

# 11<sup>th</sup> call @ Femtosecond X-ray Experiments



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

Peter Zalden on behalf of FXE

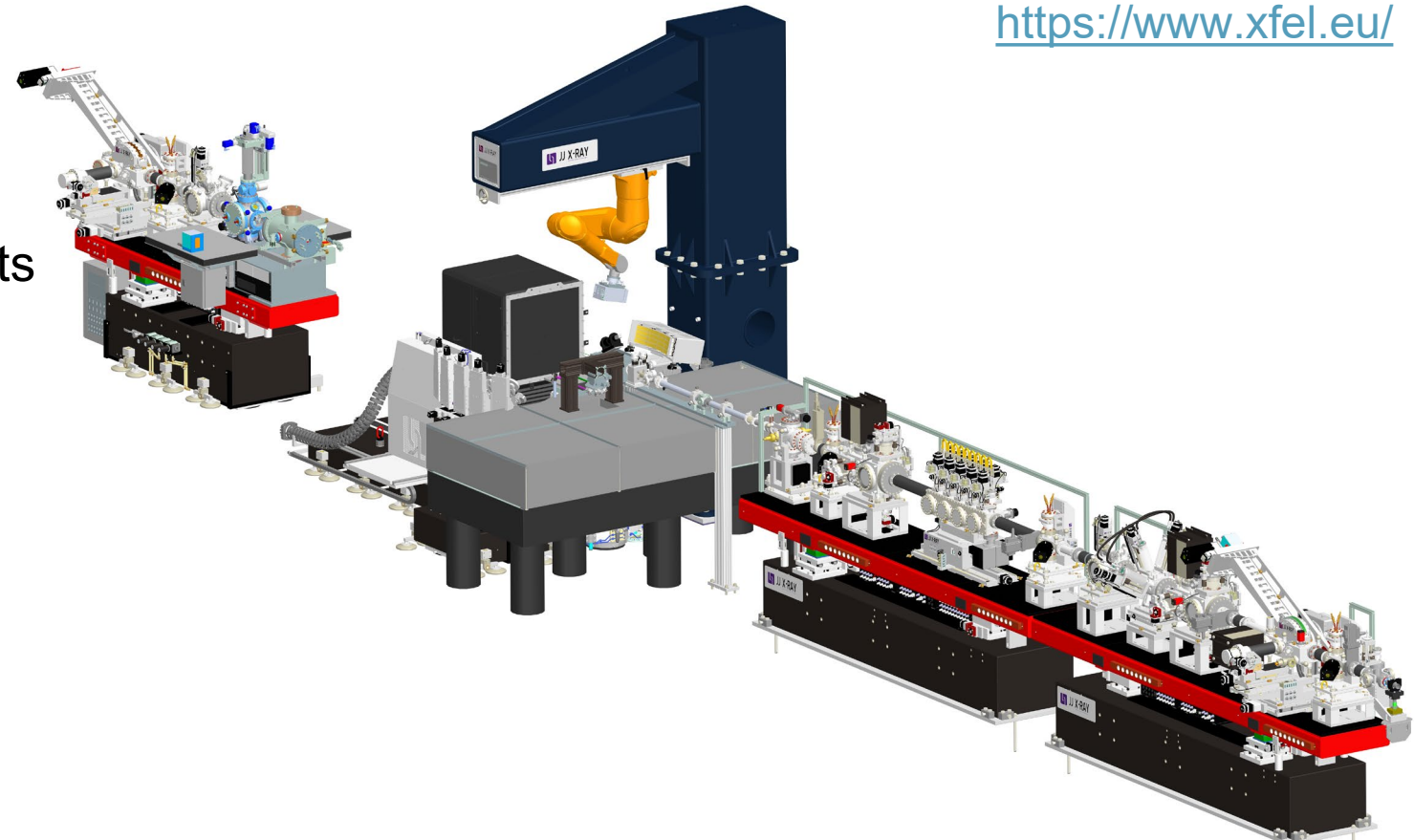
European XFEL

FXE – Femtosecond X-ray Experiments

Last town hall meeting: 12.5.2022

Agenda 20.4.2023

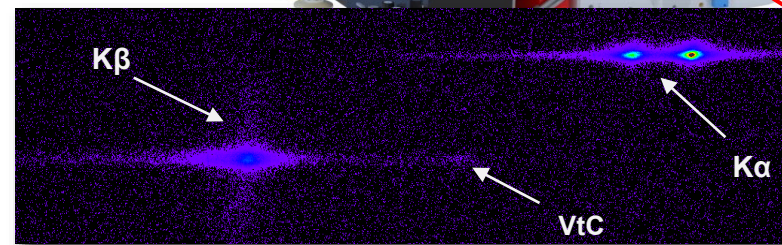
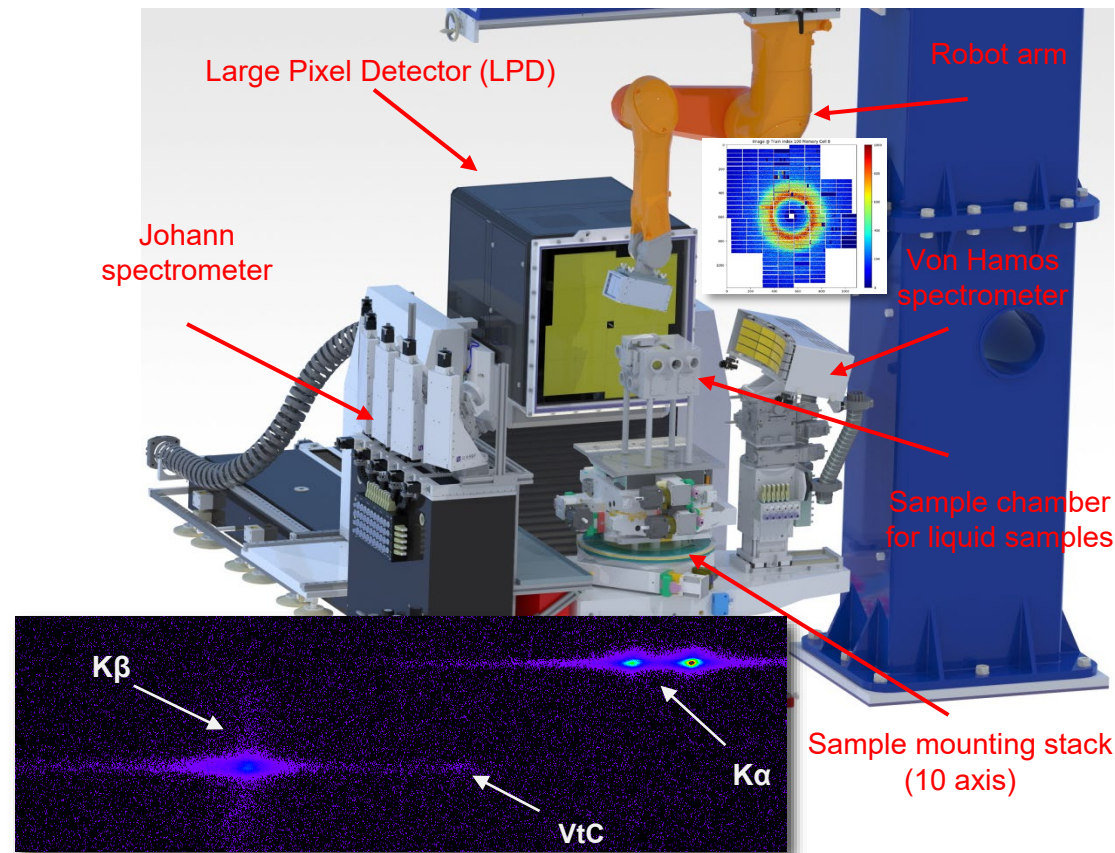
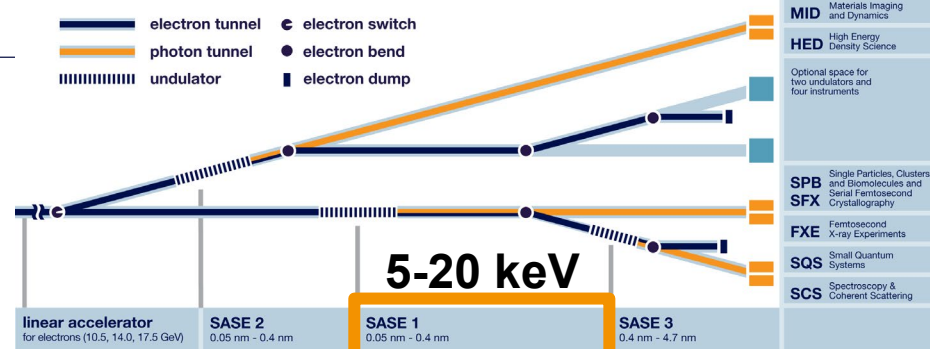
1. Overview FXE
2. News since last town hall
3. Questions/discussion



# 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
- Sample motion stack, goniometer for **single-crystal X-ray diffraction** with Jungfrau detector motion using the robot arm
- Tuneable laser excitation covering 1030, 515 nm, 257 nm (1 ps), 800, 400, 266 nm (15 or 50 fs) and an **OPA** (50 fs, 240 nm to 3 μm) with **THz** in development (LiNbO<sub>3</sub>, 0.2-0.3 THz)
- **X-ray absorption spectroscopy** (5-20 keV): **scanning** (Si111 2-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

