# hRIXS@SCS Instrument of European XFEL

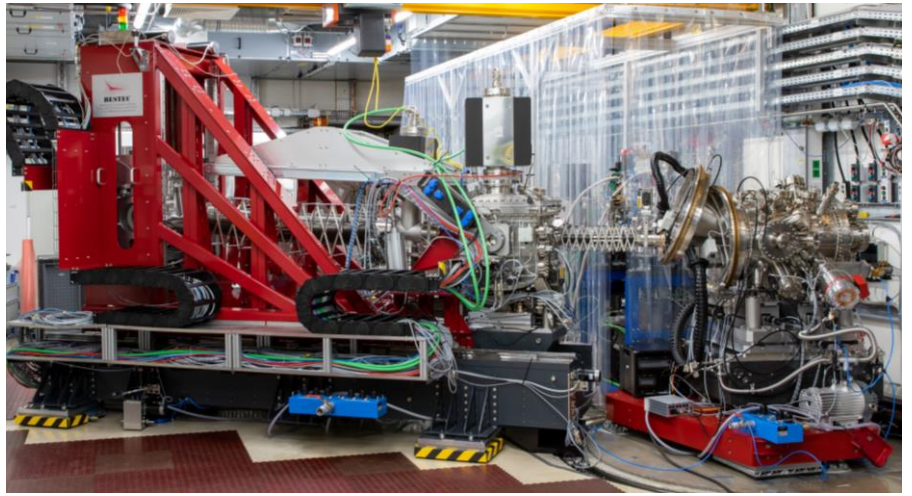
## Webinar for hRIXS user community

October 21, 2021

**Agenda**:

- Status of hRIXS instrumentation (J. Schlappa)
- Report about hRIXS commissioning (B. v. Kuiken)
- Parameters for upcoming call (J. Schlappa, Z. Yin, S. Parchenko)
- Q-A Session

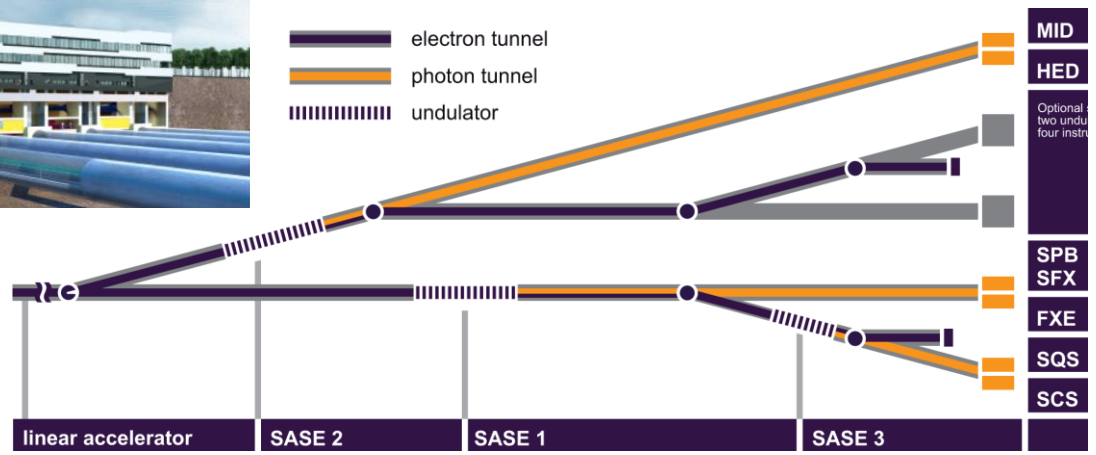
***Please Type your Questions in the Q&A Chat at Any Time***

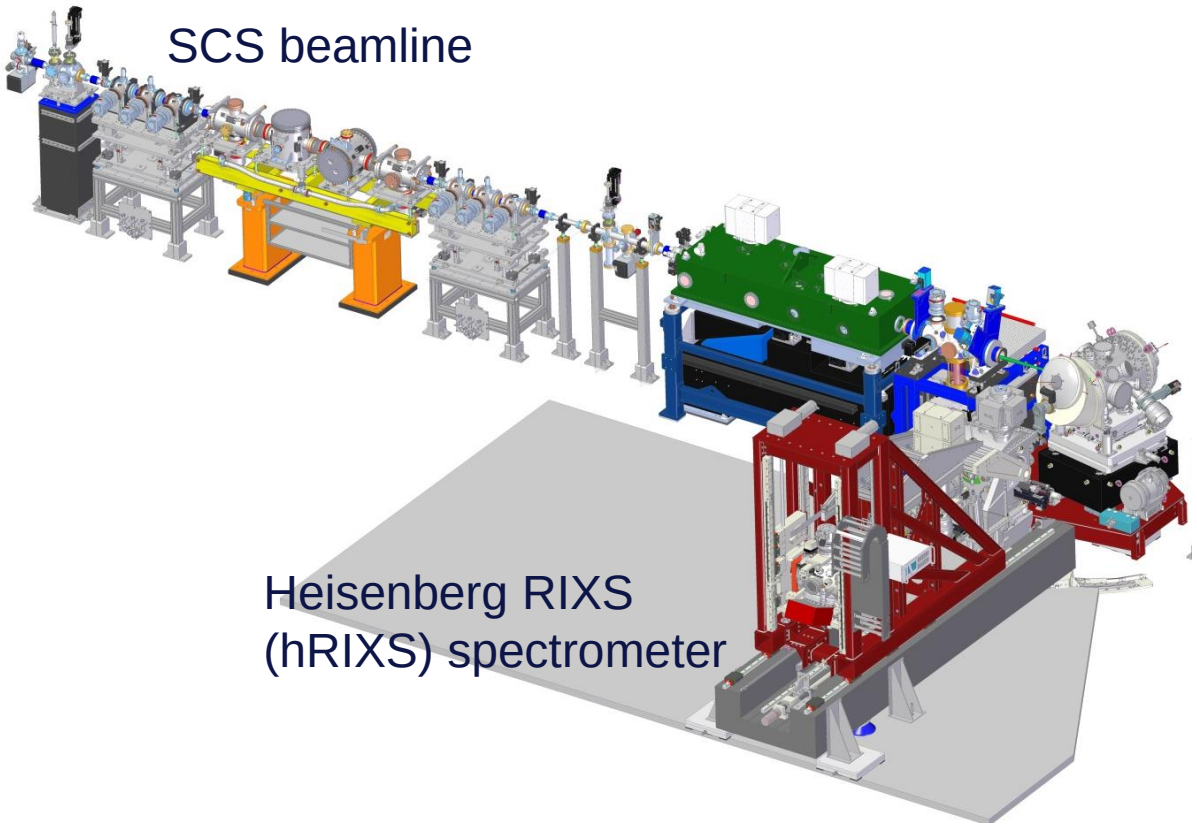


# Status of hRIXS instrumentation

Justine Schlappa
SCS instrument, European XFEL

# SCS Instrument & SASE3, European XFEL



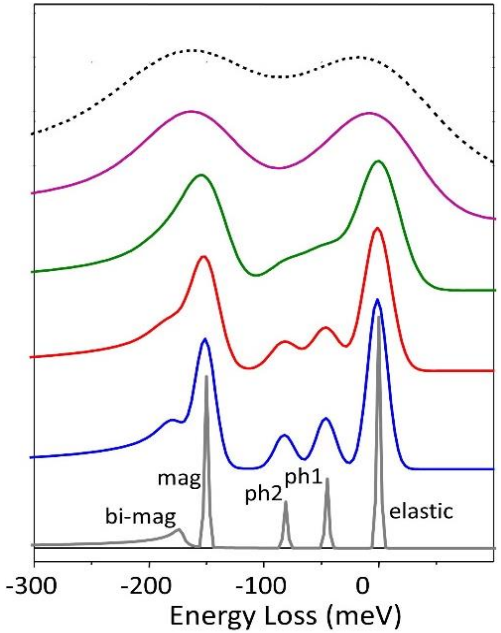




**Spectroscopy and Coherent Scattering (SCS)**:

- Soft x-ray beamline
- Time-resolved/ non-linear x-ray spectroscopies
- Time-resolved/ non-linear x-ray diffraction
- Forward- / small-angle scattering geometries
- Reflection- / backscattering geometries
- RIXS
- Solid samples
- Liquid-jet samples

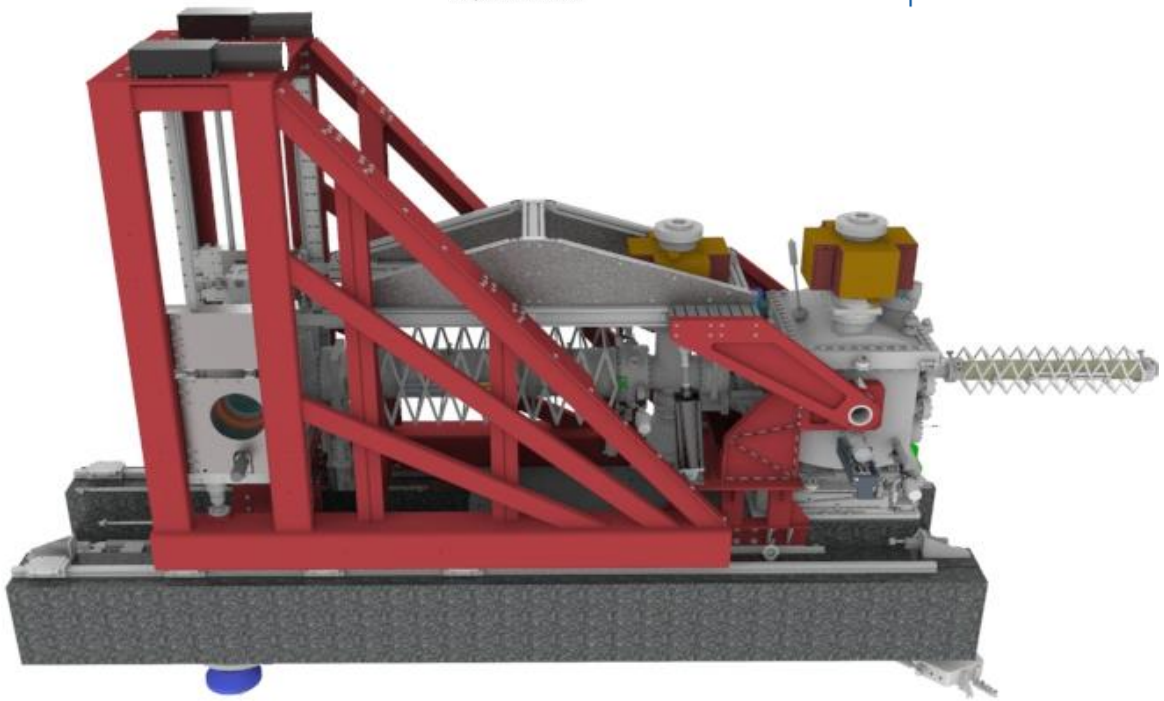
# Heisenberg RIXS (hRIXS) user consortium spectrometer

**Aim:**
Momentum-resolved &
time-resolved resonant inelastic x-ray scattering (RIXS) at the transfer limit




| E/ΔE | Δt (fs)@ 1 keV | Δt (fs)@ 300 eV |
|---|---|---|
| 7000 | 28 | 93 |
| 10000 | 41 | 137 |
| 20000 | 82 | 273 |
| 30000 | 123 | 410 |
| 40000 | 165 | 550 |
| ∞ | | |

