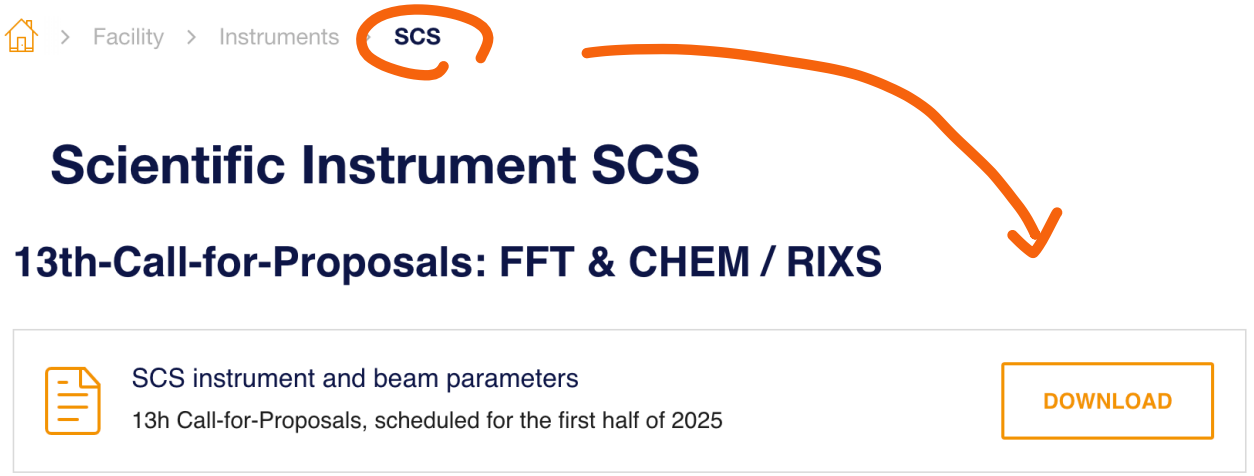
SCS instrument

User information
13th Call for Proposals

Andreas Scherz
Spectroscopy and Coherent Scattering
(SCS instrument)

27. March 2024 (updated)

contact us:
scs@xfel.eu

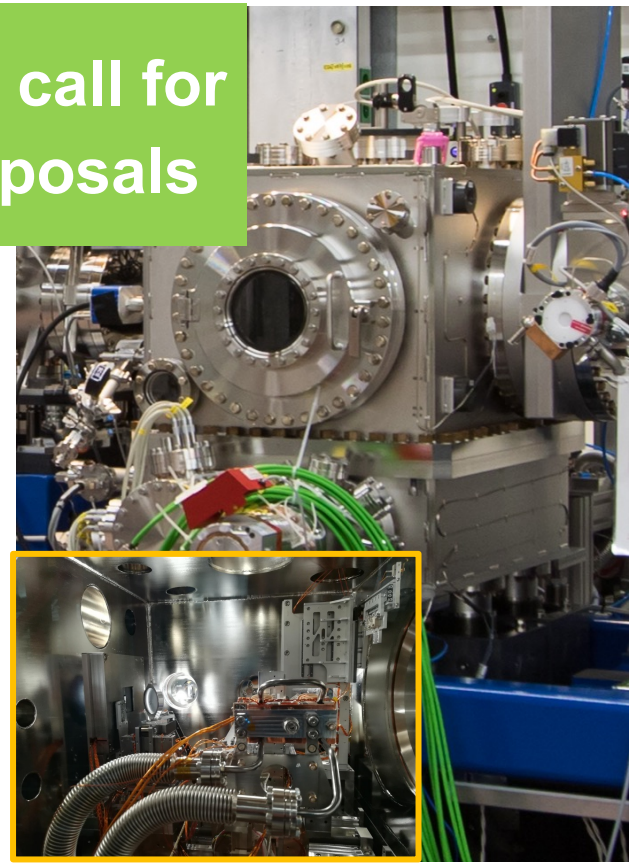


Report (2022)
SCS Instrument Review Report
R. Carley, B. Van Kuiken, L. Le Guyader, G. Mercurio, A. Scherz
doi:10.22003/XFEL.EU-TR-2022-003

