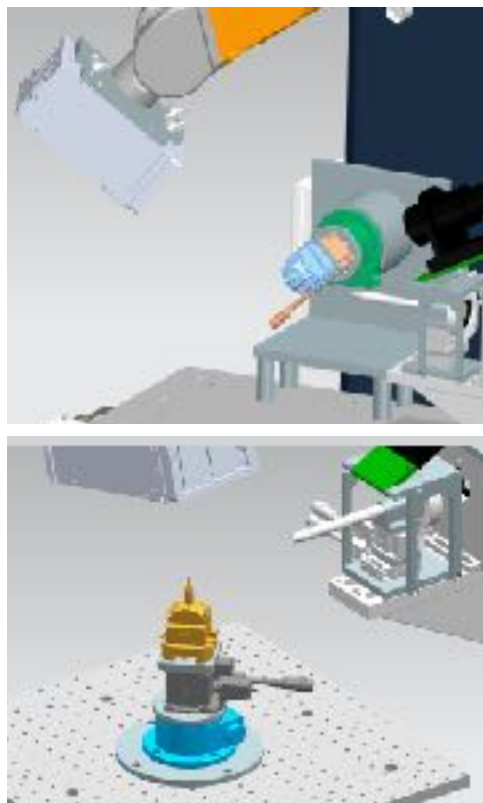


*Sharmistha Paul Dutta*

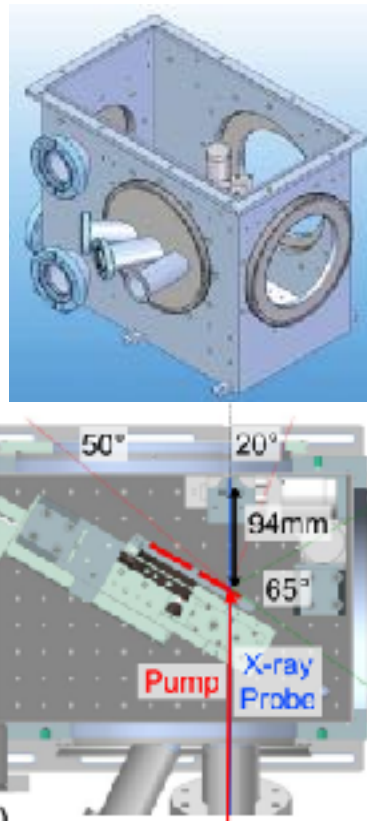


# Standard sample environment and geometries: Chemistry & Solid state experiments

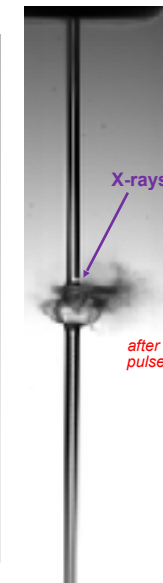
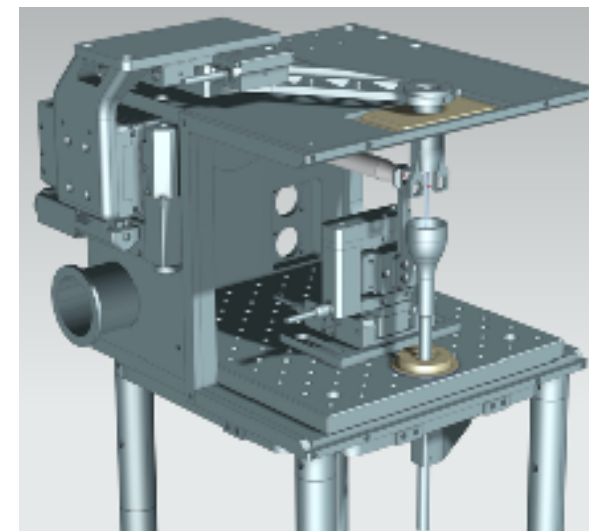
*Fixed target 10 Hz diffraction experiment (single pulse per train)*



*Destructive single-shot diffraction experiment (<10 Hz)*



*Jet speed compatible with about 0.5 MHz operation*



- 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

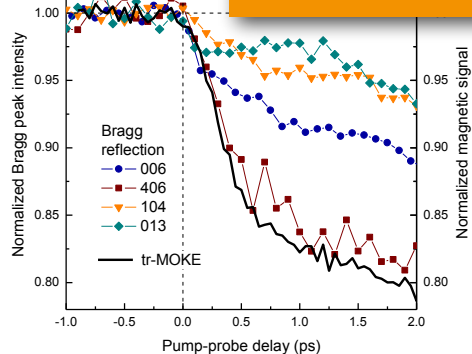
- Vacuum environment (1e-5 mbar)
- X-ray probe in transmission geometry
- Parallel X-ray emission and scattering compatible
- Diffraction up to  $8.8 \text{ \AA}^{-1}$  at 16.5 keV and  $2\theta_{\text{max}}=63^\circ$