$\Delta t = h/\Delta E$

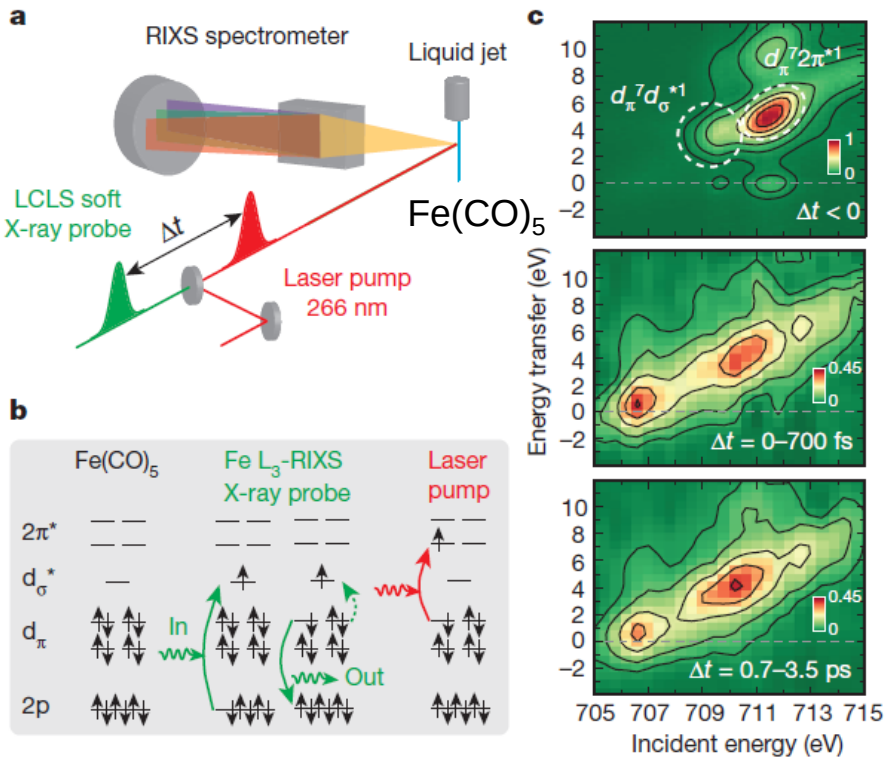


*hRIXS Proposal, User Consortium*

# Scientific Motivation for Time-Resolved RIXS

Photochemical dynamics in transition metal complexes:

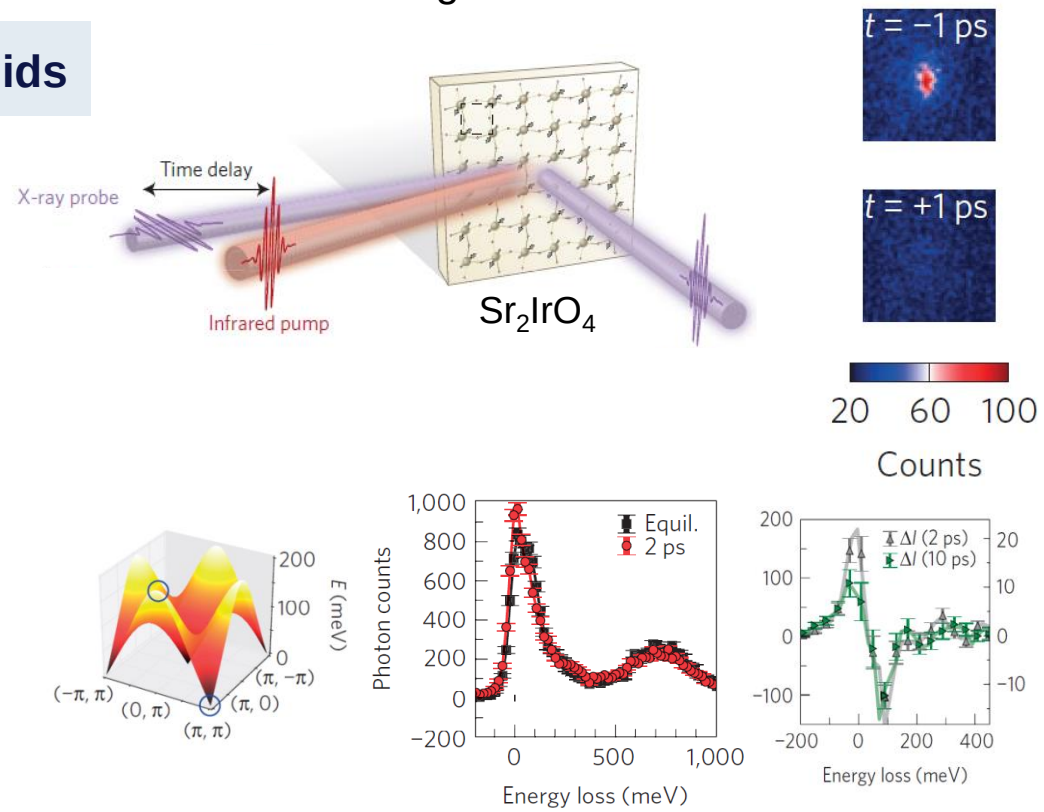
**liquids**




*P. Wernet et al., Nature 520, 78 (2015).*

Dynamics of magnetic correlations in an antiferromagnetic Mott insulator

**solids**

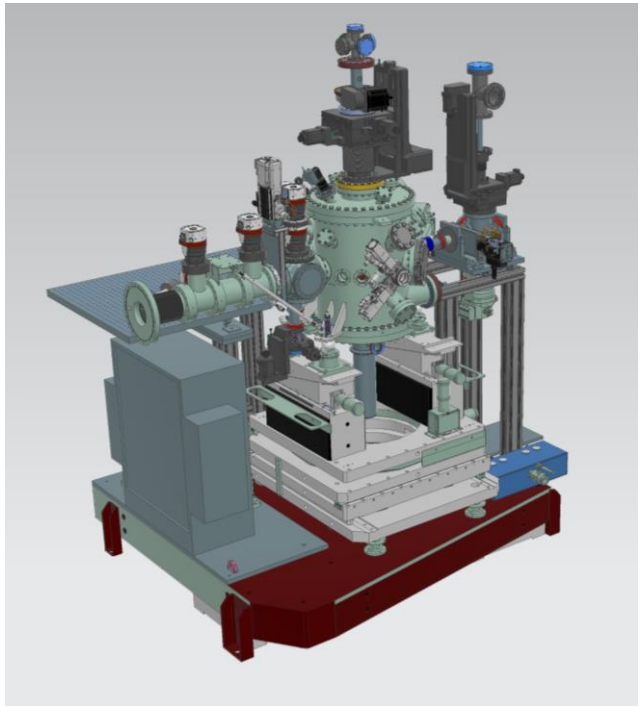



*M. Dean et al., Nature Mat 15, 601 (2016).*

# Sample environment for Time-Resolved RIXS at SCS

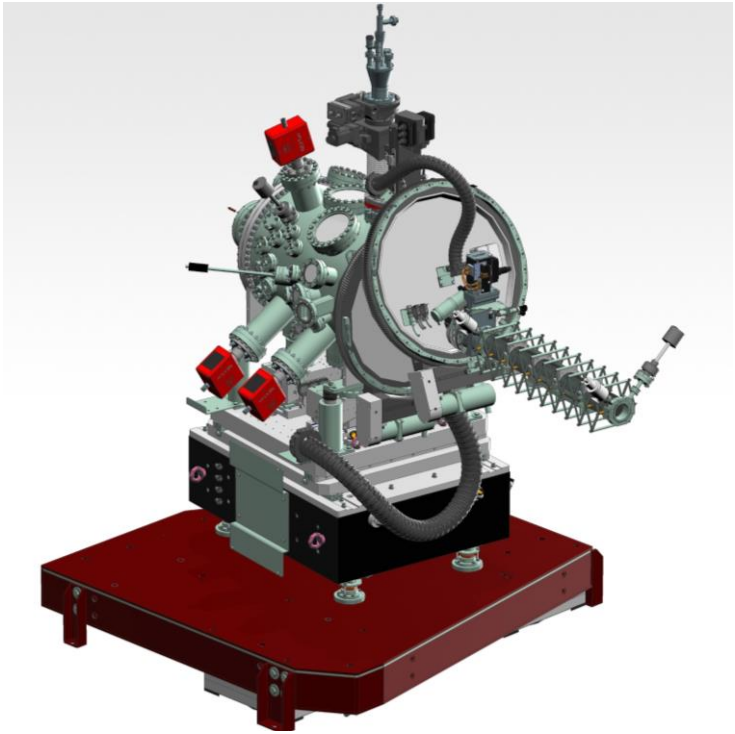
## CHEM-setup

Liquid-jets samples / chemical solid samples (setup by hRIXS UC)



## XRD-setup

Solid samples: UHV and cryogenic conditions (baseline SCS setup)



# Where are we?

- New mono grating installed in January 2021
- hRIXS spectrometer OSAT in February 2021
- X-ray commissioning of static RIXS in May 2021


# Next steps:

- Commissioning of liquid-jet environment (October/November 2021)
- Commissioning of time-resolved RIXS (February/March 2022)
- Commissioning XRD setup (starting in April 2022)


# User operation:

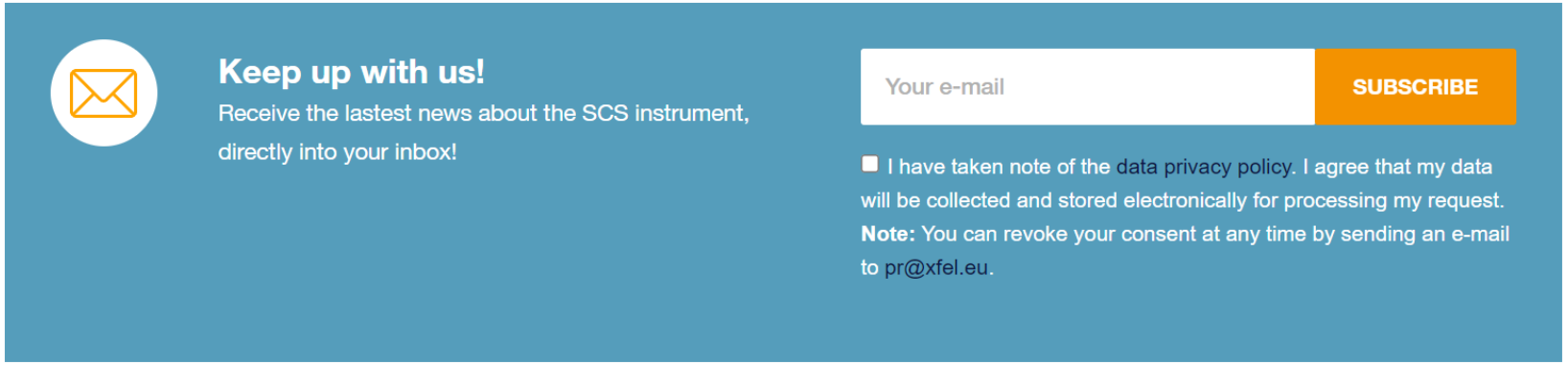
2022-II → Upcoming proposal call

Upcoming proposal call (run 8):