SCS experiment stations

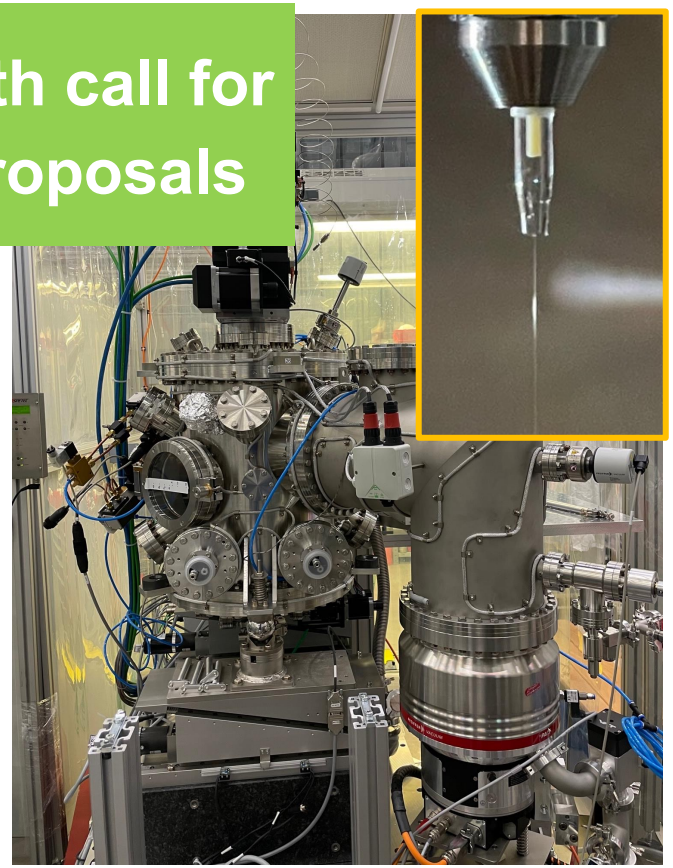
FFT experiment station
Since Oct 2018

13th call for proposals



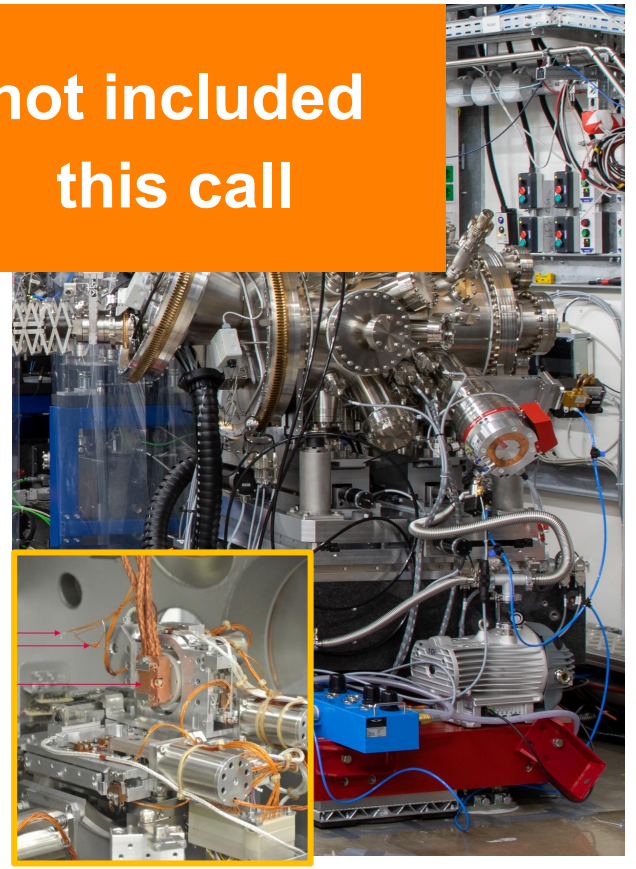
CHEM experiment station
Since Feb 2022

13th call for proposals

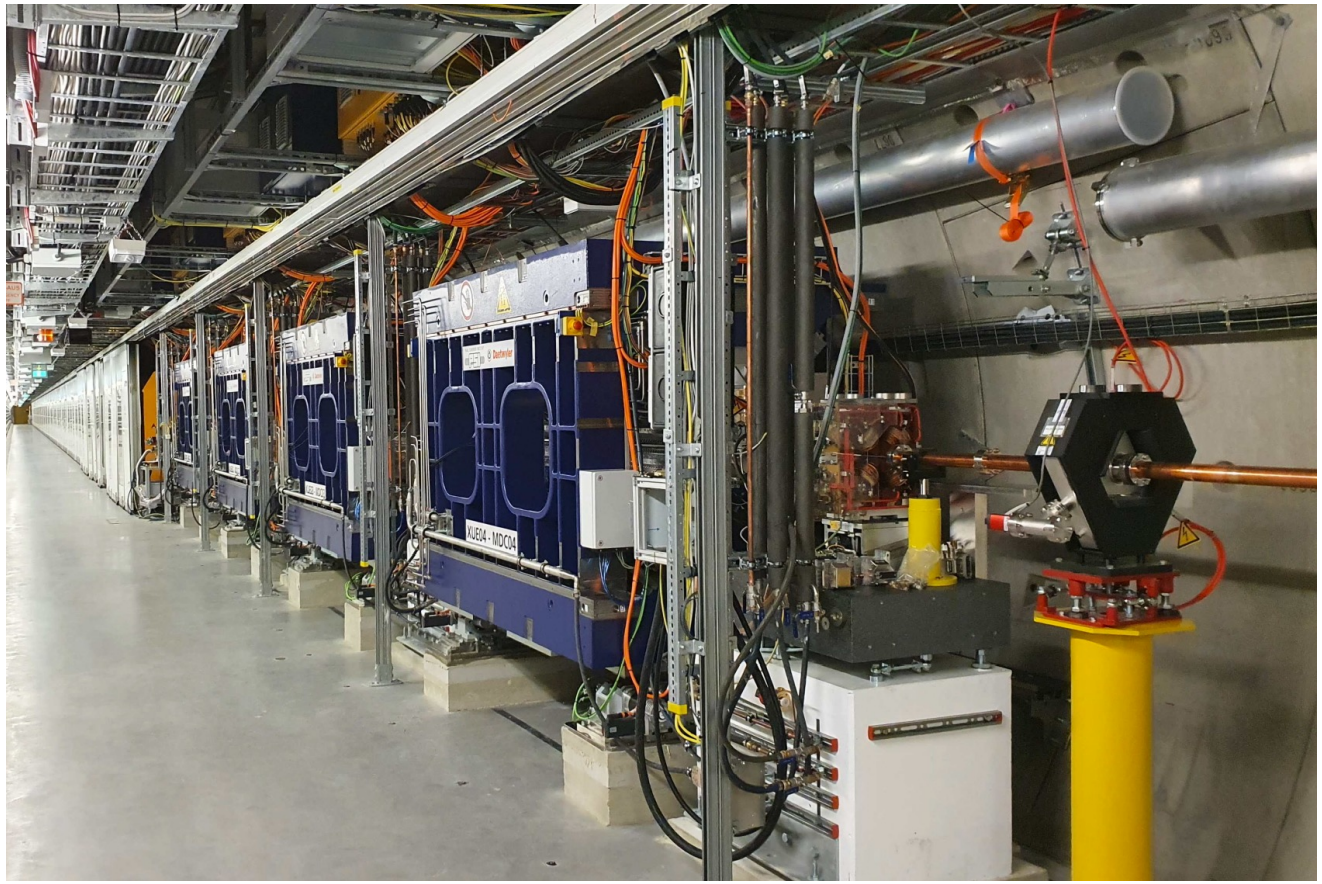


XRD experiment station
Since Sep 2022

not included this call

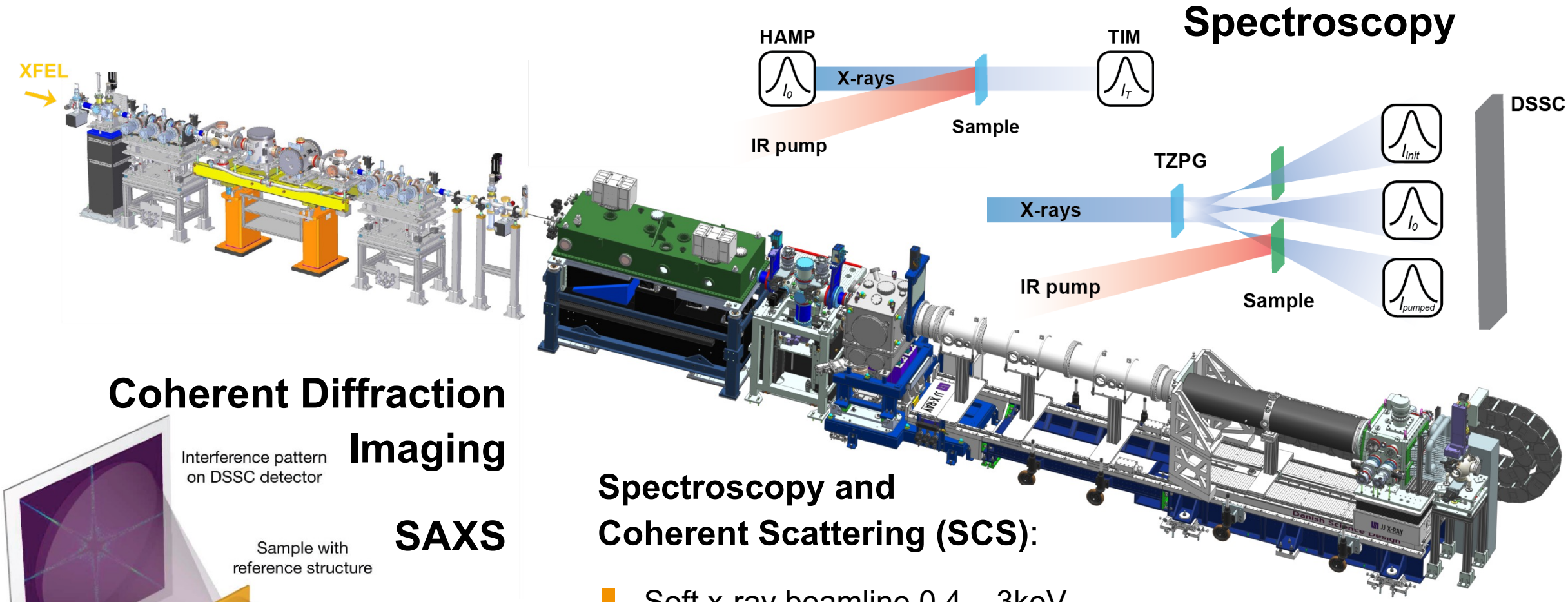


EuXFEL APPLE-X (UE90) Variable Polarization at SA3: Linear horizontal, linear vertical, left and right circular Polarizations



APPLE-X tested so far in the energy range of 700 – 900 eV. Inquire for details

SCS instrumentation for forward scattering geometries



Coherent Diffraction Imaging

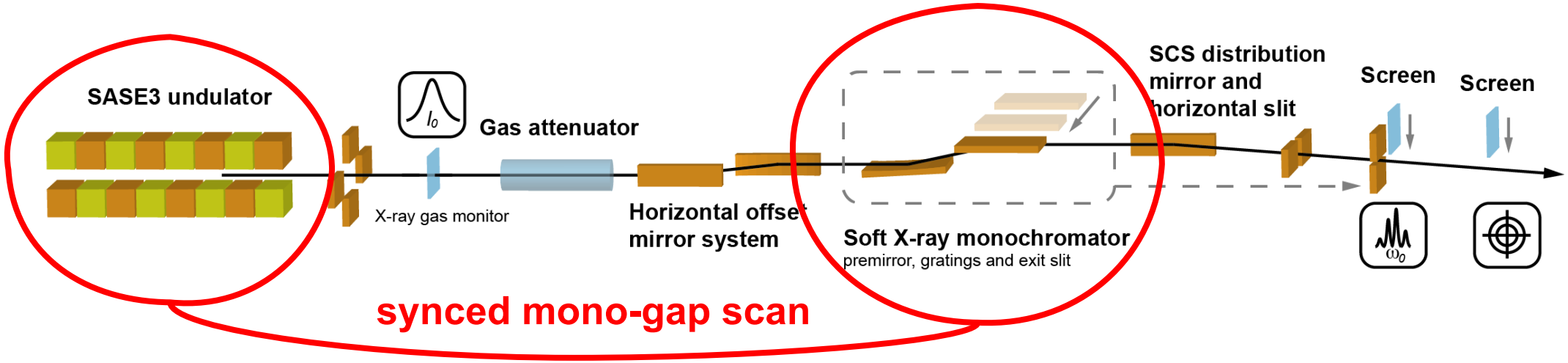
SAXS

XPCS

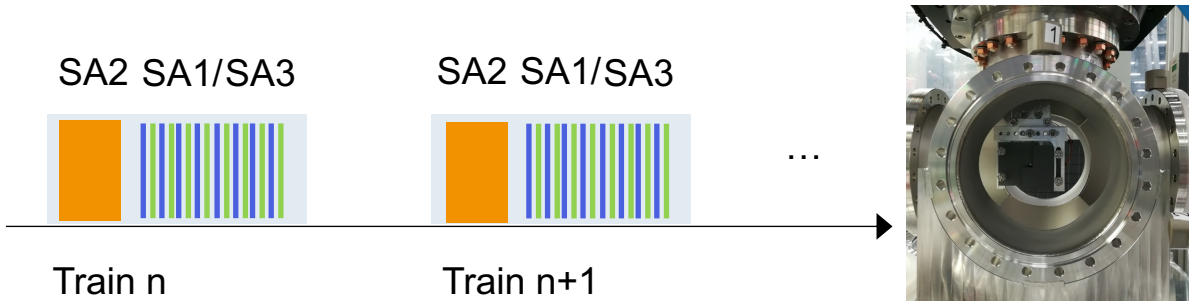
Spectroscopy and Coherent Scattering (SCS):

- Soft x-ray beamline 0.4 – 3keV
- Time-resolved/ non-linear x-ray spectroscopies
- Time-resolved/ non-linear x-ray diffraction
- Forward- / small-angle scattering geometries