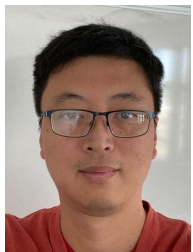


Paul Frankenberger



Siti Heder

## Postdocs



Han Xu



Xinchao Huang



Doriana Vinci



Hao Wang



Diana Bregenholt  
Jakobsen



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## Leading Scientist



Chris Milne

## PhD students



Sharmistha Paul Dutta

## Administrative Support



Maria Peter

## Scientists



Dmitry Khakhulin



Frederico Alves Lima



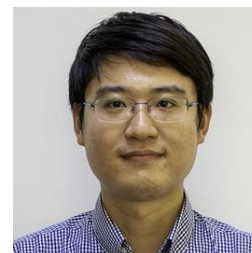
Mykola Biednov



Yohei Uemura



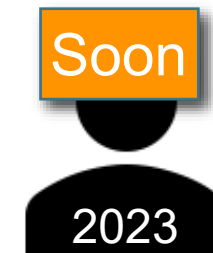
Peter Zalden



Yifeng Jiang



Fernando Ardana Lamas



Soon

2023

Instrument  
scientist

## Detector Scientist



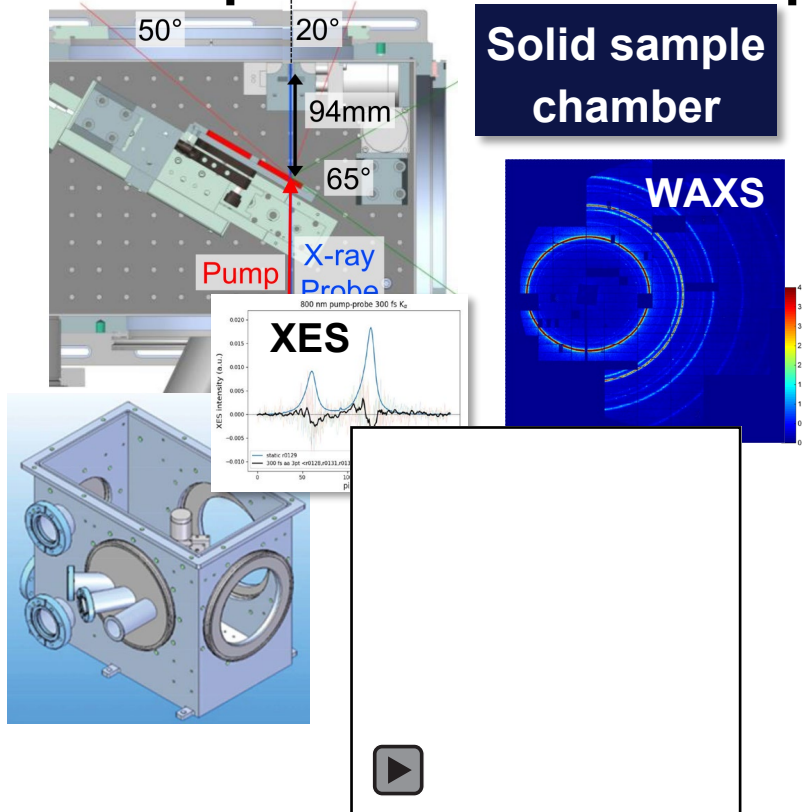
Hazem Yousef

## Recent alumni

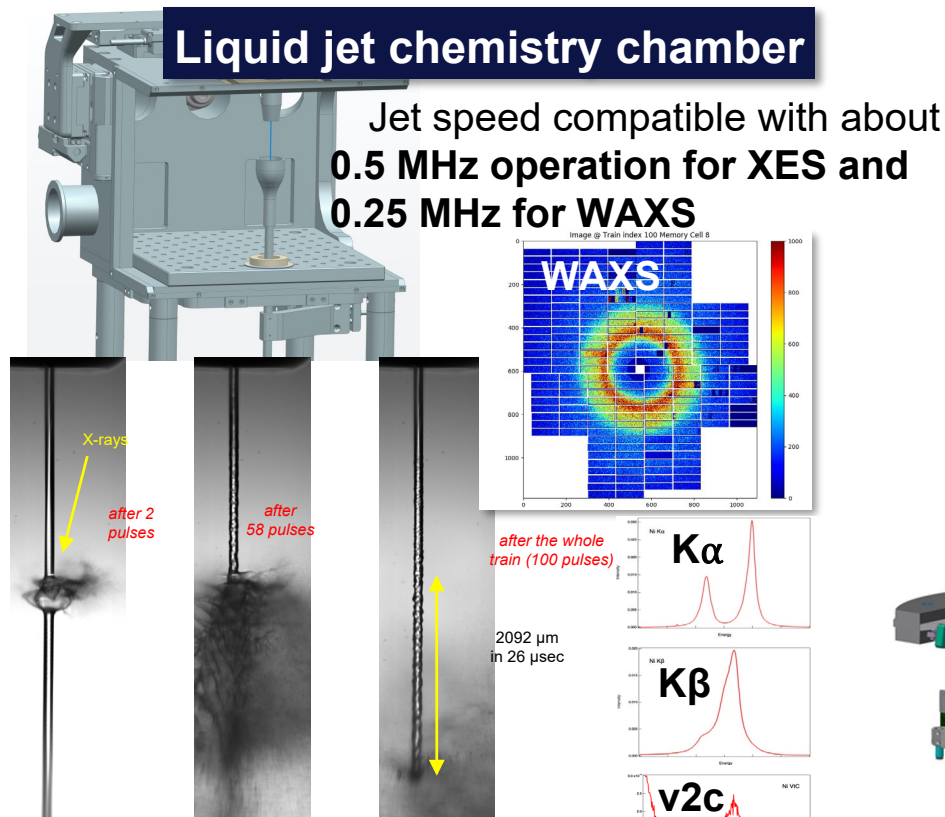
Vandana Tiwari, postdoc

# Sample environment: Liquid & Solid state experiments

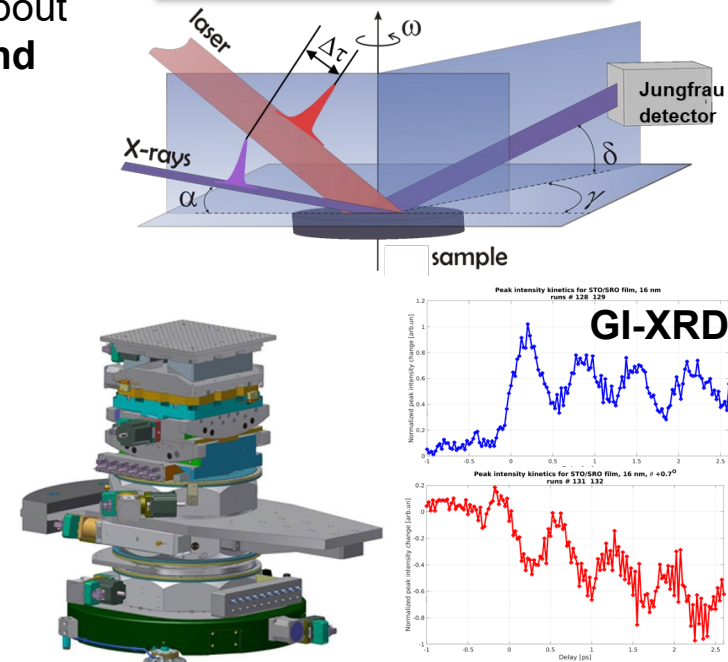