→ announcement will be send out next week

**In order to receive notification subscribe to SCS newsletter at our website:**

https://www.xfel.eu/facility/instruments/scs/index_eng.html

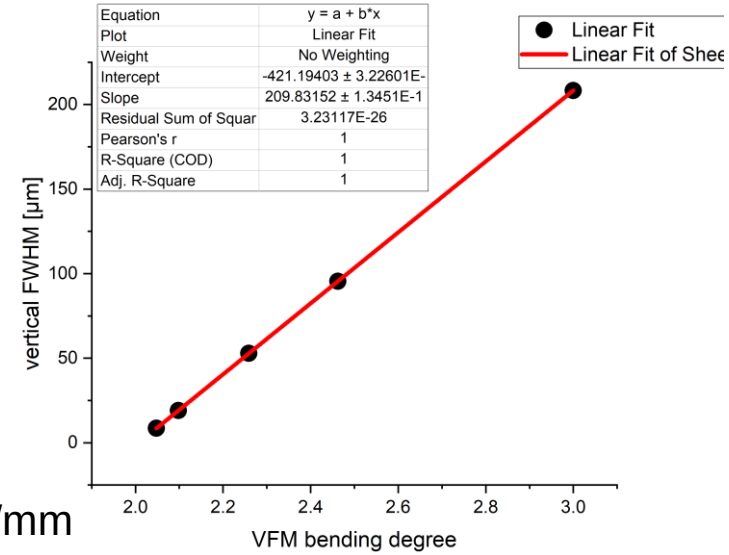


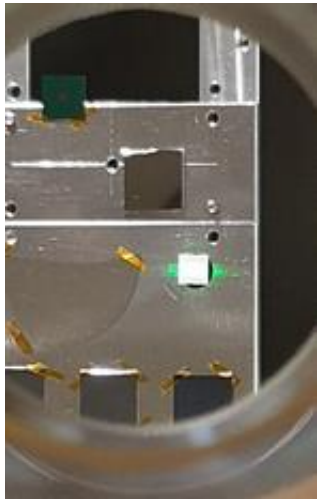
# Report about hRIXS Commissioning

Ben van Kuiken
SCS instrument, European XFEL

# Commissioning Spring 2021: Overview

- Stage 1: Beamline Optimization
  - Characterization of a new 150 l/mm high-resolution grating for beamline monochromator
  - Characterization of new interaction point at SCS instrument
- hRIXS Spectrometer Commissioning
  - Instrument commissioned at Cu L-edge, Ni L-edge and O K-edge with 3000 l/mm grating
  - The Chem endstation was used together with a solid sample holder
  - Initial alignment by optical lasers and using multi-layers with strong specular signal
  - All measurements were performed at 1.1 MHz with 400 pulses/train
  - Princeton CCD detector was used in integrating mode (1 – 10 min acquisition)



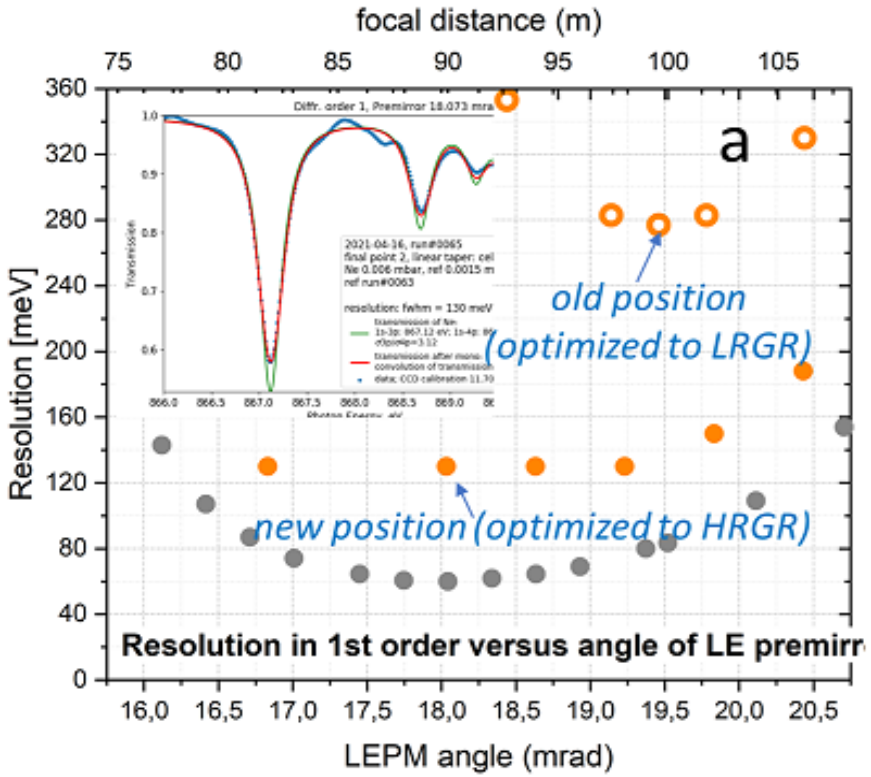



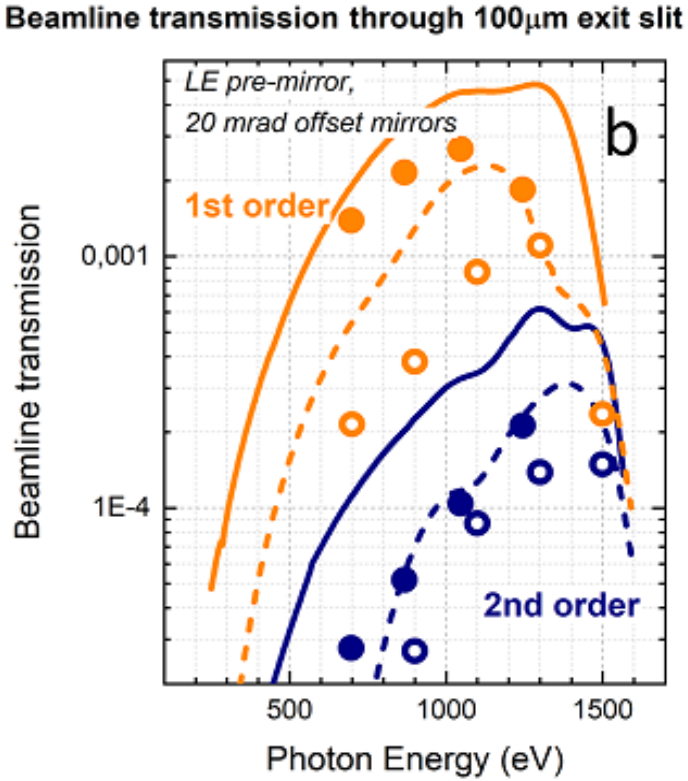
# Soft-X-ray Monochromator upgrade with higher-resolution grating:

## *Resolution optimization of HRGR by aligning angle of LE premirror at Ne absorption lines 1s-3p (867.1 eV), 1s-4p*

**New 150 l/mm grating (HRGR)**

- funded by hRIXS project
- 1yr from order, integration during winter shutdown and commissioning in 2021-I by SCS, XRO, and vacuum group
- Resolving power >7000 (Ne lines)
- resolving power > 10.000 confirmed at 530eV and 930eV using the hRIXS spectrometer (combined res.)



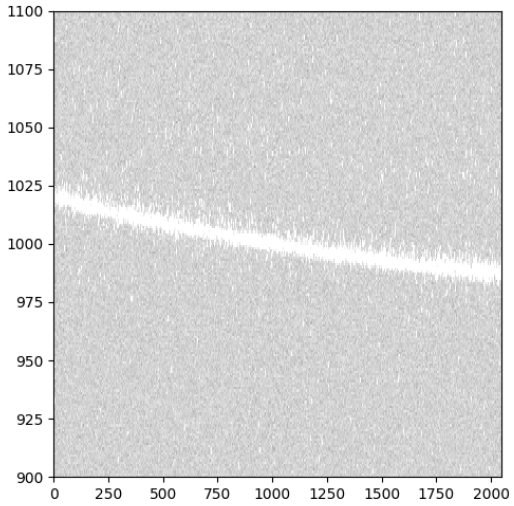




- *LRGR, measured*
- *HRGR, measured*
- *wavefront propagation*

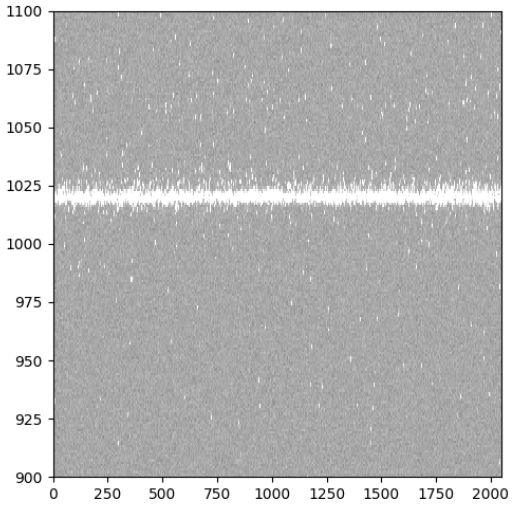
*Transmission of SASE3 beamline in 1st and 2nd diffraction orders for LRGR (solid lines and circles), HRGR (dash lines and open circles)*

# hRIXS Data Collection and Working Points

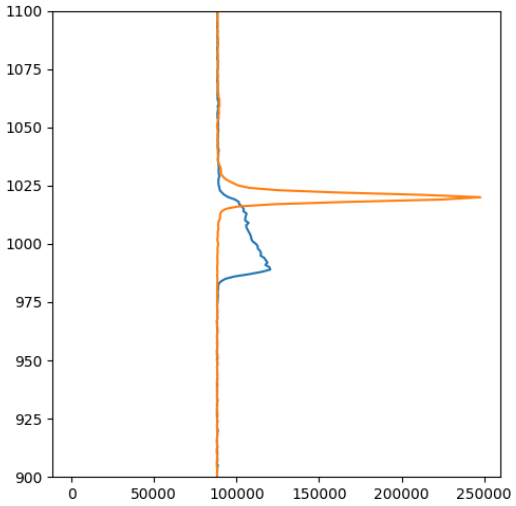
Raw Data




Curvature Corrected




Summed Spectra



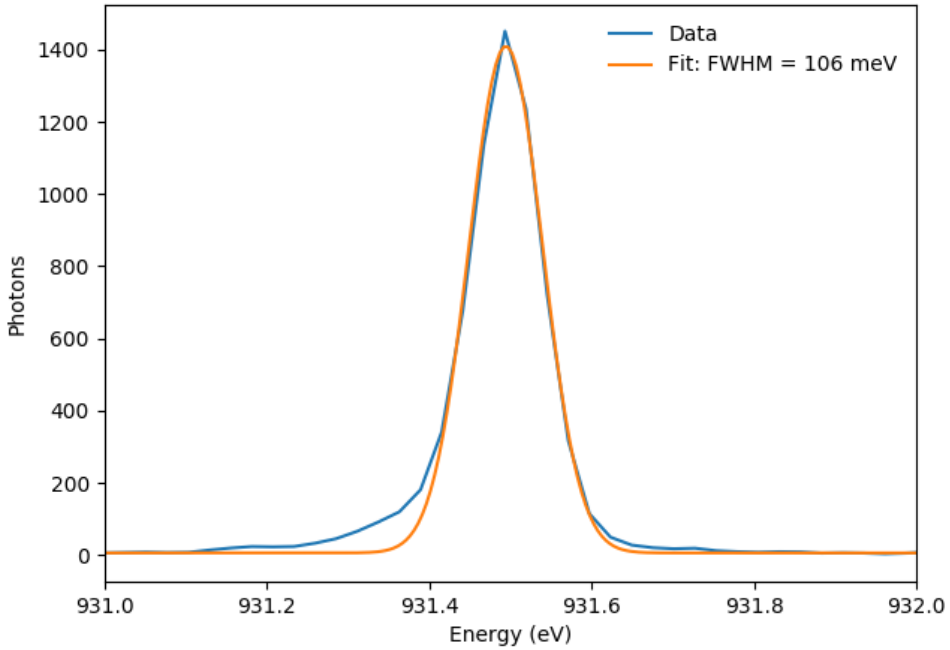

- Data is only curvature corrected
- No binning or cosmic ray removal has been performed in data shown today