Current status of beamline and implemented capabilities of the SCS instrument

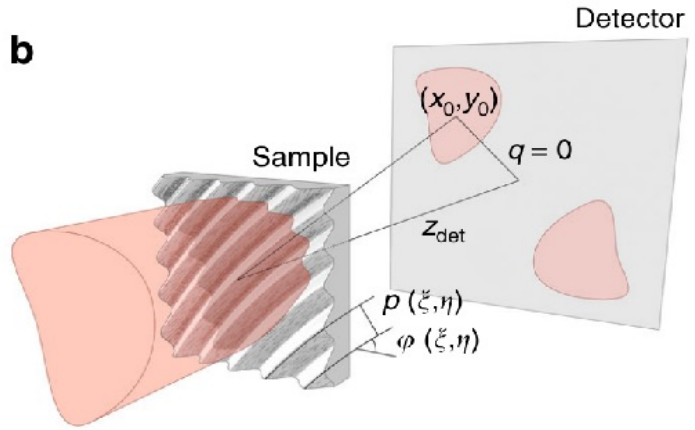


Interleaved mode with SA1

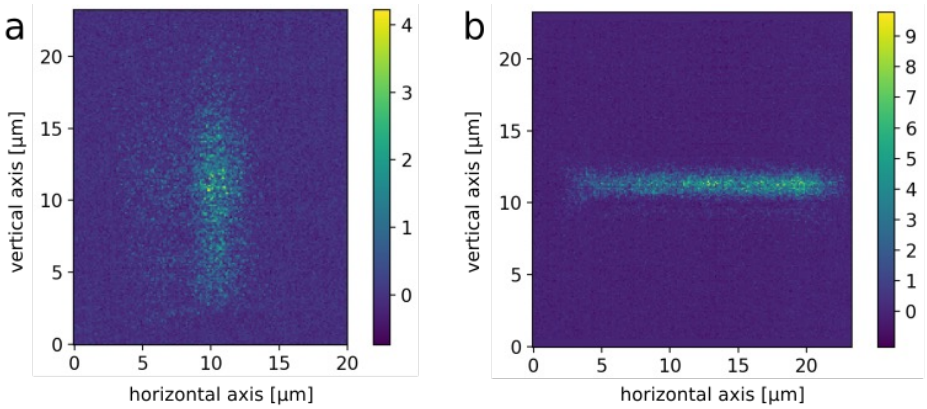


Train picker

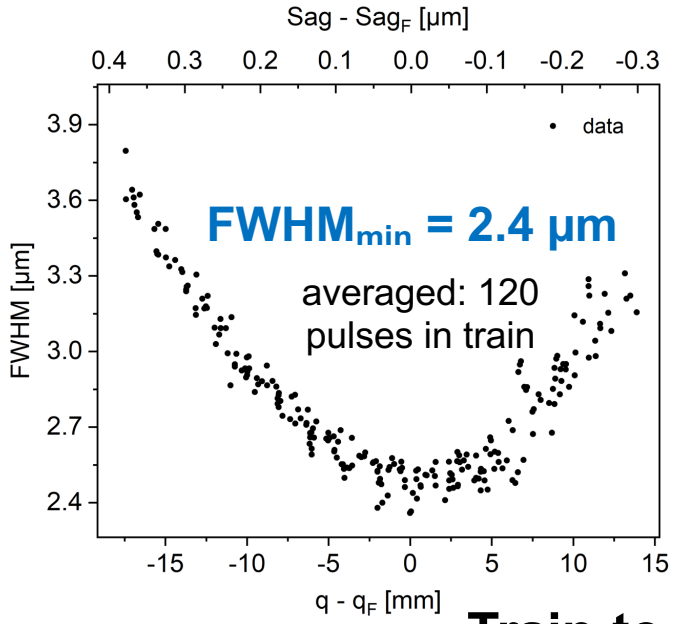
KB Focus Characterization

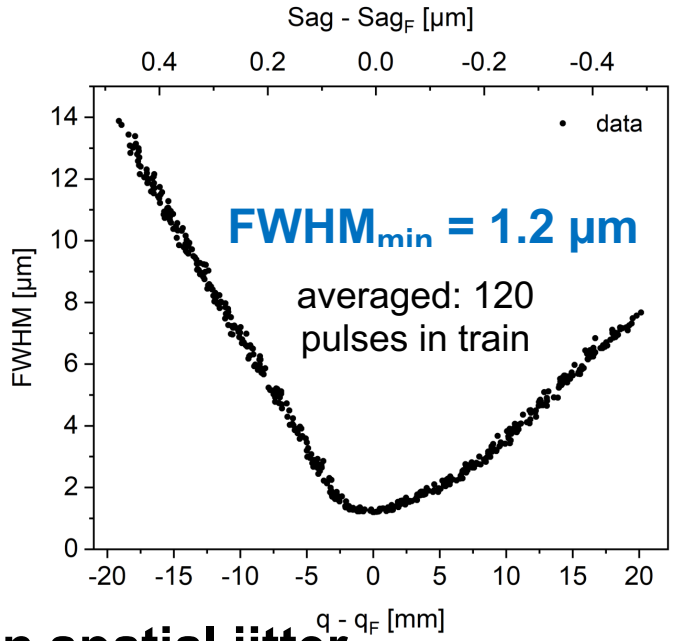


M. Schneider et al., Nat. Commun. 9, 214 (2018)

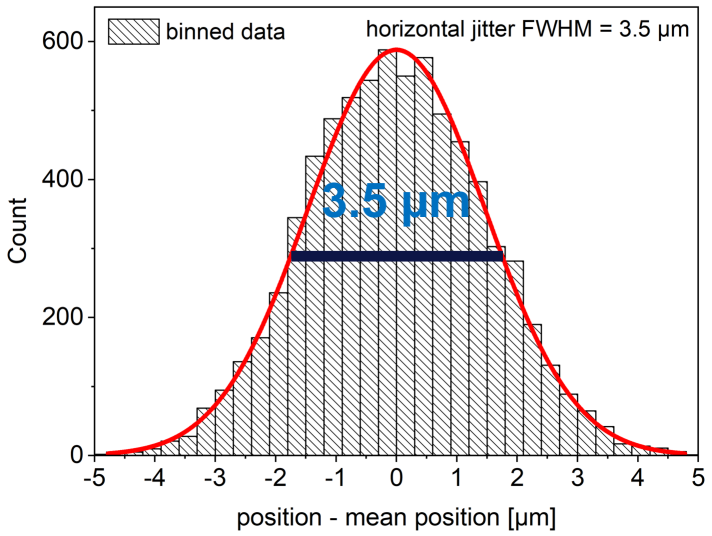


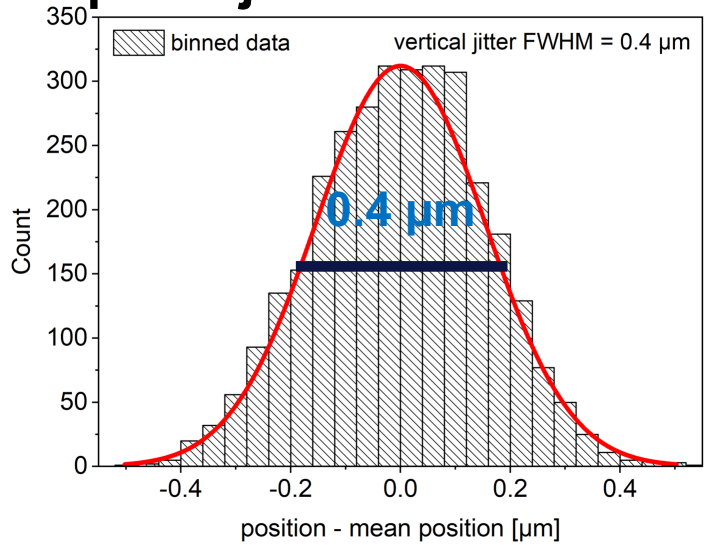
G. Mercurio et al., Proc. of SPIE Vol. 11109 (2019).
G. Mercurio et al., Optics Express, 30(12), 20980 (2022)



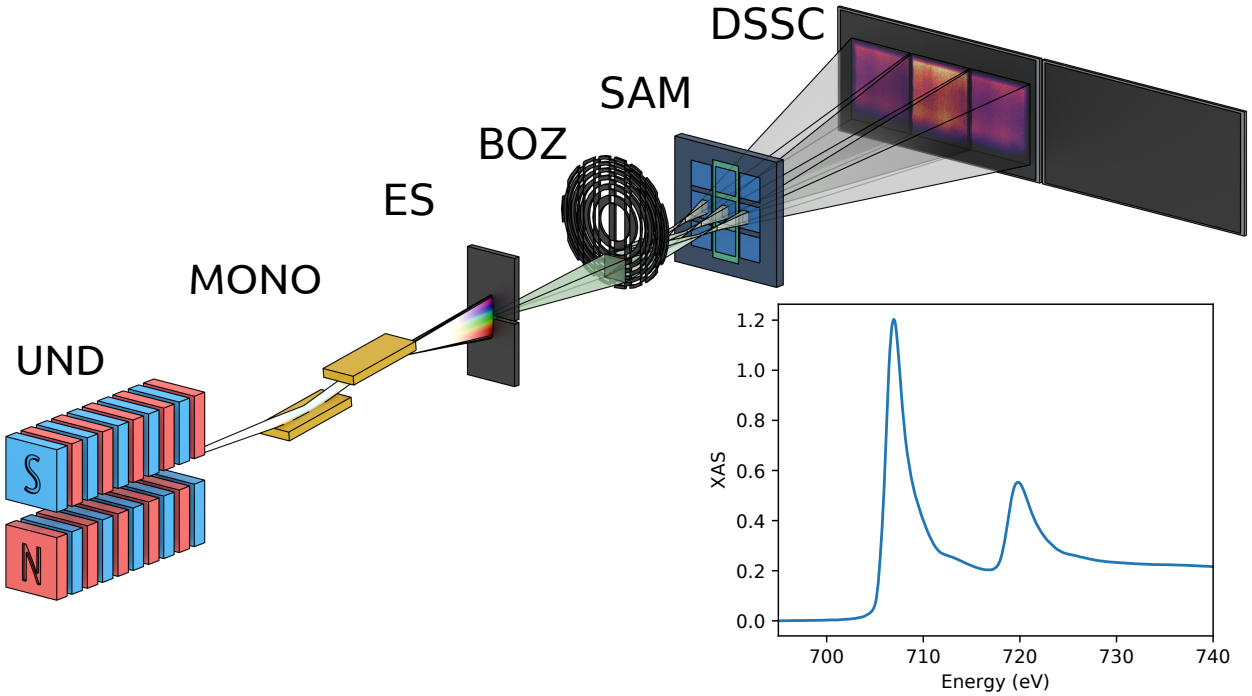


Train-to-train spatial jitter

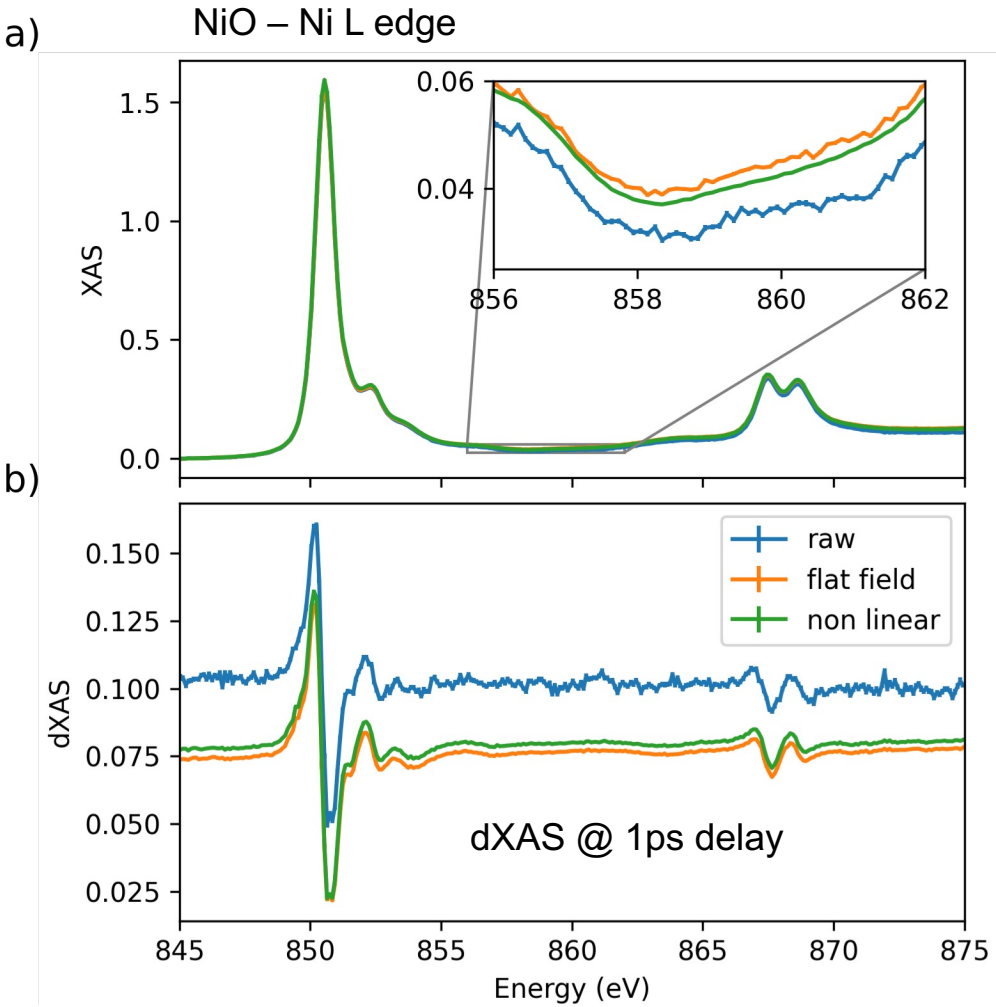




Beam-splitting off-axis zone plate for shot-noise limited MHz transient absorption spectroscopy with the DSSC detector