## Solid sample chamber



## Liquid jet chemistry chamber



## Single-crystal grazing-incidence diffraction



In collaboration with R. Shayduk (MID/EuXFEL)

- 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](mailto:dmitry.khakhulin@xfel.eu))

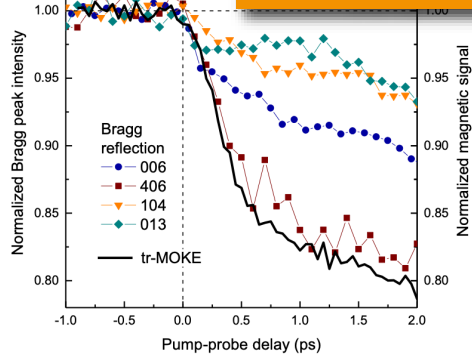
- Vacuum environment (1e-5 mbar)
- X-ray probe in transmission geometry
- Up to 15k samples accessible per filling/evacuation
- Parallel X-ray emission and scattering compatible
- Diffraction up to 8.8 Å<sup>-1</sup> at 16.5 keV and  $2\theta_{max} = 63^\circ$  courtesy of P. Zalden ([peter.zalden@xfel.eu](mailto:peter.zalden@xfel.eu))

- Helium 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<sup>-1</sup> courtesy of F. Lima ([frederico.lima@xfel.eu](mailto:frederico.lima@xfel.eu))

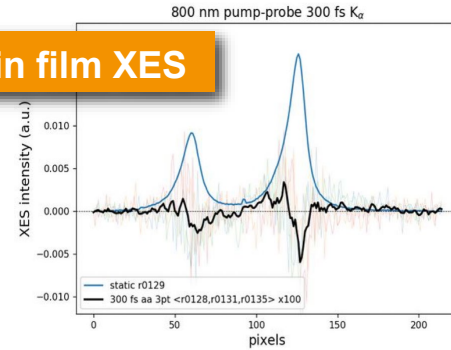
# Scientific Scope of FXE: Measuring ultrafast dynamics with hard X-rays