- He environment
- Open on 3 sides (XES, XAS, WAXS compatible)
- Parallel UV-Vis flow loop to monitor sample
- Jet diameter 25-200  $\mu\text{m}$
- XES Bragg angle range  $67-83^\circ$
- WAXS maximum Q up to  $10 \text{ \AA}^{-1}$

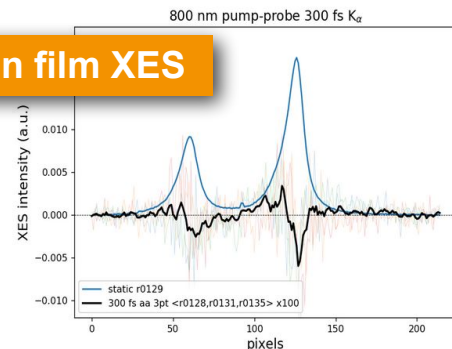
# Scientific Scope of FFE: Measuring ultrafast dynamics with hard X-rays

## Ultrafast solid-state dynamics

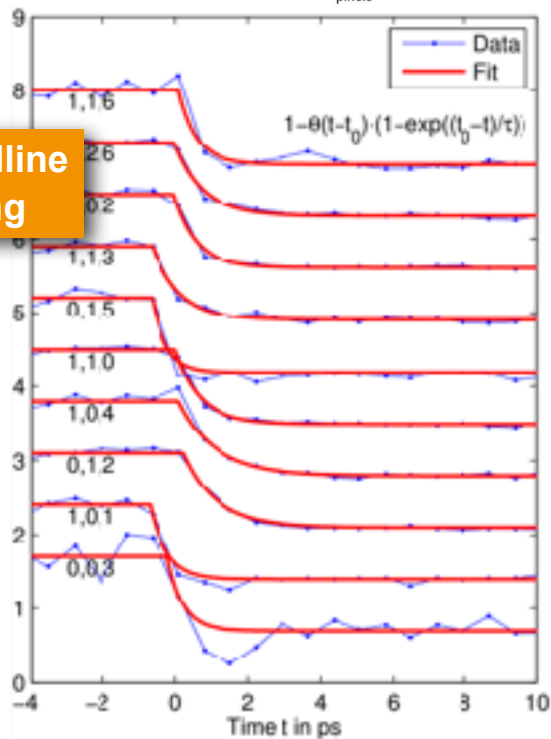
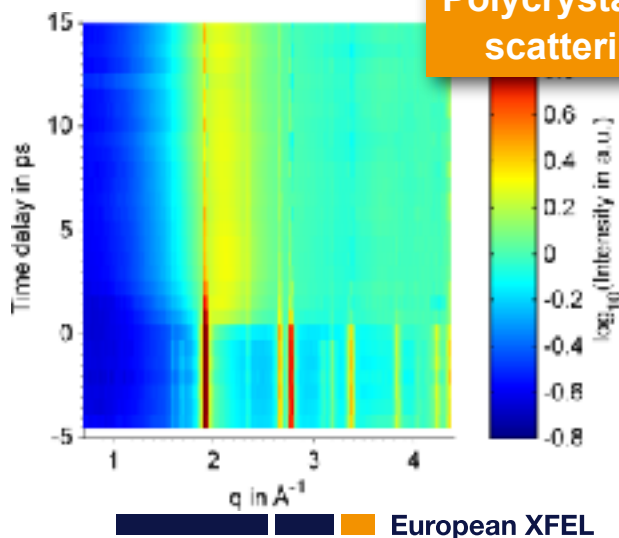
### Single-crystal XRD