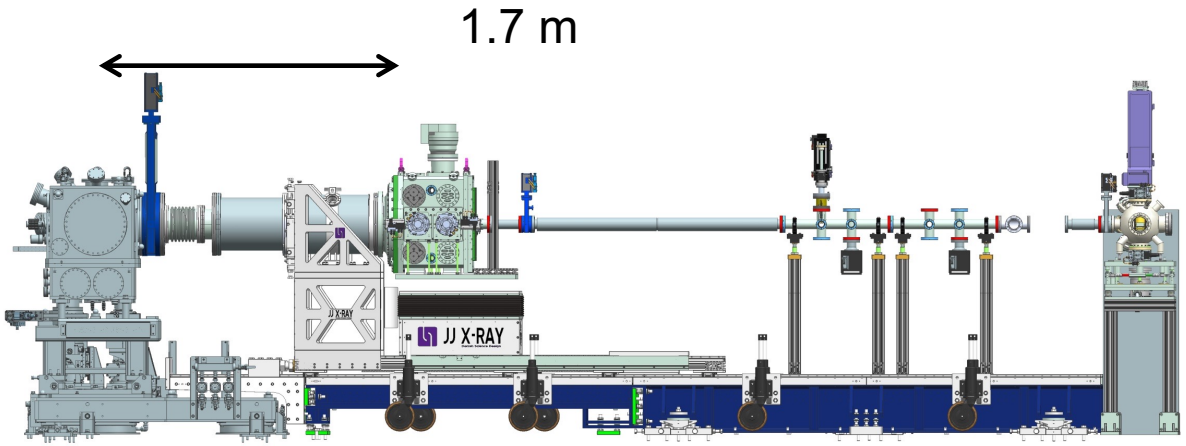


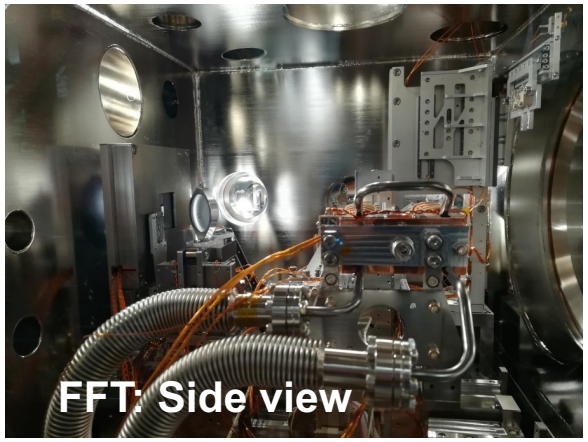
Le Guyader & al., J. Synchrotron Rad. 30, 284 (2023).
Lojewski et al., Materials Research Letters, 11(8), 655–661 (2023)
Engel et al., Structural Dynamics, doi:10.1063/4.0000206 (2023)

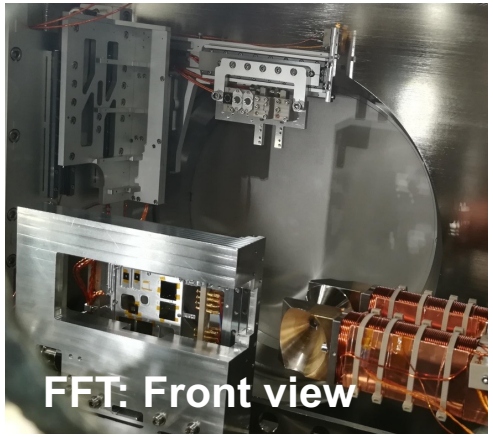


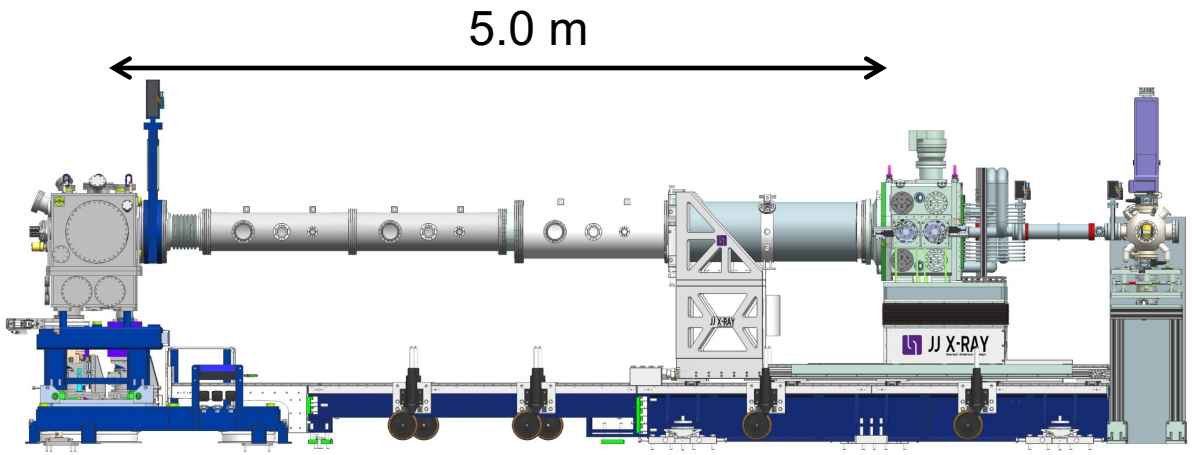
Lojewski et al., arXiv:2305.10145v1 (2023)

FFT Experimental apparatus for XAS and SAXS / CDI









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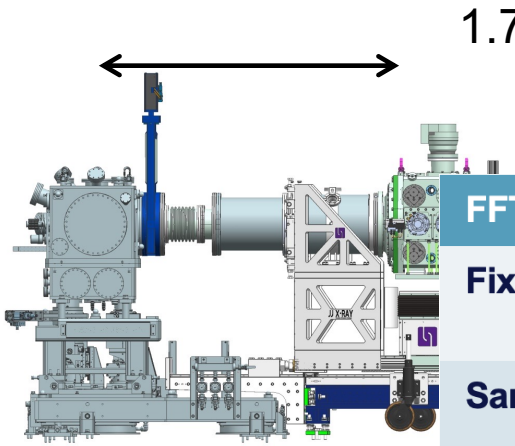
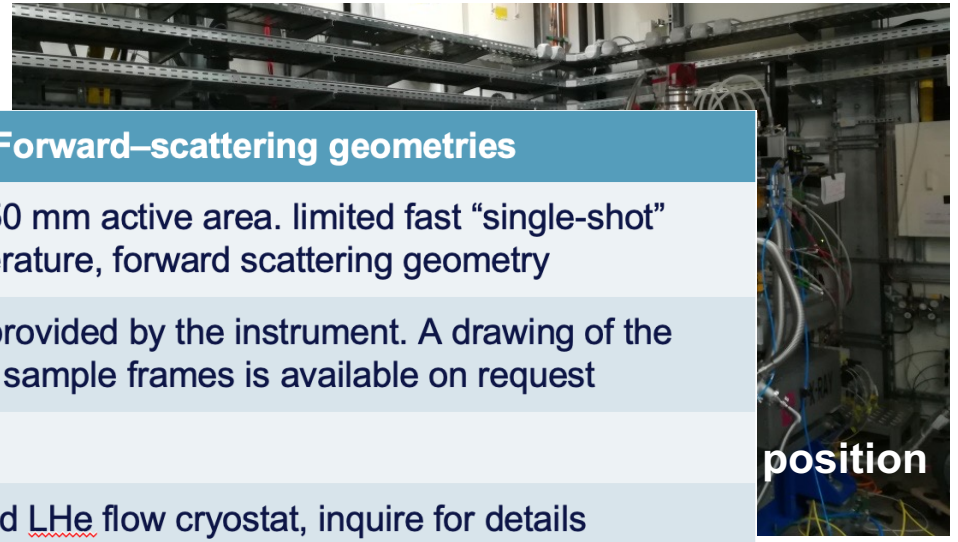
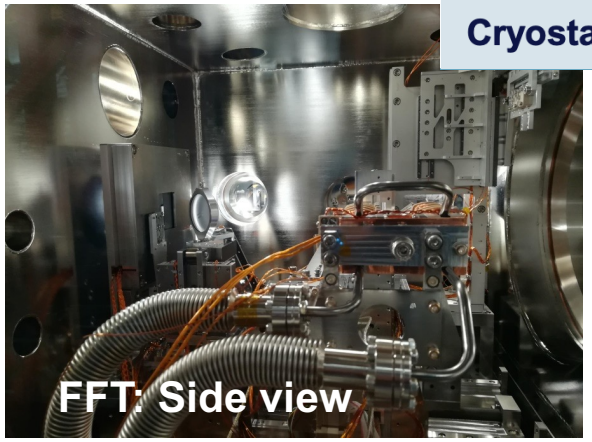
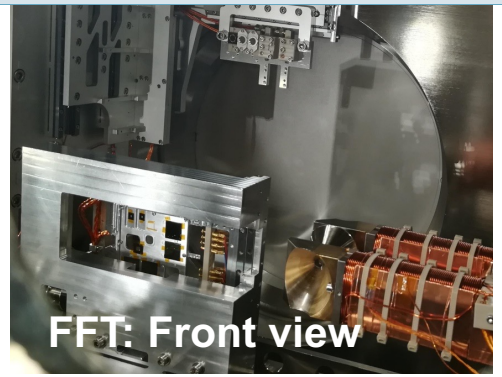
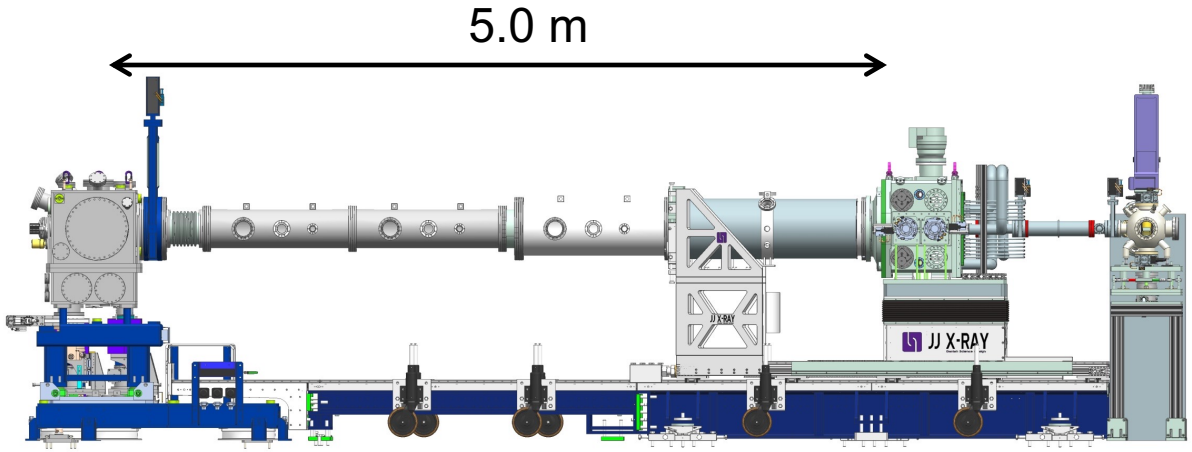


FFT experiment station - solid sample environment, Forward–scattering geometries	
Fixed target sample holder	Frame with 50 mm x 50 mm active area. limited fast “single-shot” scanning, room temperature, forward scattering geometry
Sample Frame	Standard frames are provided by the instrument. A drawing of the frame to produce own sample frames is available on request
DC electromagnet	≤ 0.35 T
Cryostat sample holder	15 – 300K, top-inserted LHe flow cryostat, inquire for details