## Ultrafast solid-state dynamics

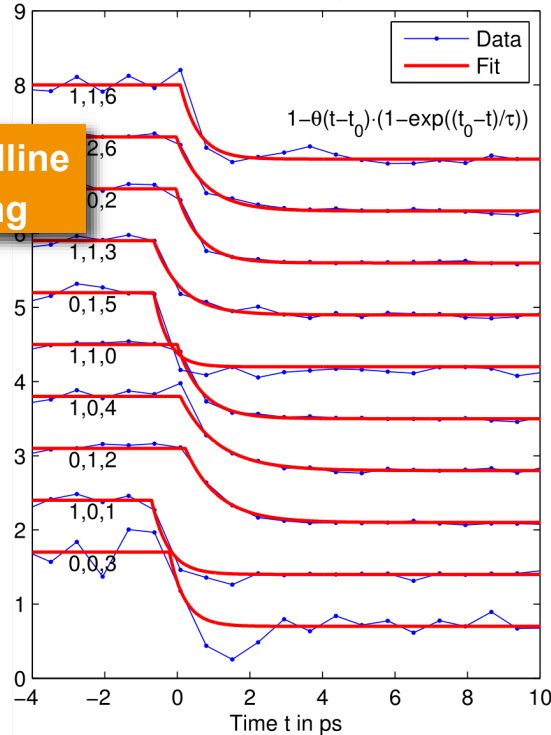
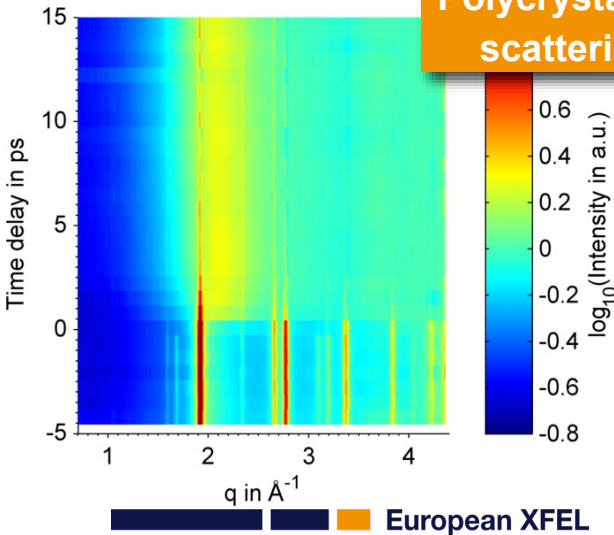
### Single-crystal XRD



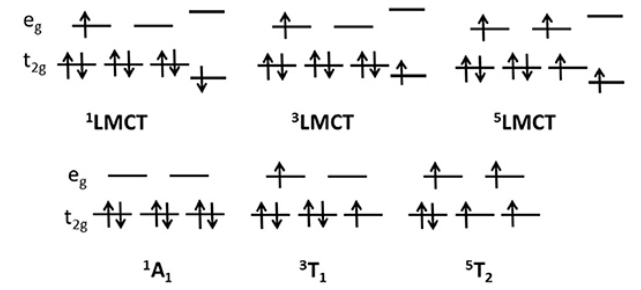
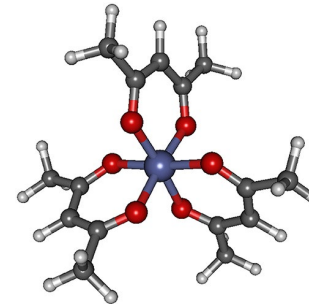
### Thin film XES