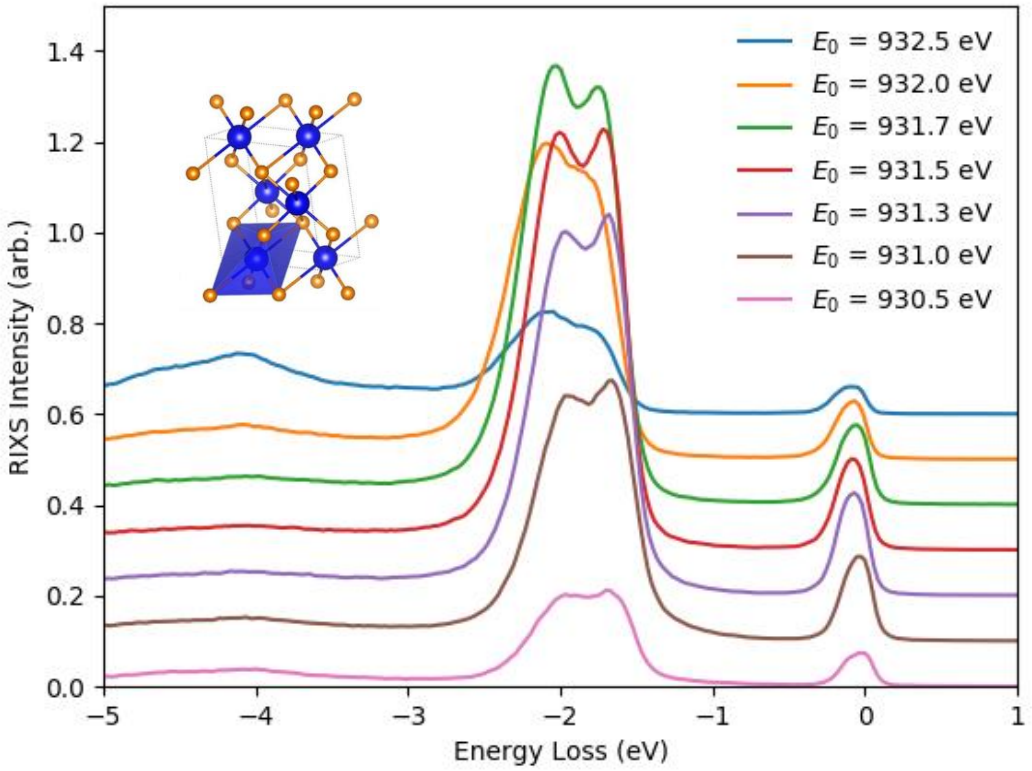
* not enough time to optimize

| 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 |

# Cu L-edge RIXS: CuO

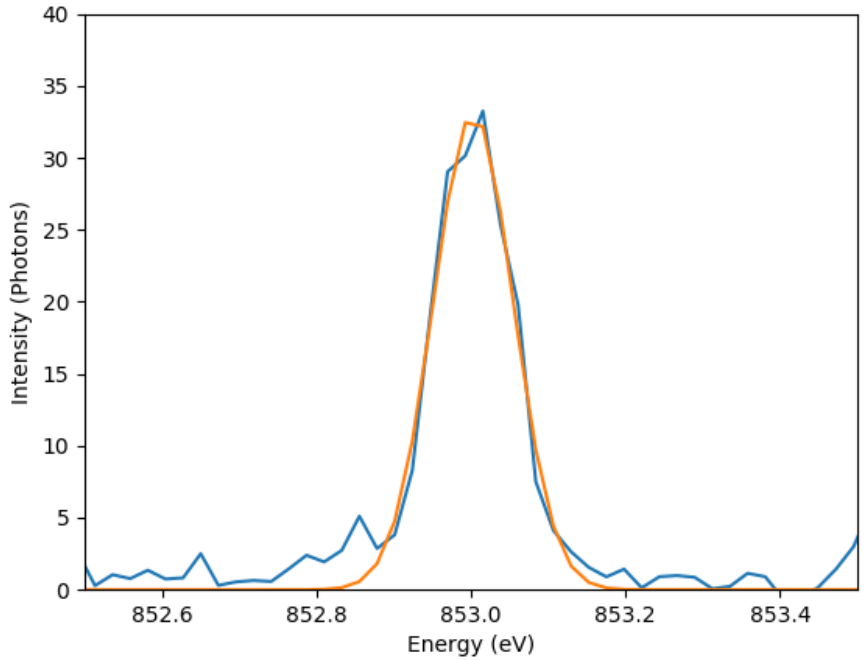
Elastic line at 931.5 eV Measured on NiO
FWHM = 106 meV
E/ΔE = ~8700

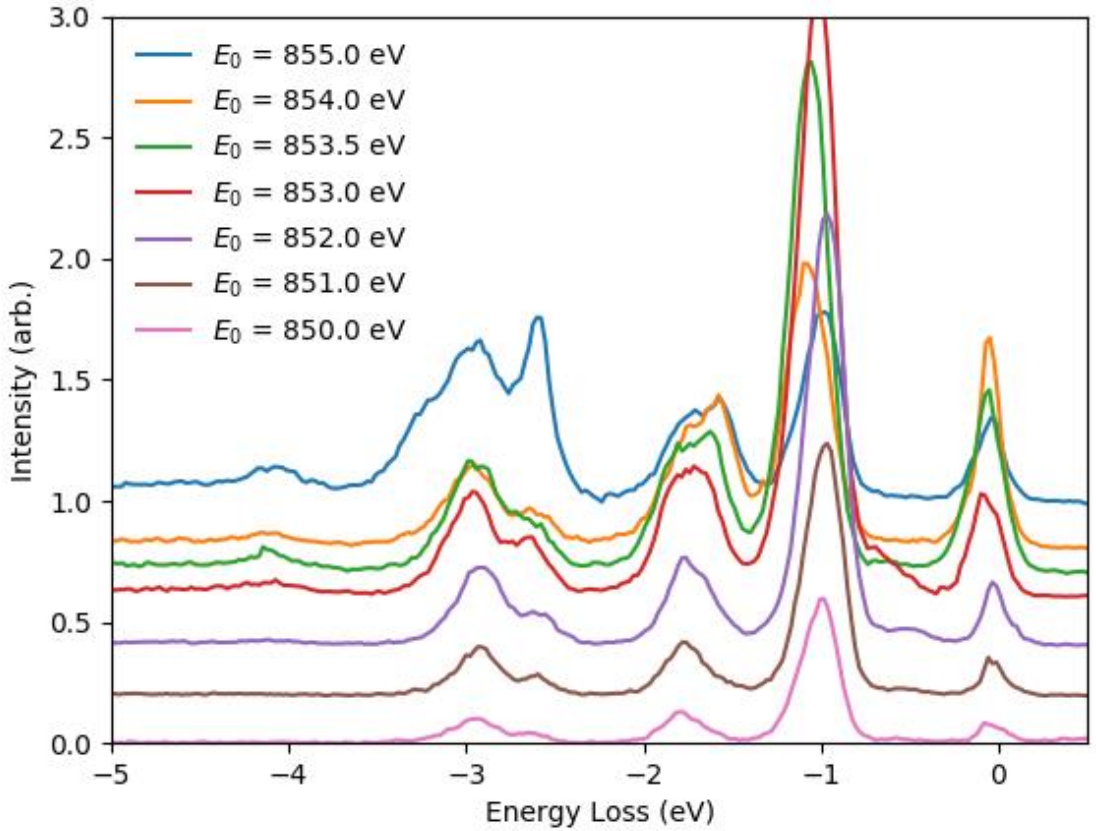


# Ni L-edge RIXS: NiO

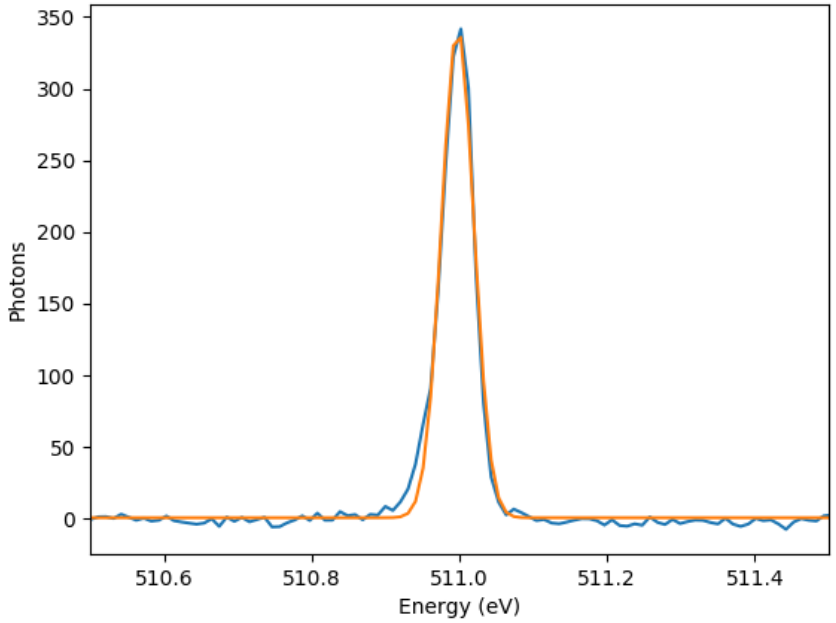
Elastic line at 853 eV Measured on CuO
FWHM = 122 meV
E/ΔE = ~6900