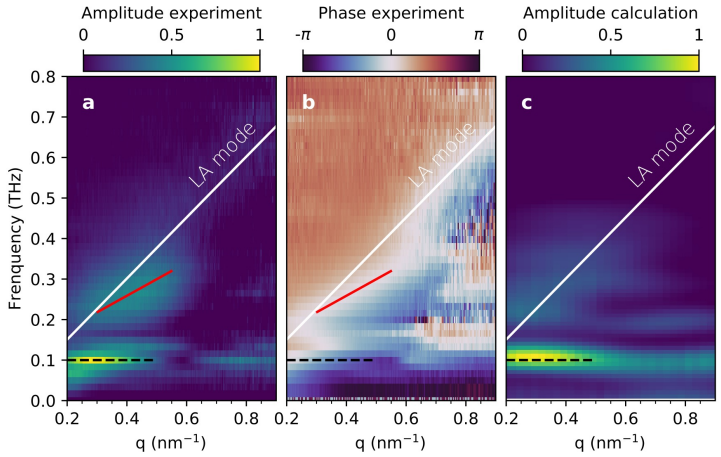




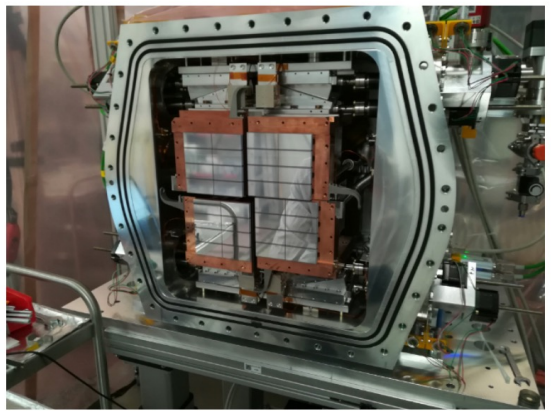
DSSC Detector for CDI, SAXS, XPCS

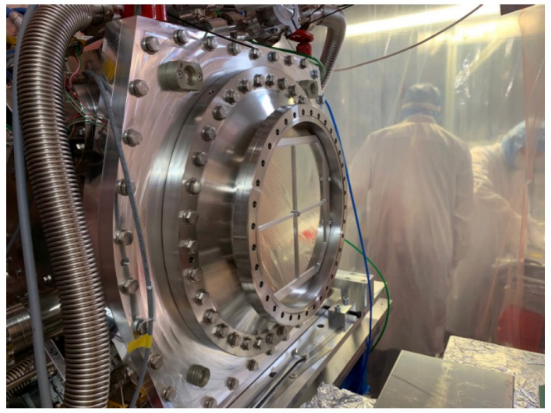
DSSC detector	SAXS, CDI, BOZ-XAS, XPCS	
Number of pixels	1024 x 1024	
Pixel coordinates	Hexagonal	Detector quadrants in windmill configuration
Pixel size	204 µm x 236 µm	
Max frame rate	4.5 MHz	
Beam hole size	Default: 4.75 mm (windmill)	The diameter of the central dead area is 8mm.
Standard detector-to-sample distance	Min: 1.02 m Max: 5.40 m Travel range: 1.5 m (under vacuum)	

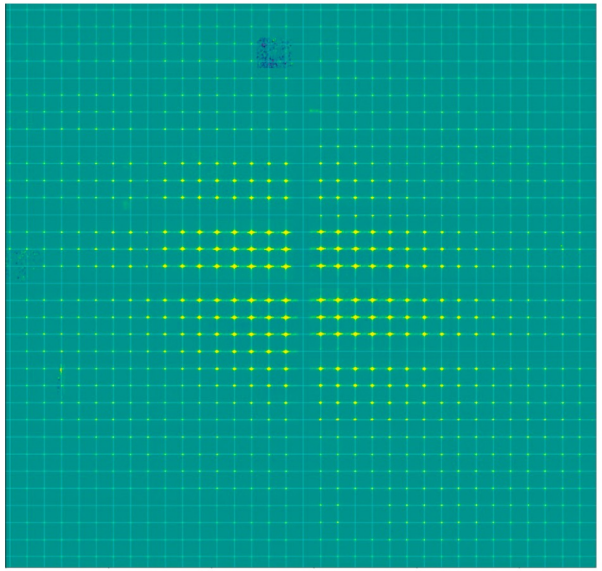
Porro et al., IEEE Transactions on Nuclear Science, 68(6), 1334–1350 (2021)
Costa et al., IEEE Access, 11, 84323–84335 (2023)

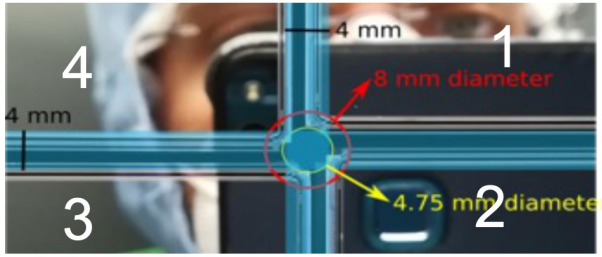


Turenne et al., Science Advances 8(13), 1–11 (2022)



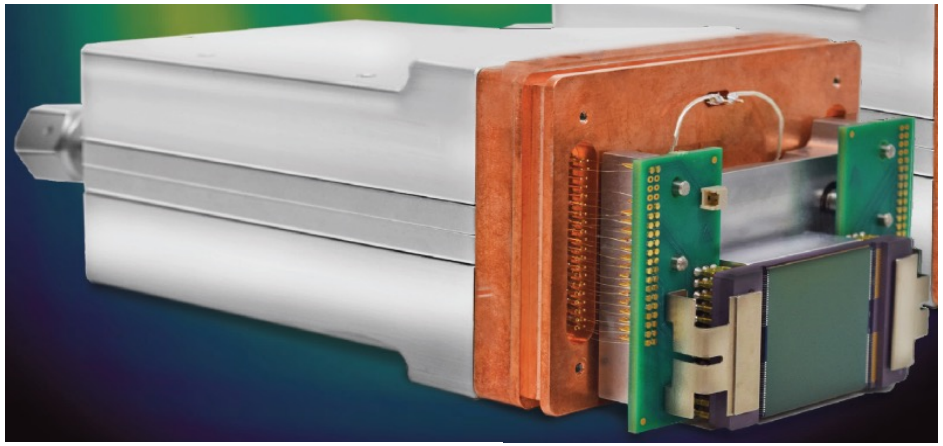




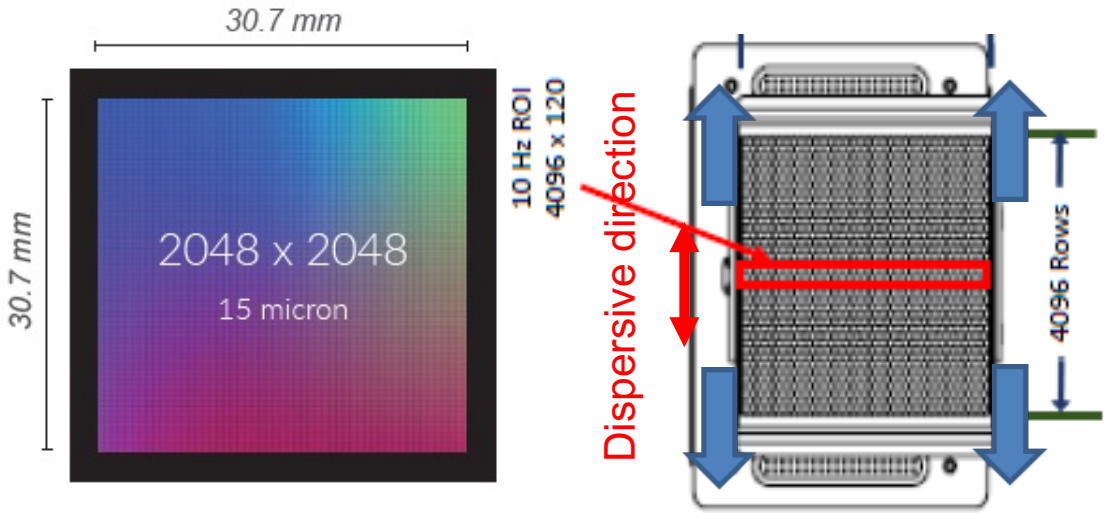


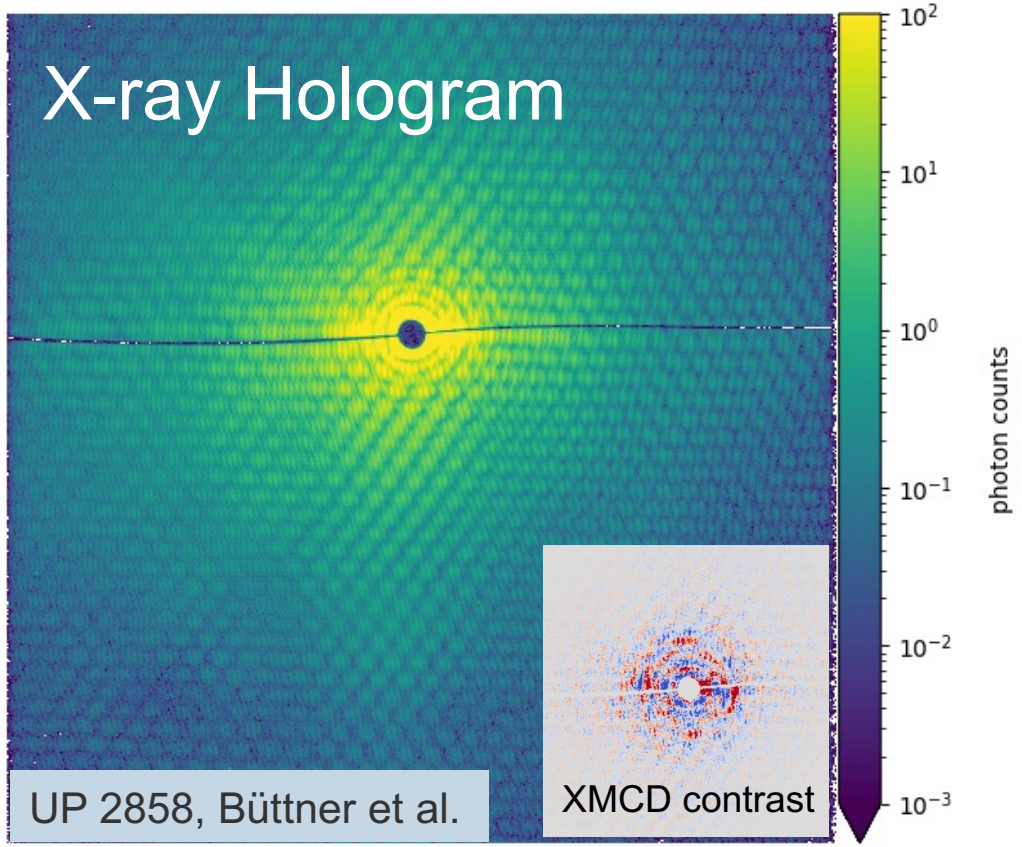
Büttner, et al.., Nature materials **20**, 30 (2021)
Turenne et al., Science Advances, **8**, 1–11 (2022)
Hagström, et al., J. Synchrotron Rad. **29**, 1454 (2022)
Hagström,, et al. Phys Rev B, **106**, 224424 (2022).
Suturin et al., Phys Rev B, **108**, 174444 (2023)