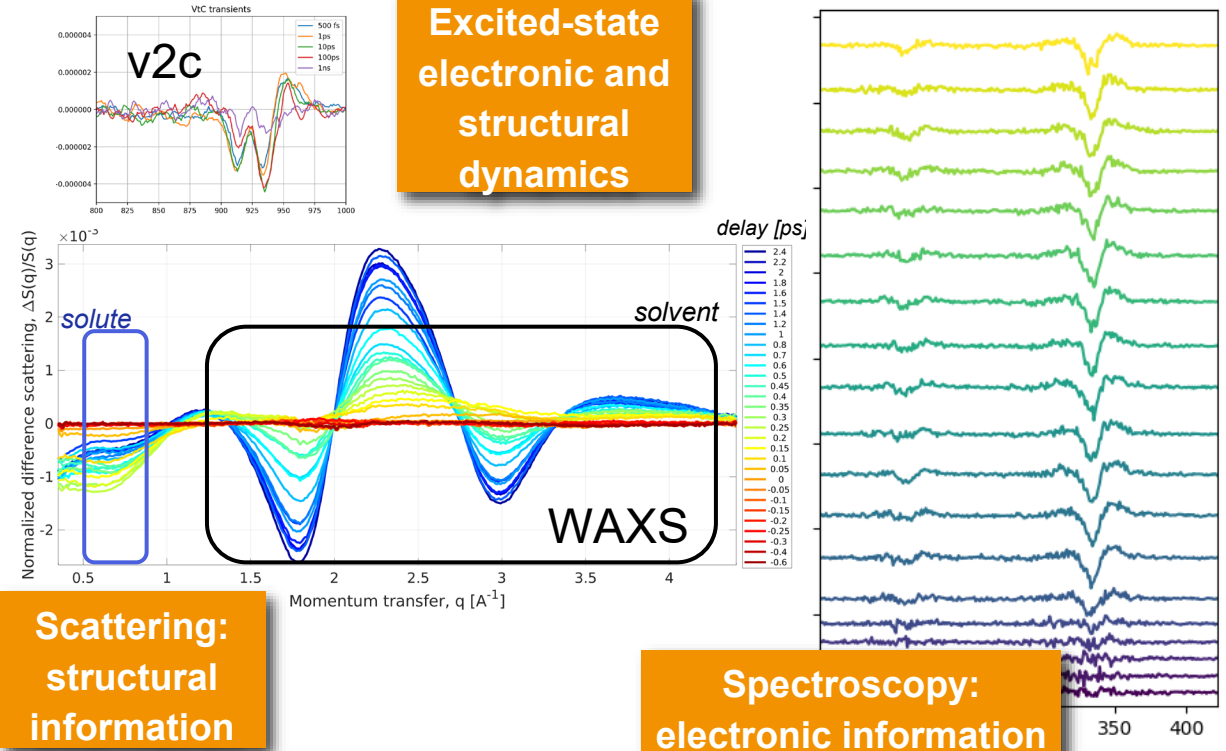
### Polycrystalline scattering



## Ultrafast (bio)chemical dynamics



### Excited-state electronic and structural dynamics



### Scattering: structural information

### Spectroscopy: electronic information

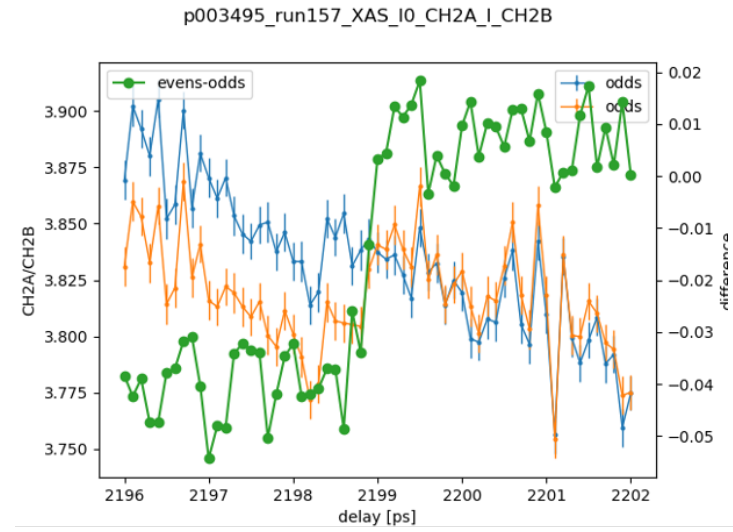
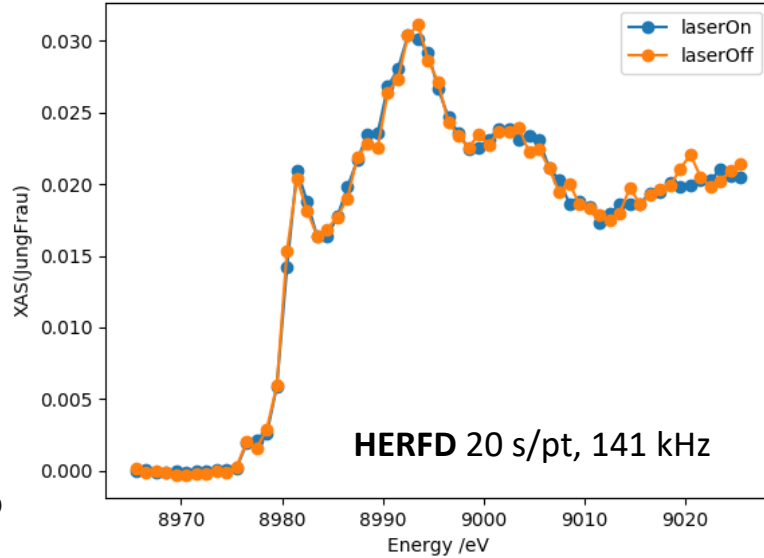
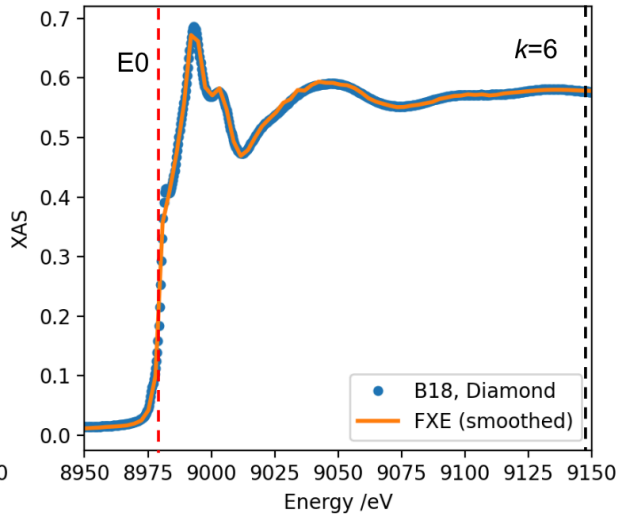