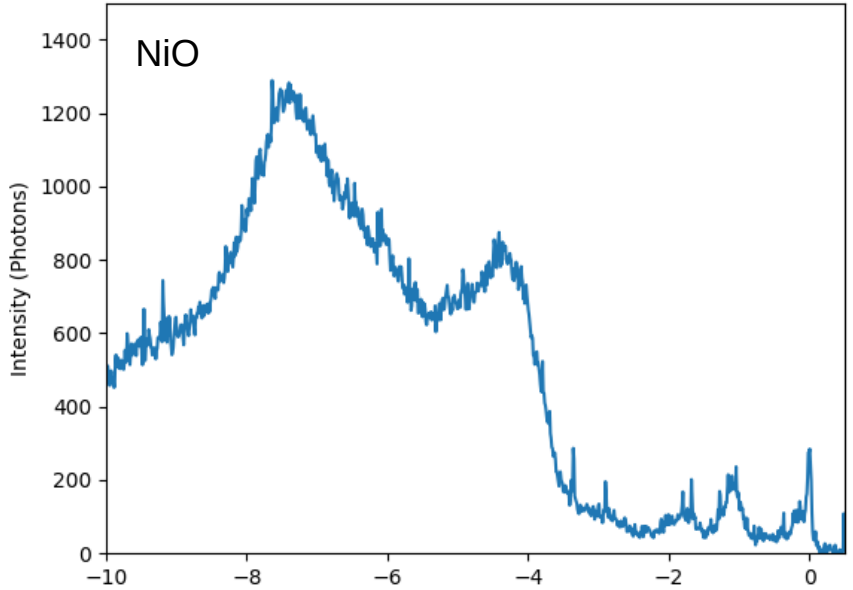


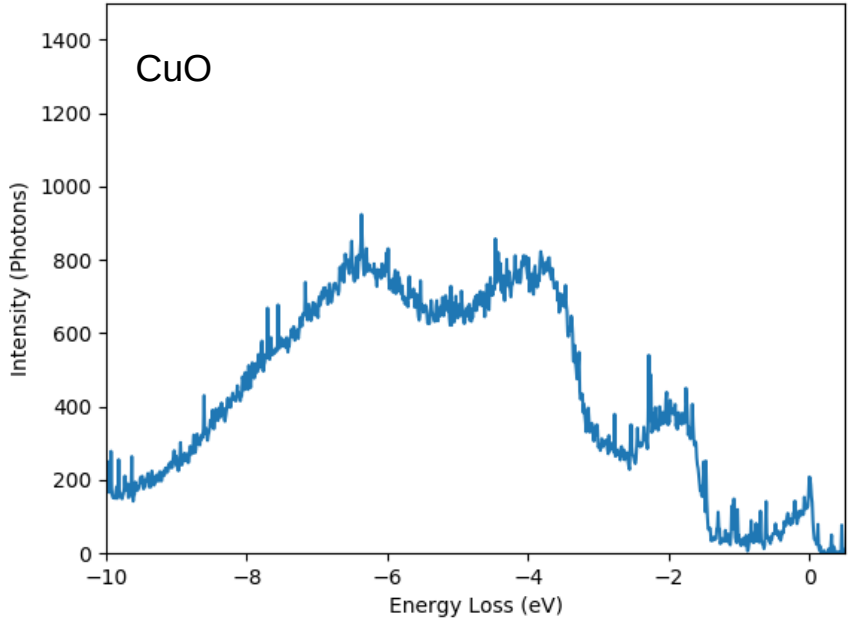
# O K-edge RIXS

Elastic line at 511 eV Measured on NiO
FWHM = 49 meV
E/ΔE = ~10500




Sum of 15
10 min spectra
E0 = 531.6 eV

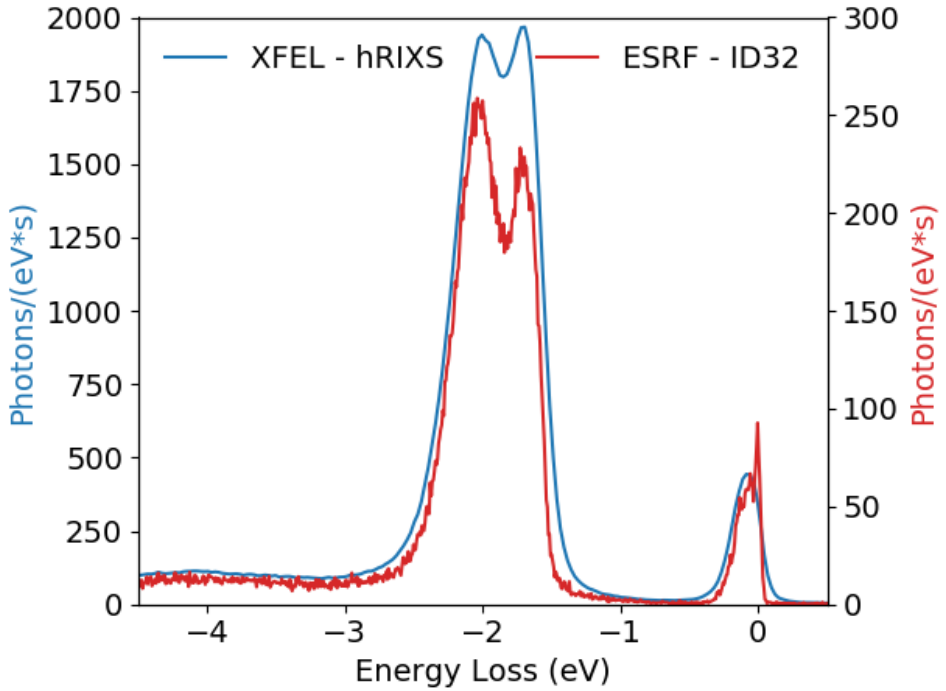



Sum of 14
10 min spectra
E0 = 530.1 eV

# Measurement Count Rates

## Cu L-edge

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



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## Cu L-edge

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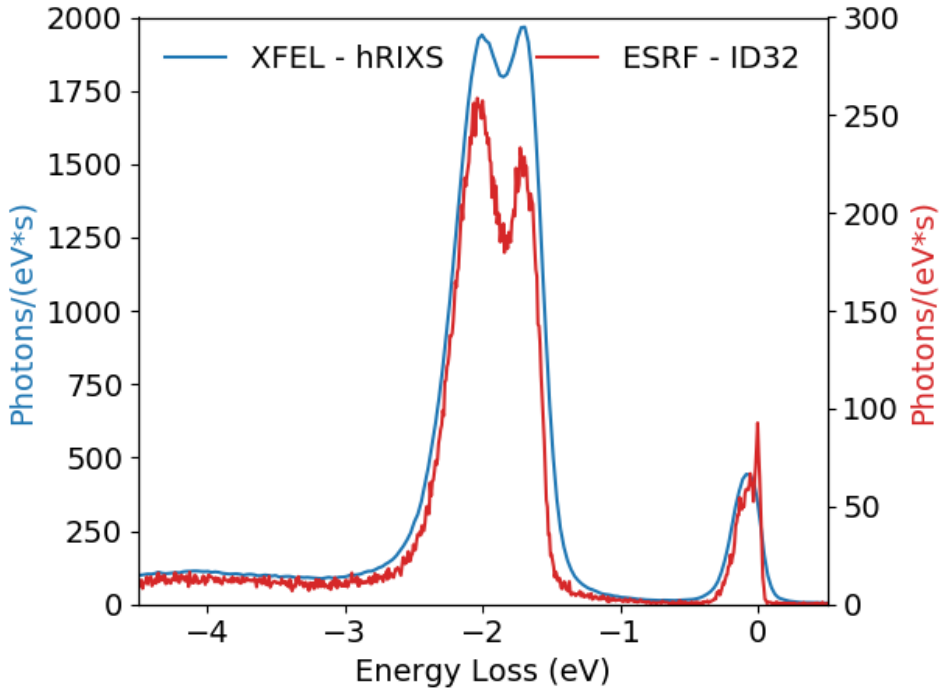
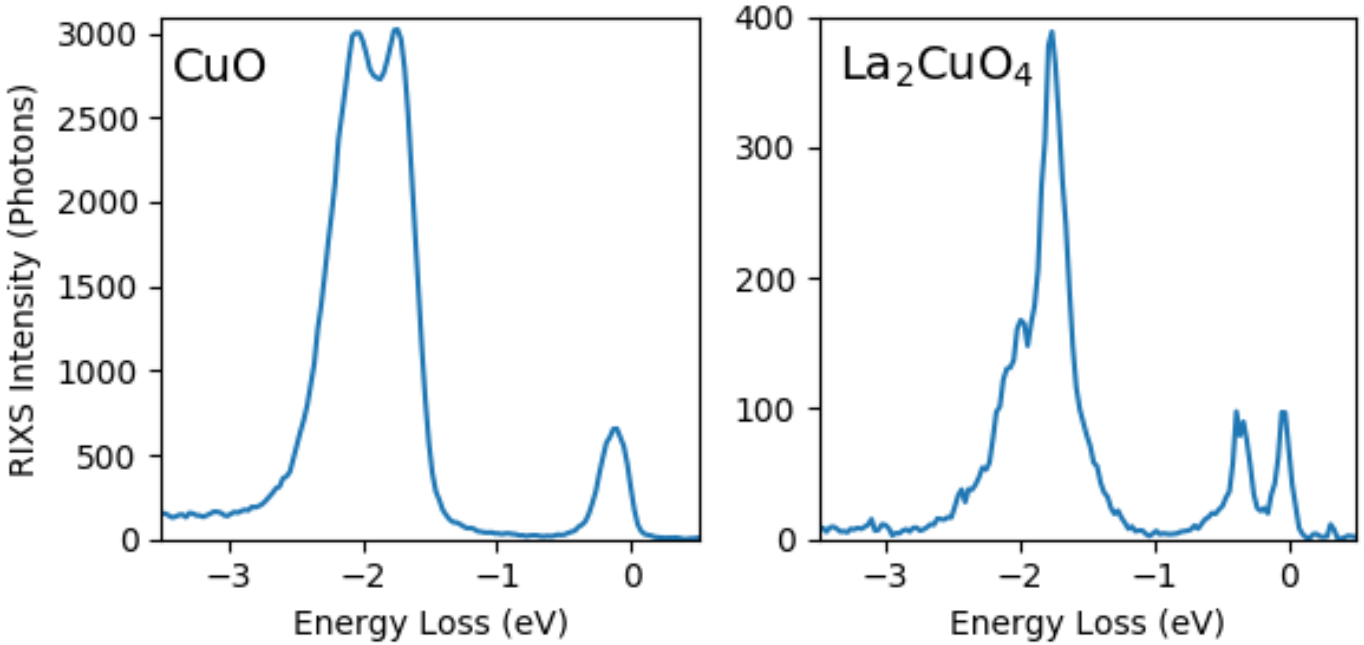


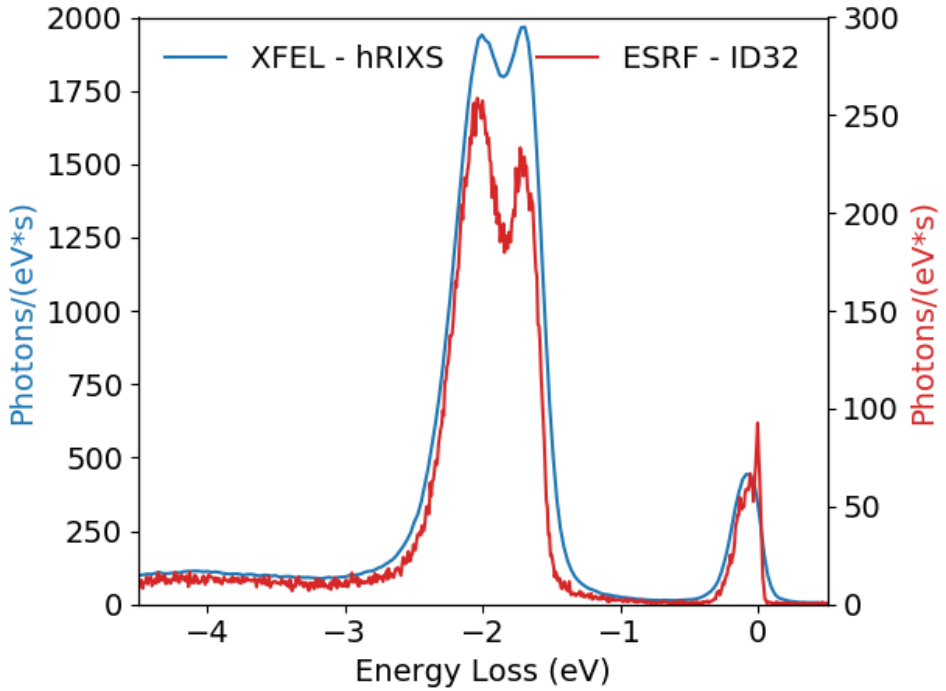




- CuO spectrum measured with 100% GATT transmission (~2 mW), 400 pulses/train, and a 1 min acquisition, 80% wt. Cu
- $La_2CuO_4$ thin film spectrum measured with 10% GATT transmission (~0.2 mW), 400 pulses/train, and a 10 min acquisition, 16% wt. Cu