Pi-MTE3 commercial detector option



PI-MTE3 Detector		
Number Pixels / Size	2048 x 2048, 15µm x15µm	Cartesian coordinates, 30.7 x 30.7 mm imaging area
Frame rate	up to 1Hz	4 port readout, inquire for details
detector-sample distance	55 - 820 mm	



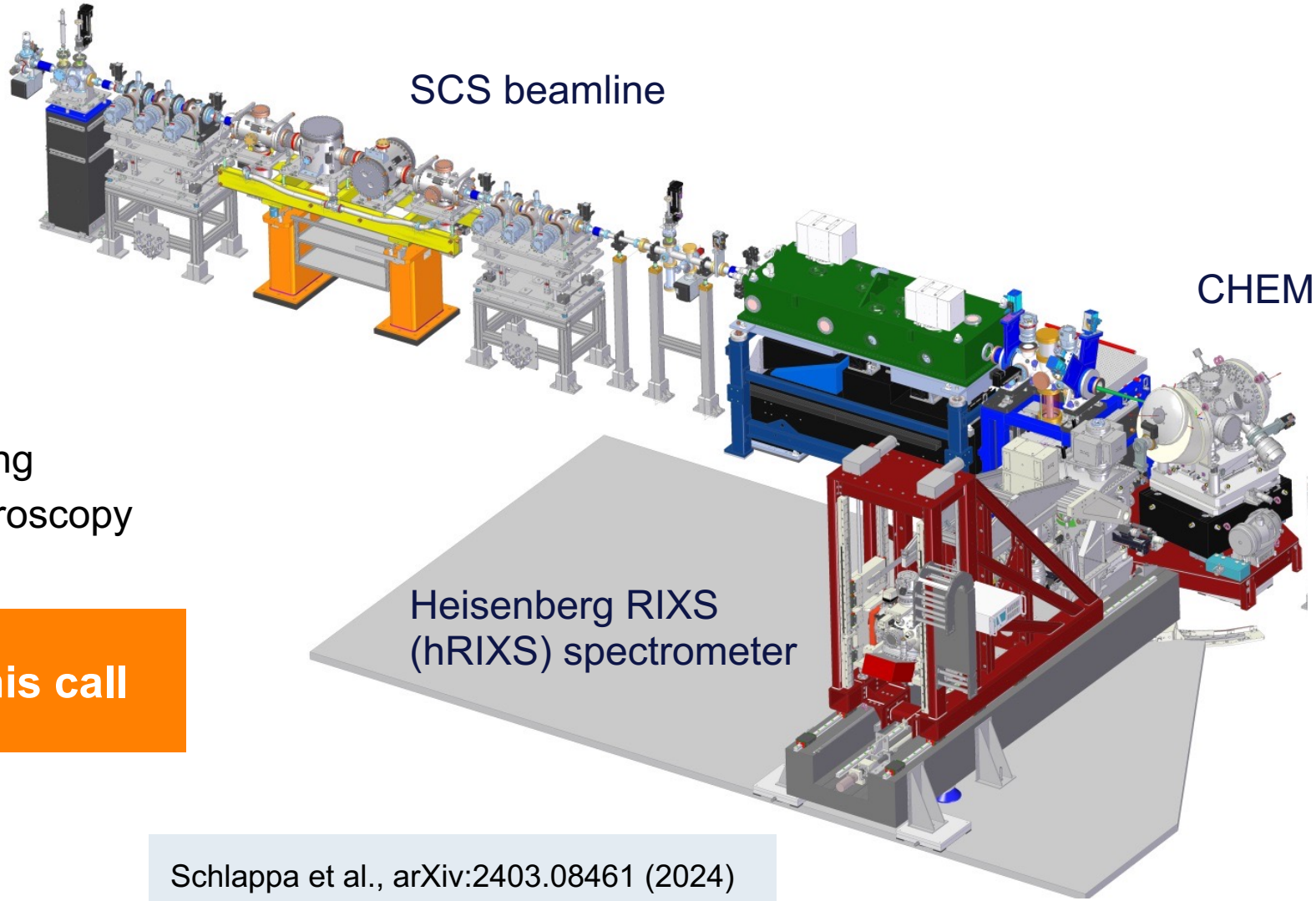


CHEM station at the SCS Instrument, 13th Call for Proposals

Spectroscopy and Coherent Scattering (SCS):

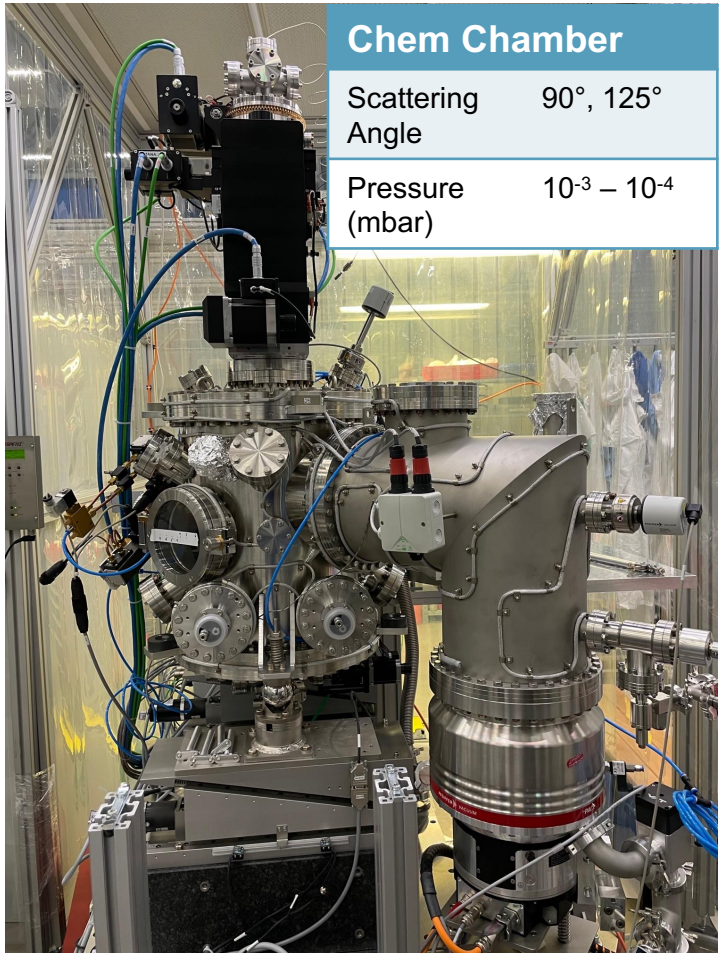
- Soft x-ray beamline 0.4 – 3keV
- Liquid jet samples
- Resonant inelastic X-ray scattering
- Transient X-ray absorption spectroscopy

Includes the N K edge this call



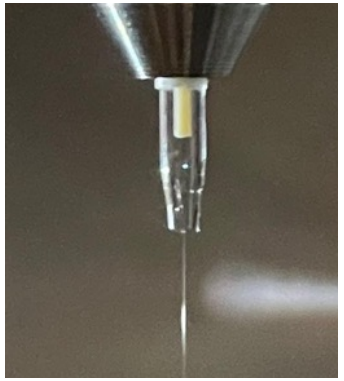
Schlappa et al., arXiv:2403.08461 (2024)

CHEM experiment station with liquid-jet sample environment

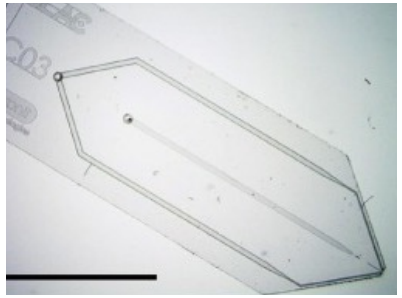


Chem Chamber	
Scattering Angle	90°, 125°
Pressure (mbar)	10^{-3} – 10^{-4}

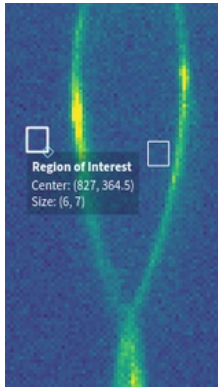
Cylindrical Jet for RIXS+PFY XAS



Flat Jet for transmission XAS



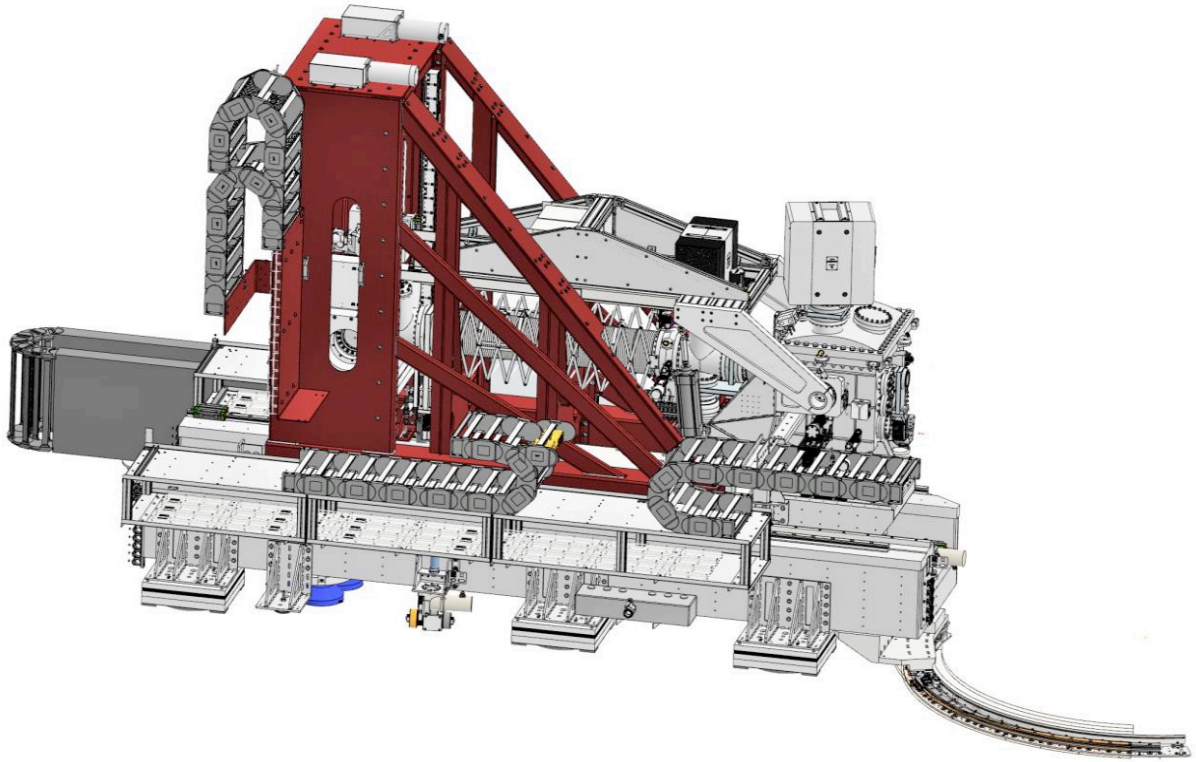
Korelek et al. Nat Commun. (2018) 9. 1353