# XAS @ FXE: Status update

November 2022

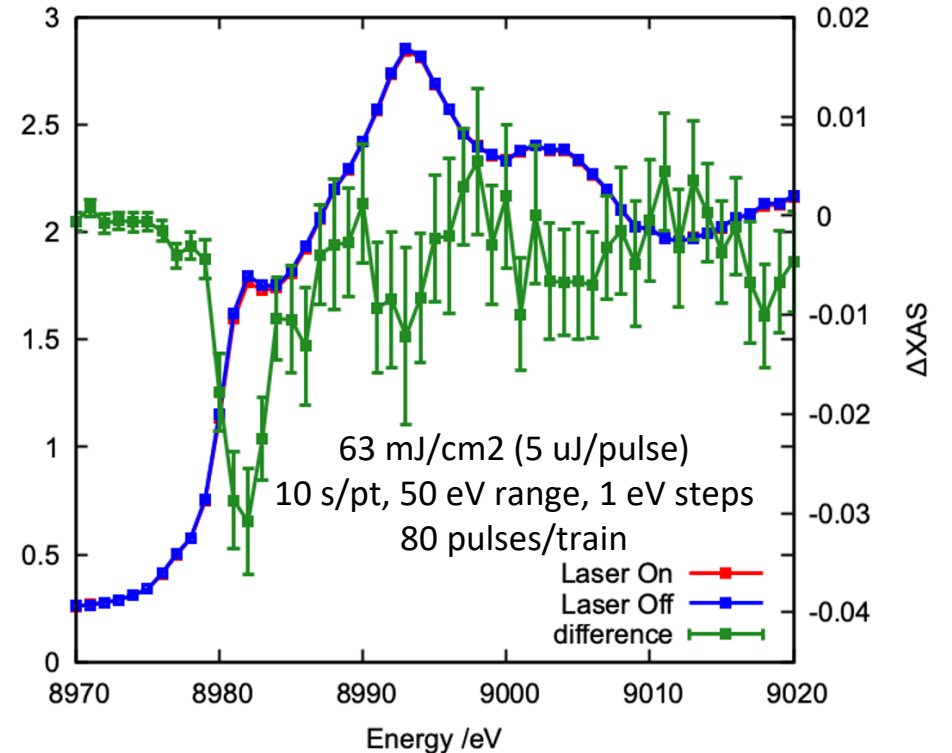
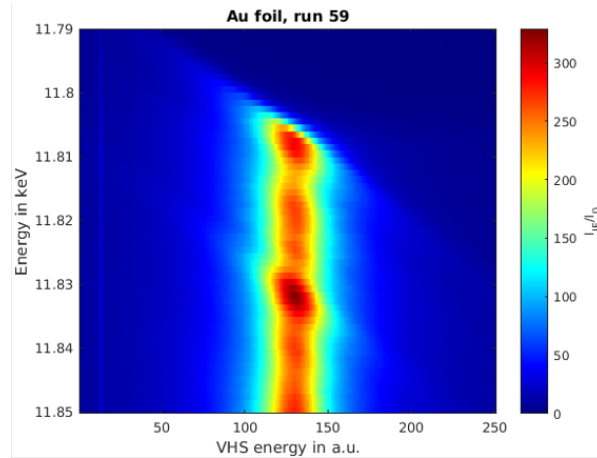
run163+164