# Measurement Count Rates

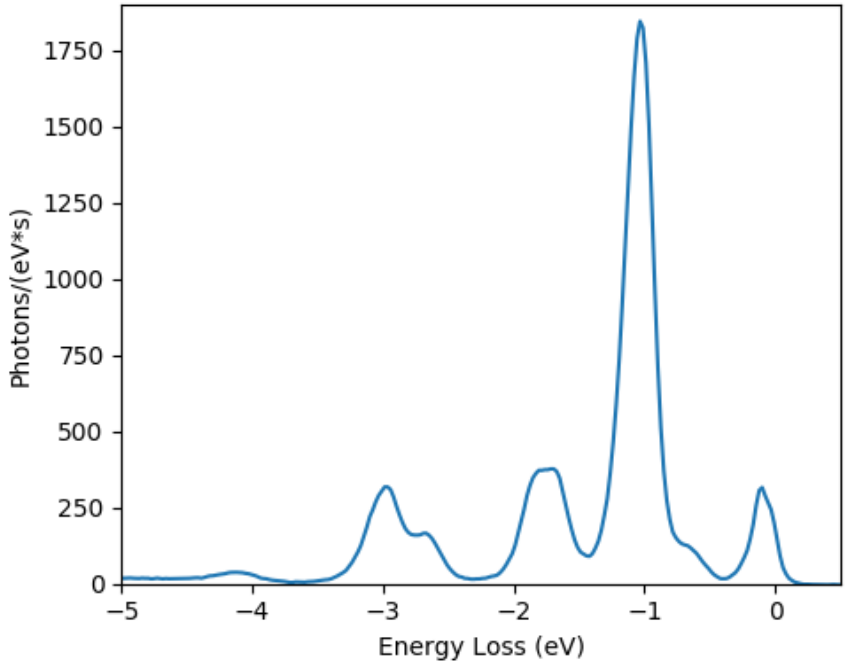
## Cu L-edge

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




## Ni L-edge

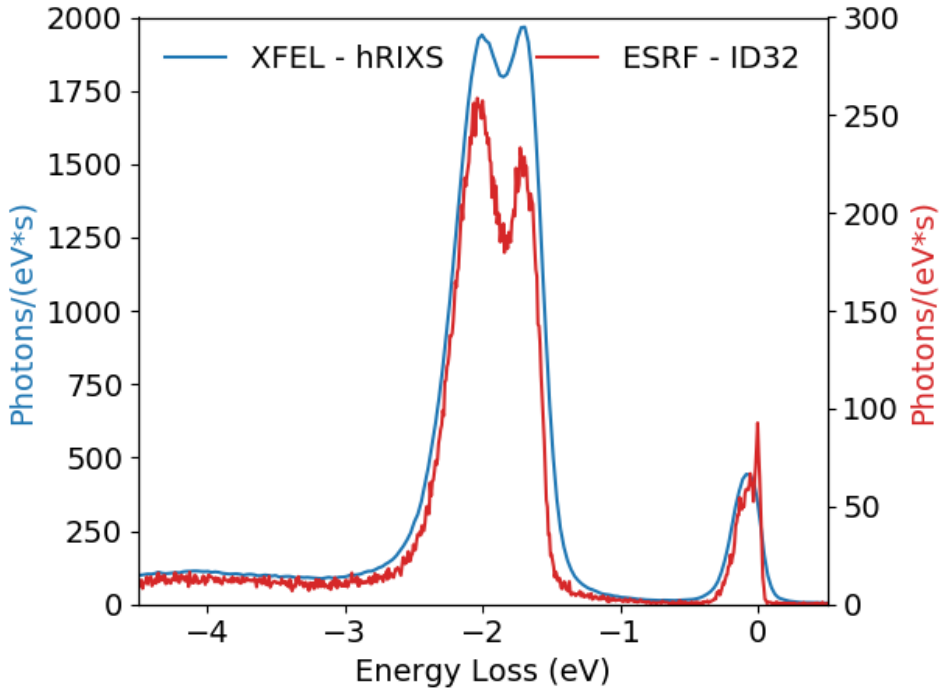
Incident Beam 1.0 x $10^{13}$ ph/s



# Measurement Count Rates

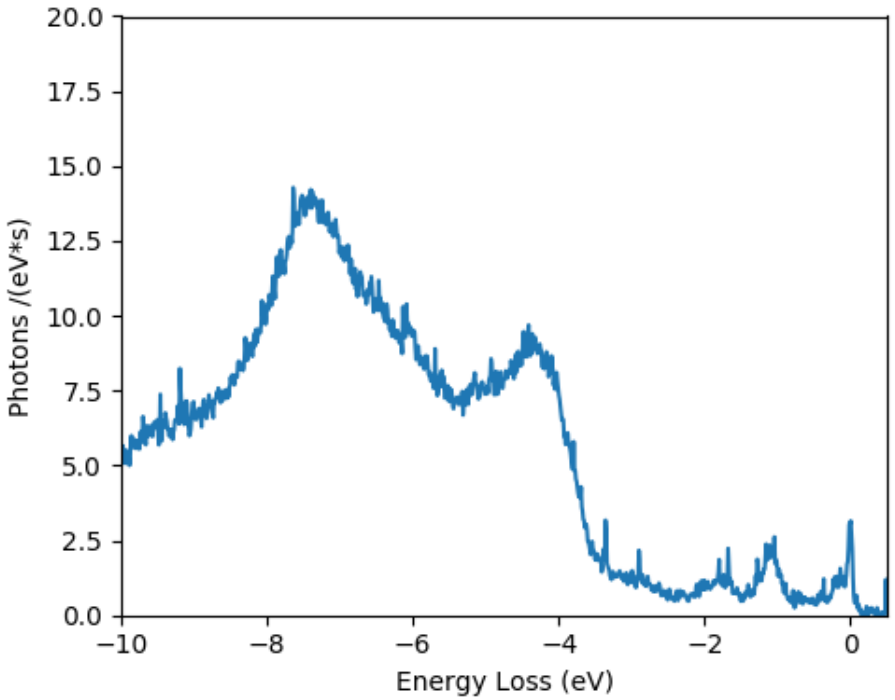
## Cu L-edge

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



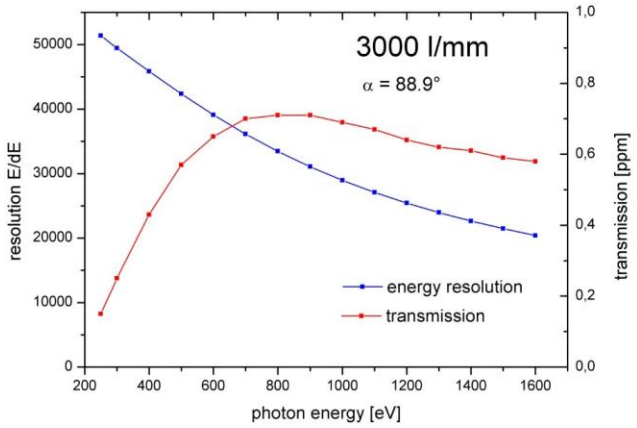

## O K-edge

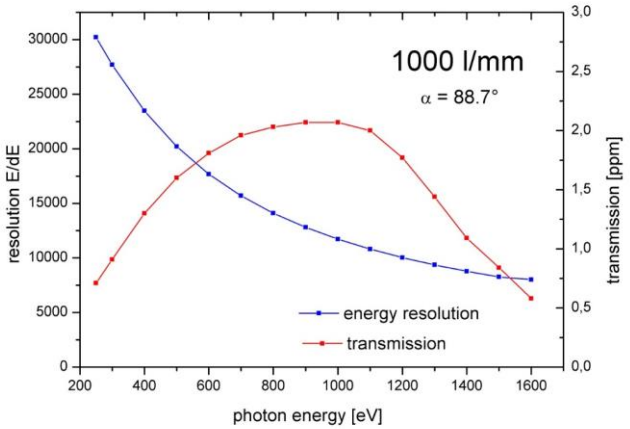
Incident Beam 1.6 x $10^{12}$ ph/s



# Expected Parameters

- 1000 l/mm grating will offer higher efficiency




- Expected Count Rates for Liquid samples
  - O K-edge measurements of liquid water (55 M) compare similarly to metal oxide O K-edge spectra (79 and 90 M for CuO and NiO, respectively)
  - A 100 mM solution of a transition metal complex (dilution factor of ~1000) with $La_2CuO_4$

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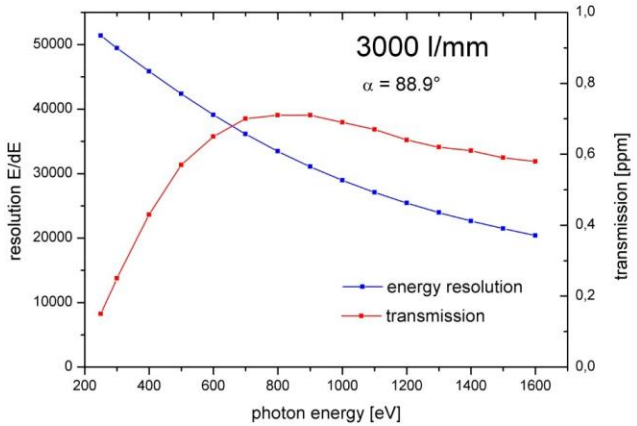


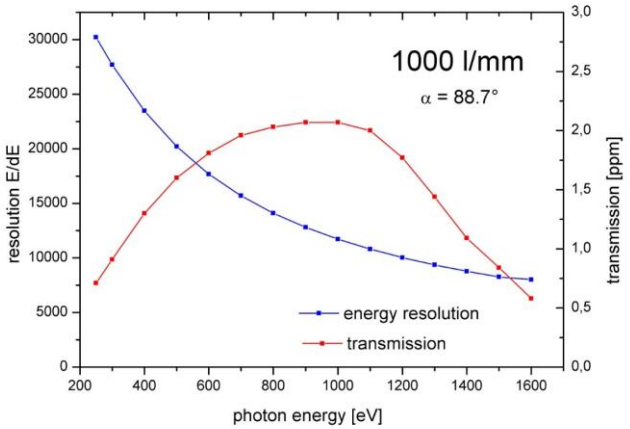


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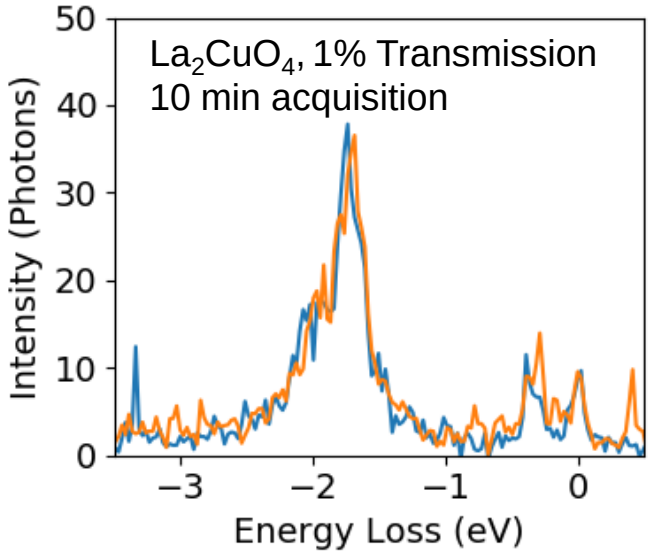

# UAC Q1 2022: Enabling Optical Pump – RIXS Probe at SCS for Solids and Liquids

- Pump-probe on Solid-state samples with Chem Chamber
  - KW6 will be used to commission laser in-coupling and diagnostics
  - KW8 will be dedicated to pump-probe measurements on solid samples at Cu and Ni L-edges

- Pump-probe measurements on Solution Samples
  - KW11 will commission the cylindrical liquid jet system at O K-edge
  - KW13 will be dedicated to pump-probe at Fe L-edge

# Acknowledgement

***European XFEL:***

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***University of Helsinki:***

Simo Huotari

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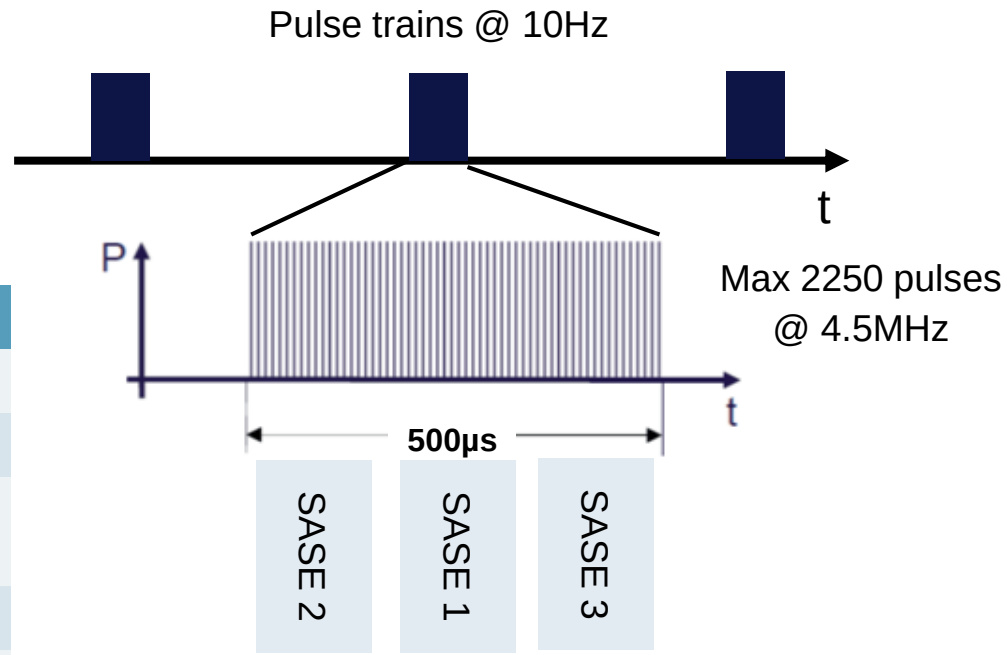
***ERSF**:* Nick Brookes