	Cylindrical Nozzle (RIXS)	Flat Jet (BOEZ)
Jet Dimension	20 – 50 µm diameter	1 – 4 µm thick
Solvents*	Water, Ethanol, Octane	Water
Flow Rate	~1 ml/min	~3 ml/min
X-ray Spot Size	Tunable 200 µm – < 10µm	line focus (200 x 10 µm H x V)

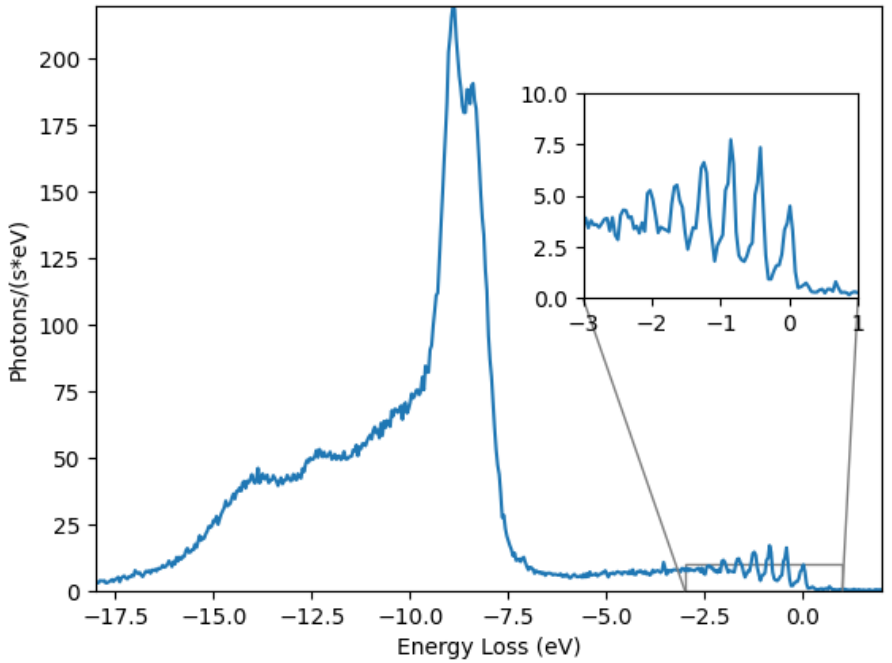
***Contact SCS staff to discuss additional solvents and sample details (recirculation, cooling, etc)**

hRIXS parameters for run 13



hRIXS parameters	
Photon energy	0.5 – 1.5 keV
Combined resolving power	Up to 10.000 (mono HR) 3.000 (mono LR)
Transmission	~10^{-6}
Time resolution	Limited by mono: 80-150 fs (mono HR) 30-50 fs (mono LR)
Scattering angle -> CHEM	90 deg, 125 deg

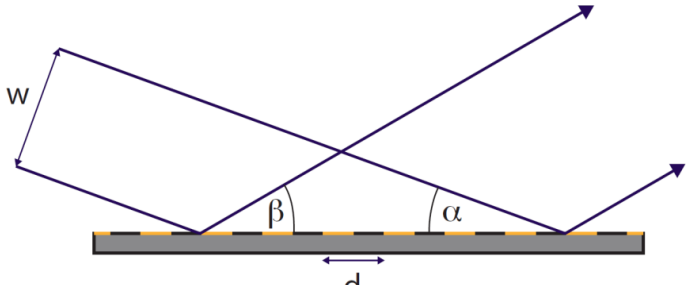
O K-edge RIXS of Liquid Water



Schlappa et al., arXiv:2403.08461 (2024)
Gerasimova et al., Journal of Synchrotron Radiation, 29(5), 1299–1308 (2022)

Monochromator settings SCS beamline:

The use of monochromator leads to pulse stretching.
Energy resolution to be compromised for time resolution and vice versa.



Time delay: $\Delta\tau_{rms} = \frac{1}{c} w_{rms} d_0 \lambda$

Low-resolution grating

LR grating	
Line density	50 l/mm
Resolving power	3.000 (1st order)
Pulse stretching	30-50 fs
X-ray pulse energy	up to 30 µJ

→ Moderate combined energy resolution
→ High temporal resolution

High-resolution grating

HR grating	
Line density	150 l/mm
Resolving power	Up to 10.000 (1st order)
Pulse stretching	80-150 fs
X-ray pulse energy	up to 5 µJ

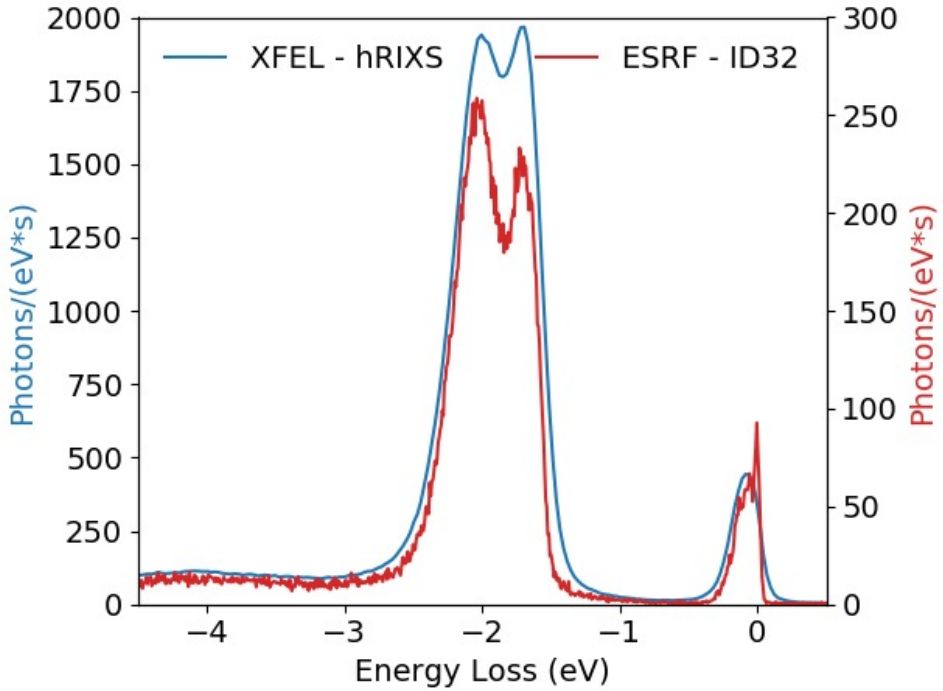
→ High combined energy resolution
→ Moderate temporal resolution

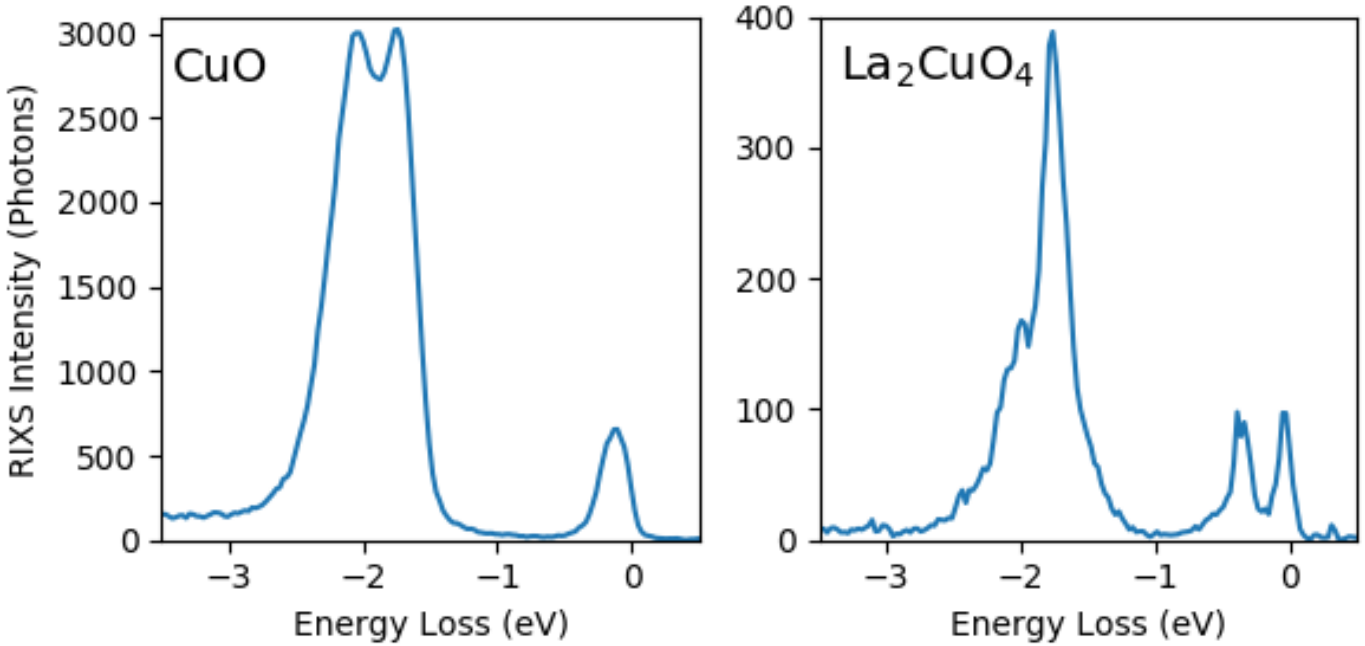
Gerasimova et al., Journal of Synchrotron Radiation, 29(5), 1299–1308 (2022)

Measurement Count Rates

Cu L-edge

Incident Beam 1.3 x 10^{13} ph/s





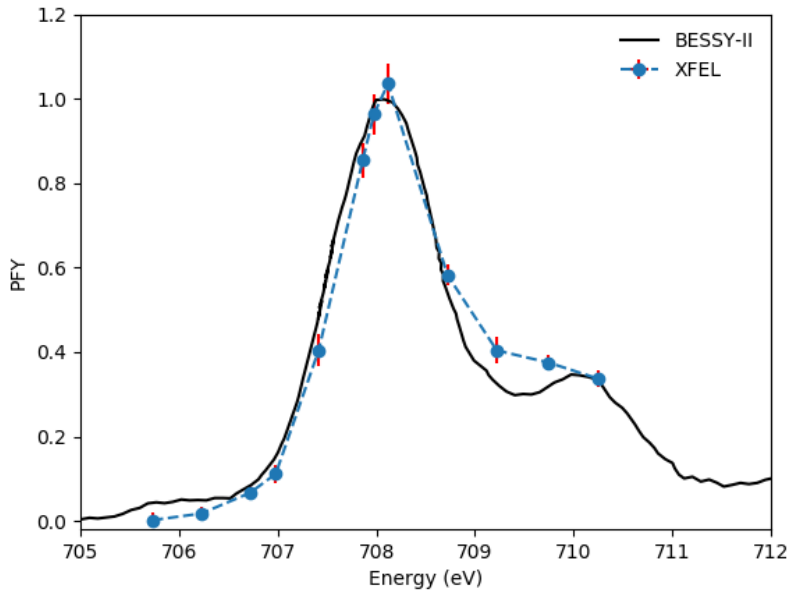
- CuO spectrum measured with 100% GATT transmission (~2 mW), 400 pulses/train, and a 1 min acquisition, 80% wt. Cu
- La_2CuO_4 thin film spectrum measured with 10% GATT transmission (~0.2 mW), 400 pulses/train, and a 10 min acquisition, 16% wt. Cu