Cu(dmp)2, 20 mM, 200 μm liquid jet



## Next steps:

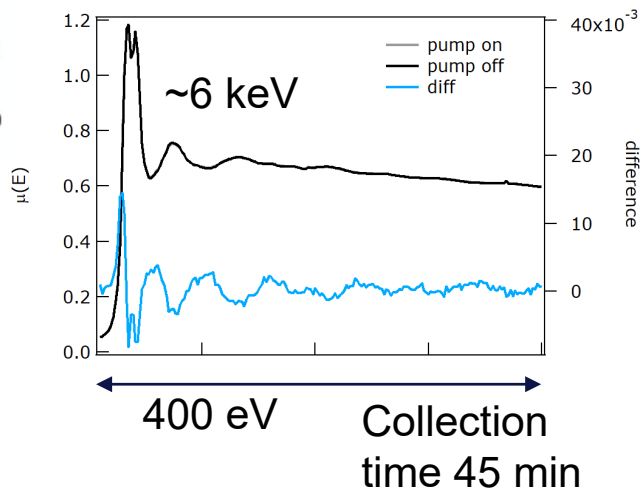
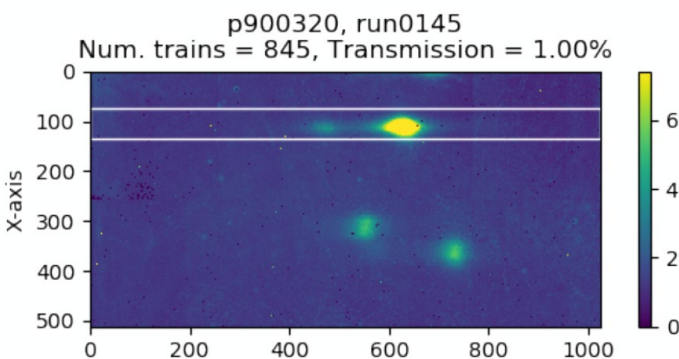
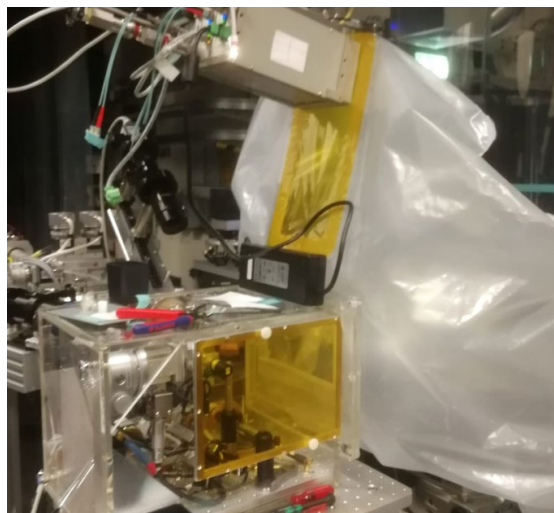
- Investigate other X-ray energies and edges
- Continue detection optimization



February 2023

# New sample environment: Goniometer in Helium environment

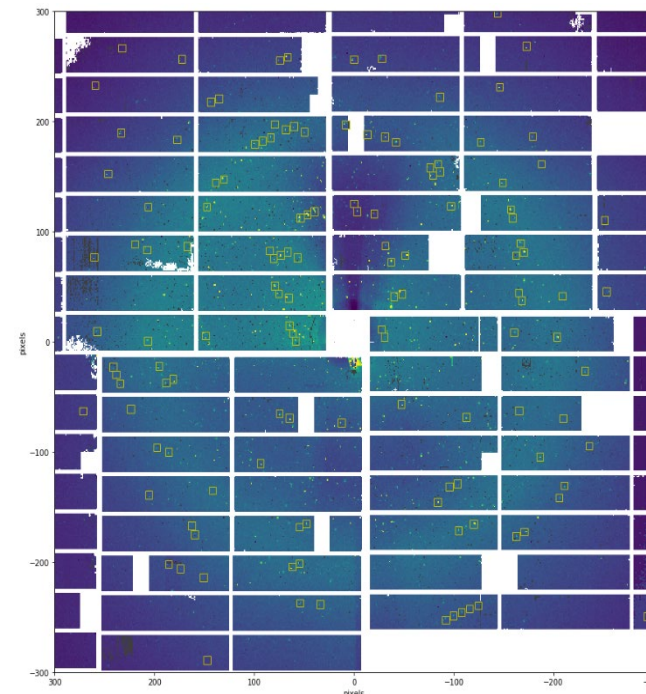
- Thin film targets
- Ideal for low  $E_{ph}$  spectroscopy (Ti, V, Cr K edges)
- tr-EXAFS possible
- Simultaneous diffraction
- 20 pulses/train (94 kHz)



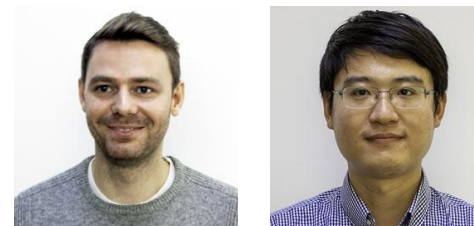
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# SFX-type expts@FXE

■ Validation of SFX detection with *Lysozyme*



- *smSFX proved itself feasible and efficient at FXE*
- *Combination of high rep.-rate and high photon energy (15 keV) allows for solving small molecule structures with high fidelity after a short acquisition time*



August 2022

## Call 11: Contact us with any questions or for more details



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