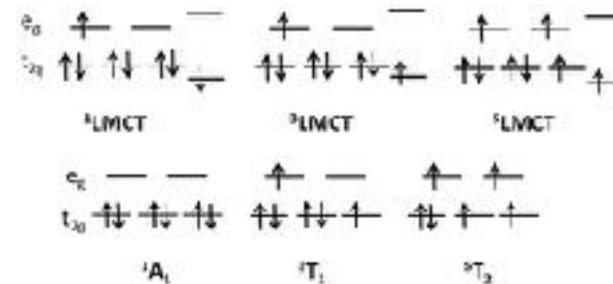
### Thin film XES



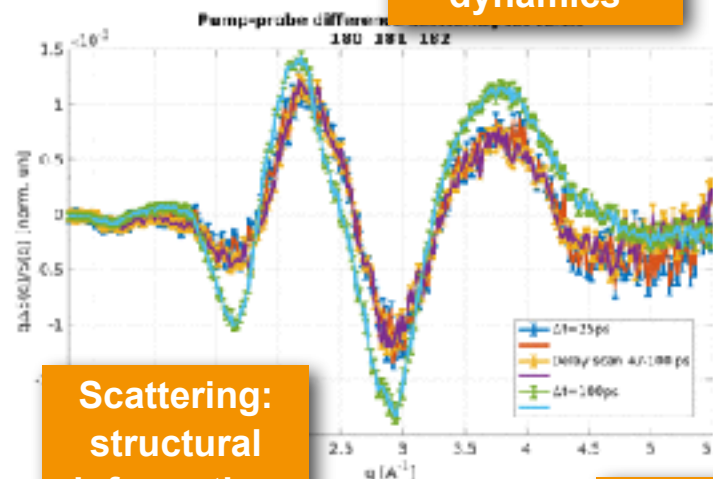
### Polycrystalline scattering



## Ultrafast (bio)chemical dynamics

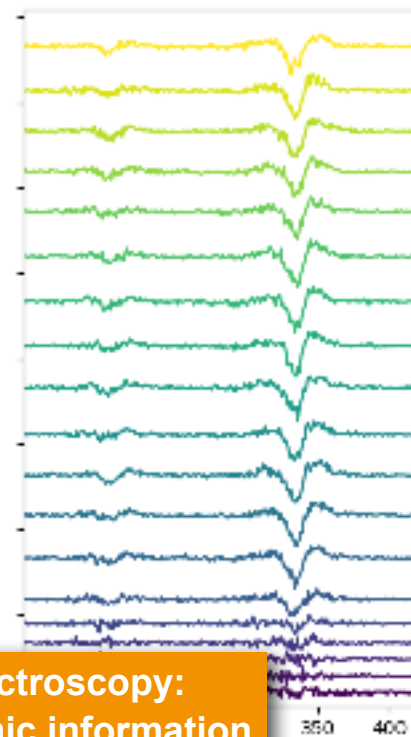


### Excited-state electronic and structural dynamics



### Scattering: structural information

### Spectroscopy: electronic information



# Run 8: Liquid chemistry chamber standard setup

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## Pump laser parameters

**Wavelength range**

490 nm - 800 nm (TOPAS OPA)  
800/400/267 nm (Harmonics)

**Pulse duration**

< 60 fs

**Typical pulse energies @ 1.1 MHz repetition rate**

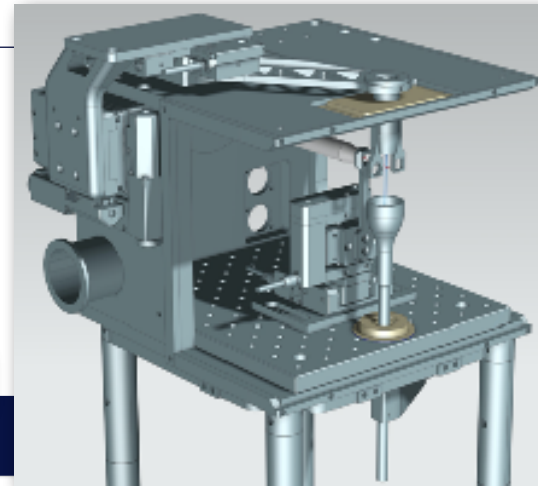
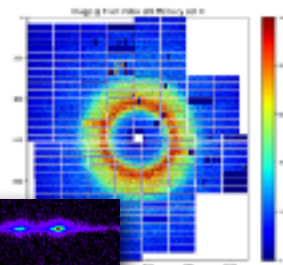
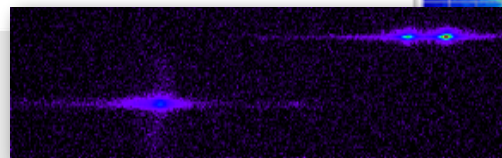
> 10 uJ for TOPAS and xHG at 267 nm, 40 uJ and 120 uJ at 400 nm and 800 nm, correspondingly

**Focus size**

100 um

**Polarisation**

Linear vertical or horizontal



## Sample geometry details

**Liquid jet diameter**

100 um

**Sample volume**

>25 mL

**Sample Pump**

HPLC

**Environment**

He atmosphere

**Sample-Scattering detector distance**

> 10 cm

**Parallel X-ray emission measurements**

Cr K $\alpha$ /K $\beta$ /VtC  
Fe K $\alpha$ /K $\beta$   
Co K $\alpha$ /K $\beta$   
Fe K $\alpha$  and Co K $\alpha$   
Ni K $\alpha$ /K $\beta$ /VtC  
Others possible, please contact FXE for details

**Von Hamos Bragg angle range**

Vertical 70 – 83°

**Wide-angle scattering range**

0.5 – 7 Å<sup>-1</sup> (photon energy dependent)

**Experimental geometry**

Quasi-collinear with Incidence angle between the laser and X-ray beams: 15 degrees or 3 degrees, in horizontal plane.

## X-ray parameters

**Incident X-ray energies**

7, 9.3 or 12.5 keV

**Repetition rate**

100-500 kHz

**Typical pulse energies**

> 2 mJ

**Focus size**

10 um

**Polarisation**

Linear horizontal