Edge	Energy (eV)	ΔE (meV)	E/ΔE
Cu L_3	930	106	8 700
Ni L_3	853	122*	6 900*
O K	530	49	10 400

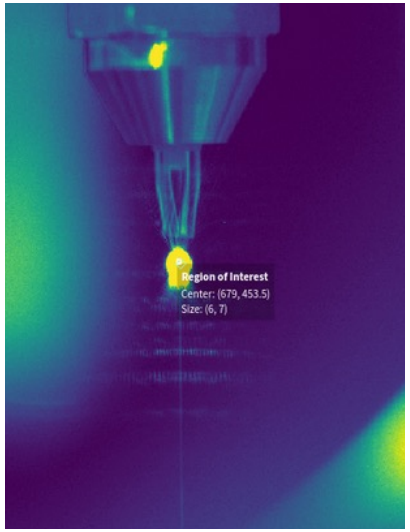
* not enough time to optimize

RIXS of Solution Samples

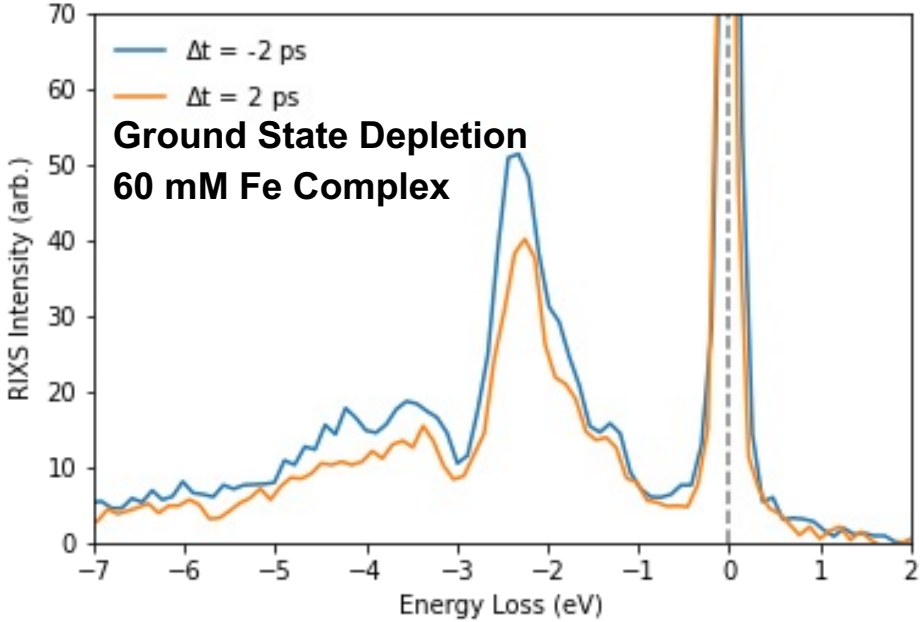
XAS Measured by PFY



Optical Laser for trRIXS



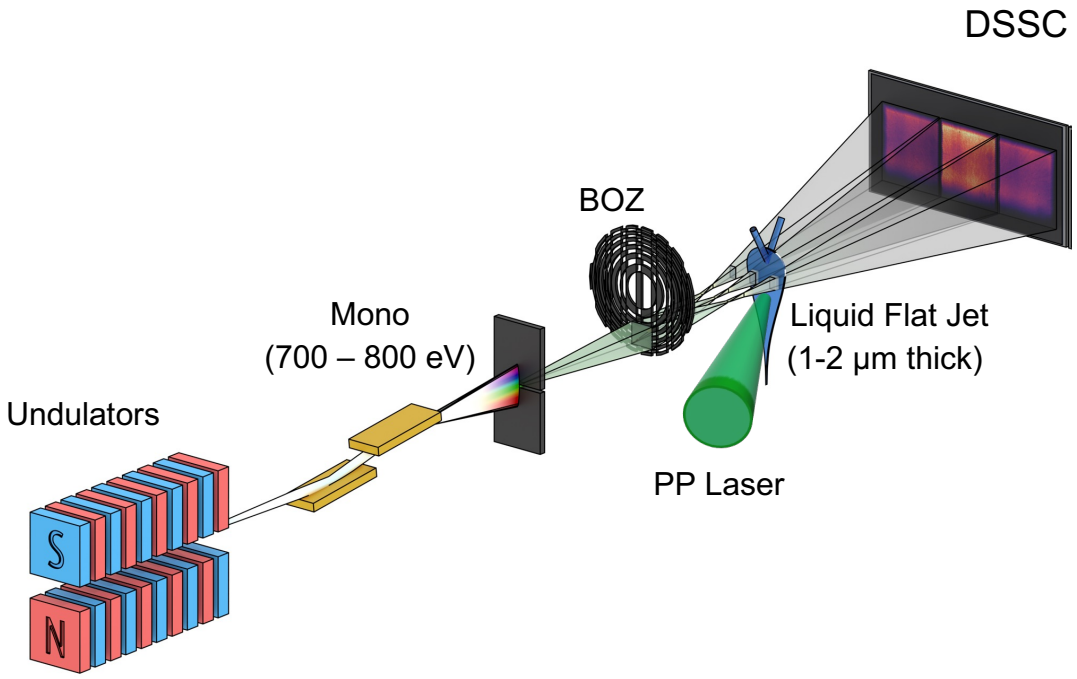
RIXS on Samples ≥10 mM



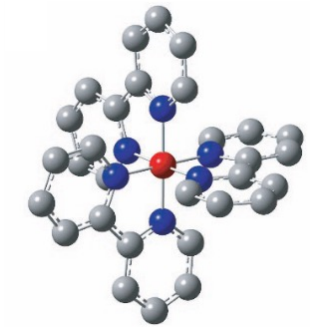
User-assisted commissioning (2022)

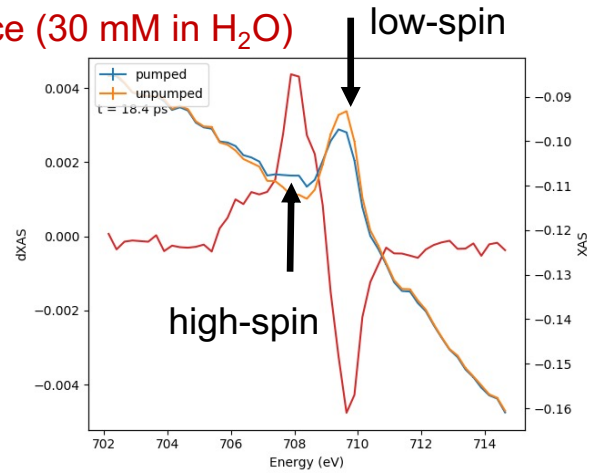
Ultrafast Transient Soft X-ray Absorption Spectroscopy in Solution at MHz Repetition Rate for Dilute Systems and Biomolecules

Beam-Splitting Off-Axis Zone Plate Setup

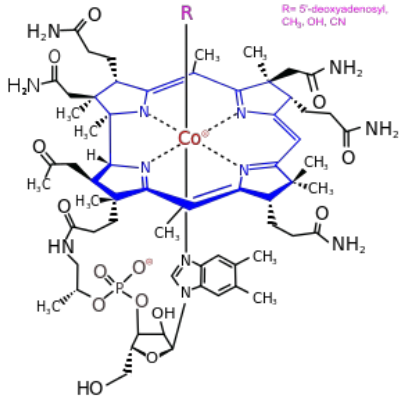


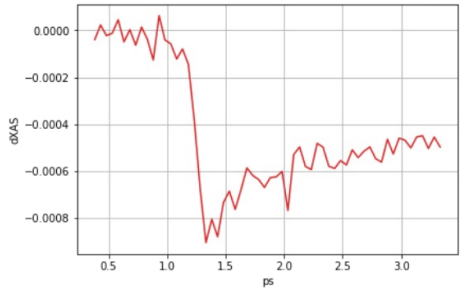
Fe Spin Crossover Reference (30 mM in H_2O)

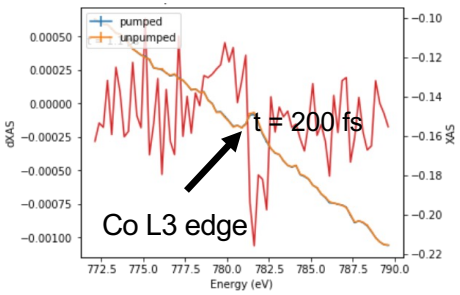




Vitamin B12 (7 mM in H_2O)



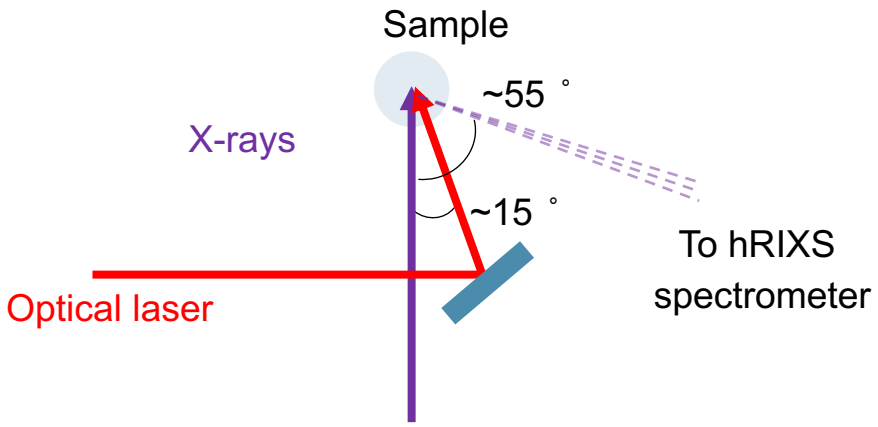




time-resolved changes are in the range of **100 µOD** => Enabling studies of biologically and catalytically relevant molecules in solution that are inherently dilute

Optical delivery to FFT and CHEM

Laser in-coupling geometry for FFT and CHEM



Optical laser system	SASE3 PP laser	
Center wavelength	800 nm	
Pulse duration	15 or 50 fs	
Repetition rate and Pulse energy	2 mJ @ 113 kHz, 800 nm 0.2 mJ @ 1.13 MHz, 800 nm	Other working points exist. Inquire for details
Wavelength tunability	Conversions from 800 nm / 50 fs: SHG (400 nm) , THG (266 nm), OPA: wavelength between 350 nm and 2.5 microns Please inquire for details on pulse energies	
Spot size	~100 µm	
Polarization	Linear and circular	
Operation	Burst mode synchronized to FEL with jitter <50 fs