# Parameters for upcoming call

Justine Schlappa, Zhong Yin, Sergii Parchenko
SCS instrument, European XFEL

# SASE3 parameters for run 8th

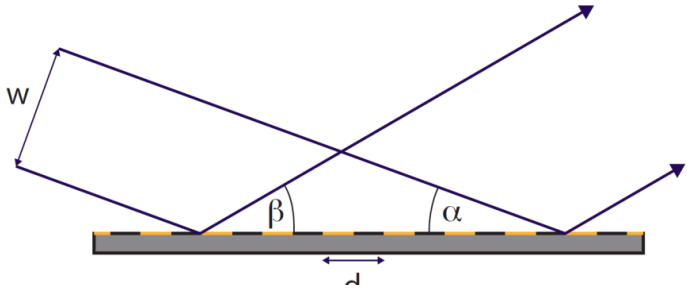
| XFEL beam parameters | |
|---|---|
| **Photon energy** | 0.5 keV – 3.0 keV |
| **Bandwidth SASE3** | 0.5 – 1.0 % |
| **X-ray pulse energy SASE3** | 5 mJ (< 1.5 keV)<br>2 mJ (> 1.5 keV) |
| **X-ray pulse duration SASE3** | 10 – 25 fs |
| **Train repetition rate** | 10 Hz (or train picker) |
| **Repetition rate in pulse train** | Up to 4.5 MHz<br>1.1 MHz for the use of liquid jet |
| **Number of x-ray pulses per train** | 400<br>Assuming equal distribution per instrument at 2.25 MHz FEL operation |
| **X-ray polarization** | Linear horizontal<br>Might become available: linear vertical and circular |




Using alternate mode between SASE1 and SASE3 we can get up to 400 pulses at 1.1 MHz rate.

# Monochromator settings SCS beamline:

The use of monochromator leads to pulse stretching.
Resolution has to be compromised for time resolution.




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 |

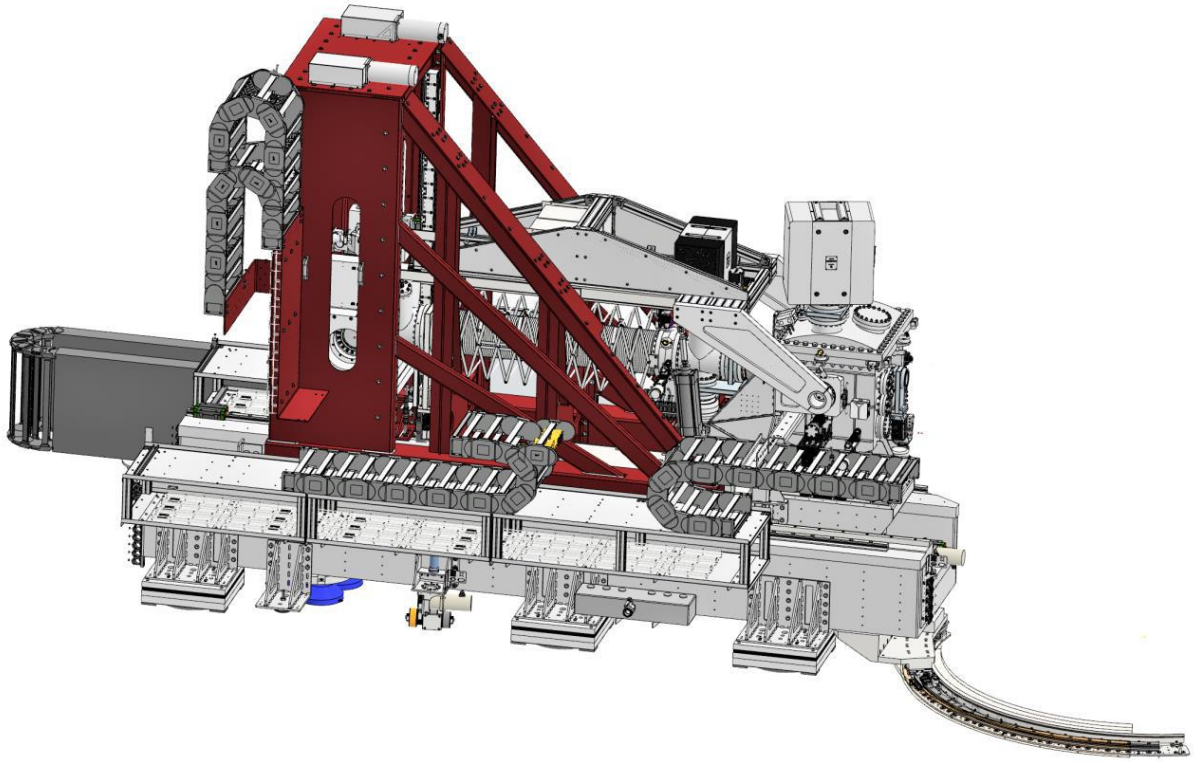
→ Moderate combined energy resolution
→ High temporal resolution

## 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

# hRIXS parameters for run 8th



| hRIXS parameters | |
|---|---|
| **Photon energy** | 0.5 – 1.5 keV |
| **Combined resolving power** | Up to 10.000 (mono HR)<br>3.000 (mono LR) |
| **Transmission** | ~$10^{-6}$ |
| **Time resolution** | Limited by mono:<br>80-150 fs (mono HR)<br>30-50 fs (mono LR) |
| **Scattering angle** | Fixed, angles depend on experimental station |

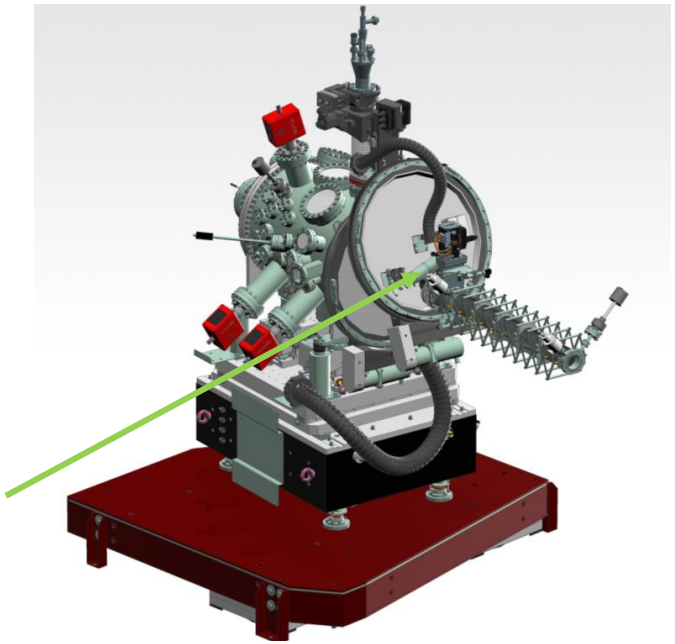
- Continuous motion will be commissioned in beginning of 2022-II and will not be offered yet

# XRD setup (baseline SCS) in run 8th

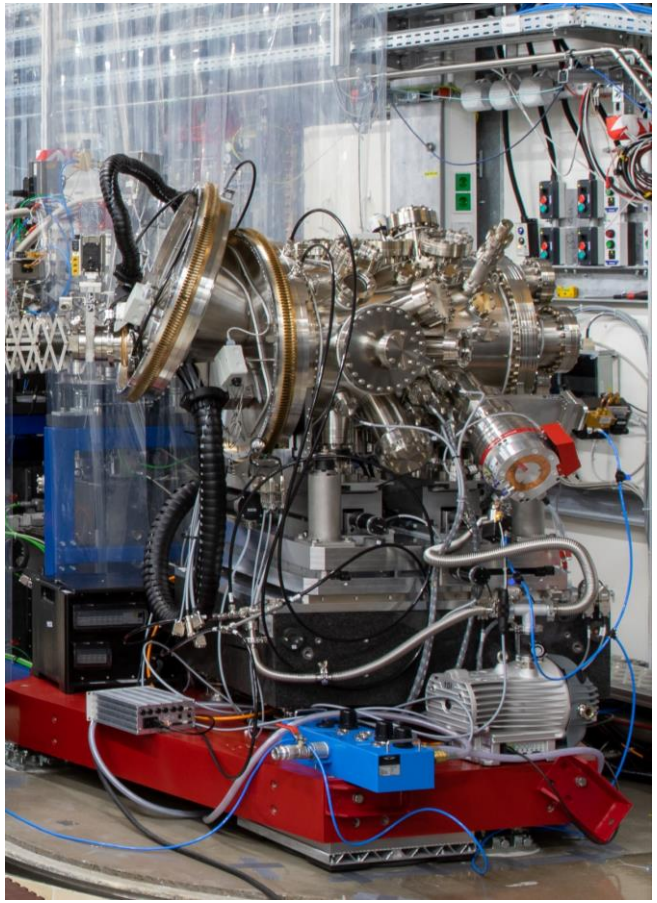
- Time-resolved spectroscopy from solid samples:
  - UHV ($p < 10^{-9}$ mbar)
  - Maximum sample size: ~ 1 $cm^2$
  - Triple-rotating flange to change scattering angle of hRIXS:

65 deg ≤ 2Θ ≤ 145 deg

  - Cryogenic temperatures

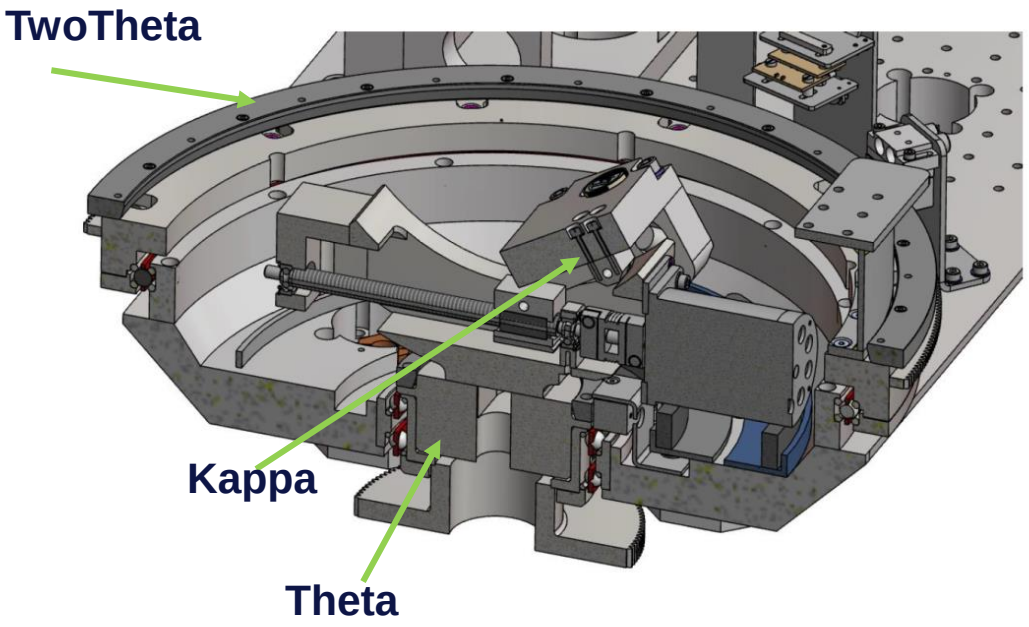


Triple-rotating flange



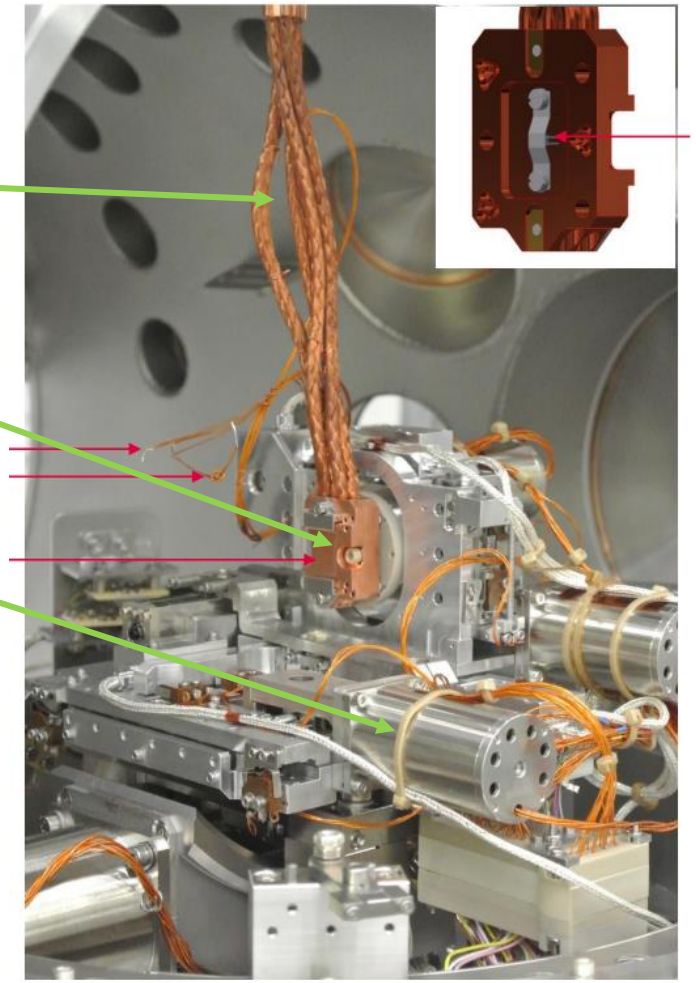
- Technical/offline commissioning starting in April 2022
- No continuous motion of hRIXS during user experiment in run 8th , fixed angle

# XRD inner mechanics

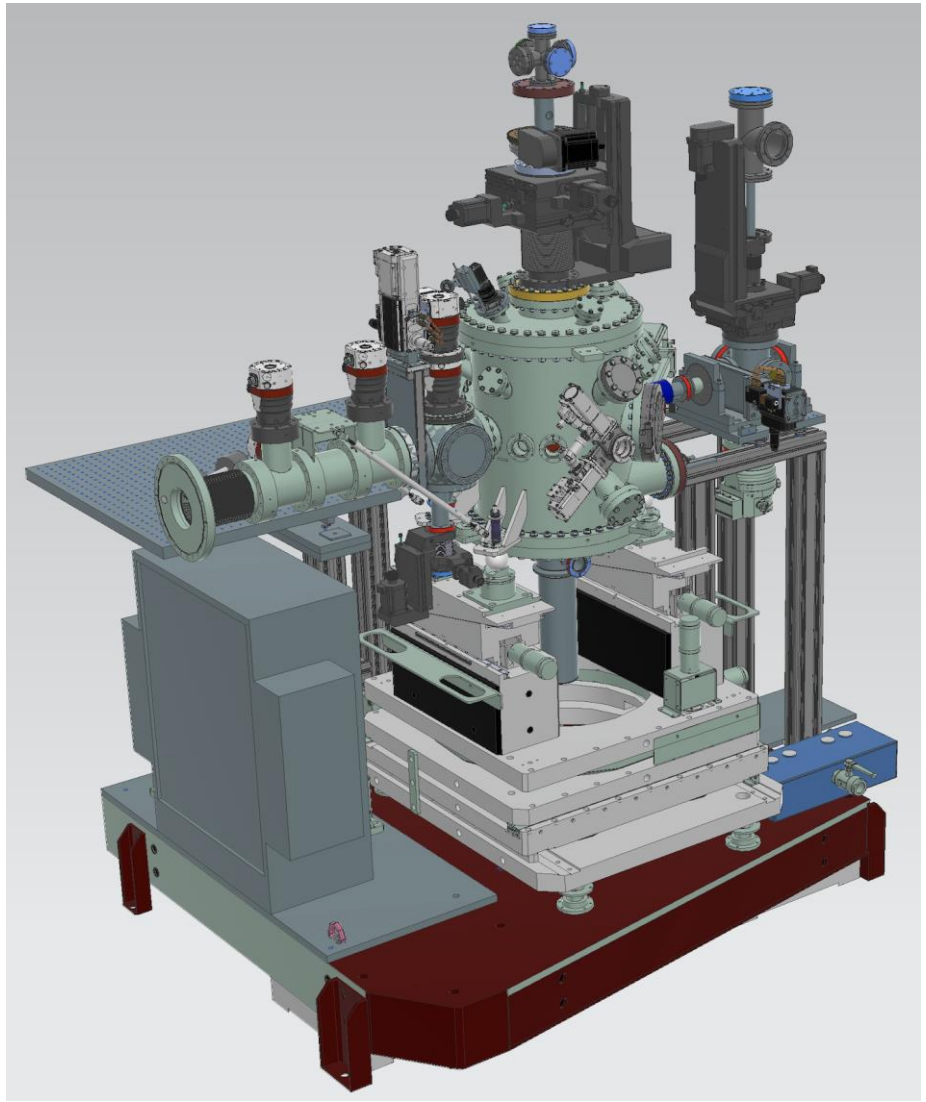



- In-vacuum diffractometer
- Sample: 6 DOF
- Temperatures: RT – 20 K (specification)
- Sample transfer system

| Motion | Range | Repeatibility |
|---|---|---|
| TwoTheta | ± 180 deg | < 1 µrad |
| Theta | ± 180 deg | < 1 µrad |
| Kappa | ± 30 deg | < 1 µrad |
| Azimuth | ± 90 deg | < 0.0002 deg |
| X | ± 5 mm | 0.5 µm |
| Y | ± 5 mm | 0.5 µm |
| Z | ± 5 mm | 0.5 µm |

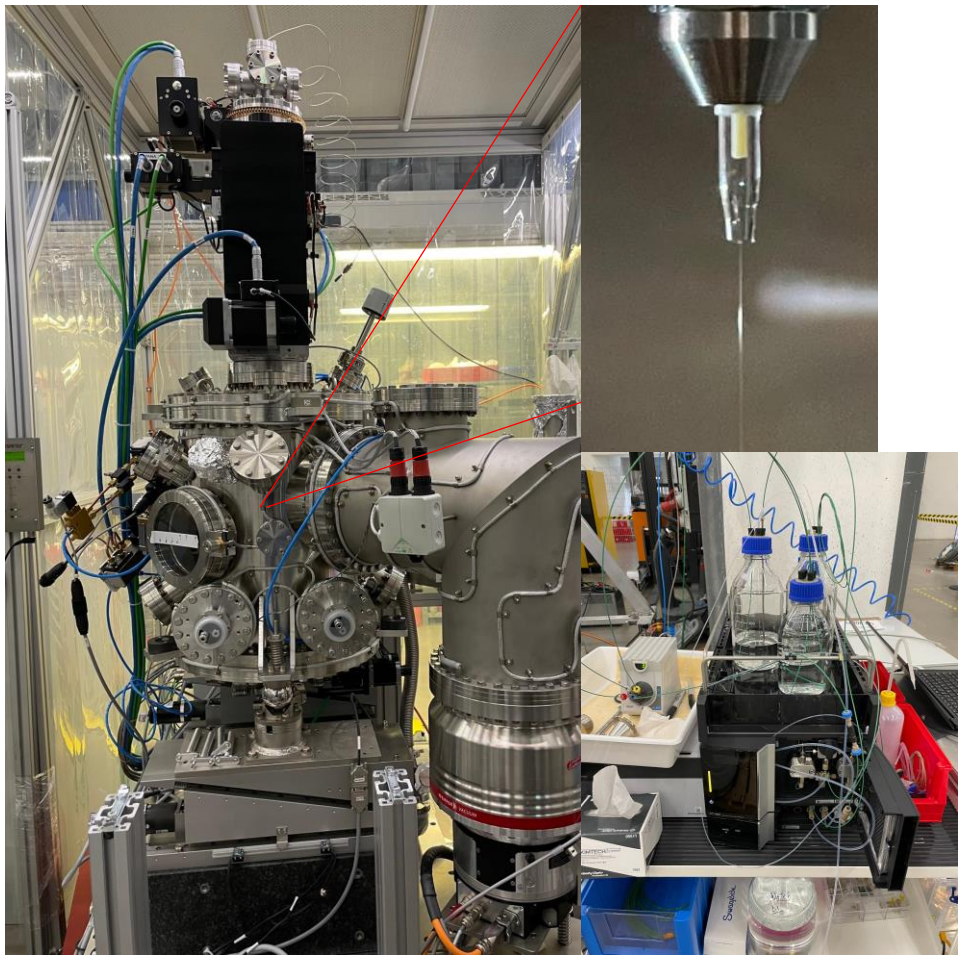


# Chemistry Chamber (by the hRIXS UC)



- **Objectives:**
  - **dedicated experimental chamber for hRXIS studies of chemical systems in the liquid phase**
  - **Cylindrical liquid Jet**
  - **Three differential pumping stages (DPS)**
  - **Highly flexible and motorized sample and chamber aligment**
  - **Multi purpose sample holder**
  - **Multitude of diagnostic tools for, i.e. X-ray spot size, spatial and time overlap**
  - **XAS in TFY**

# CHEM Chamber liquid jet system

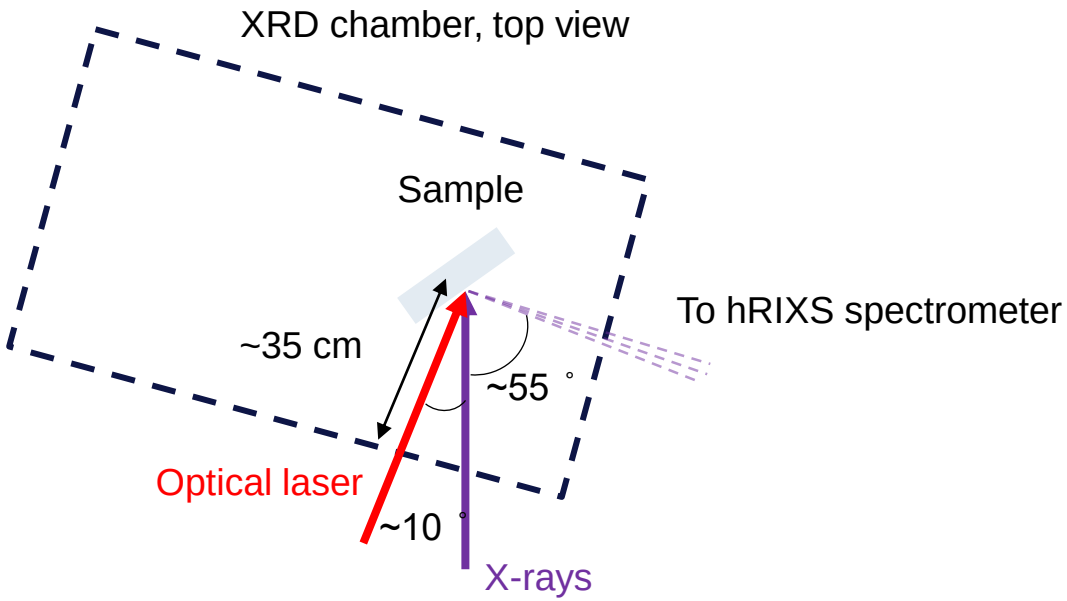


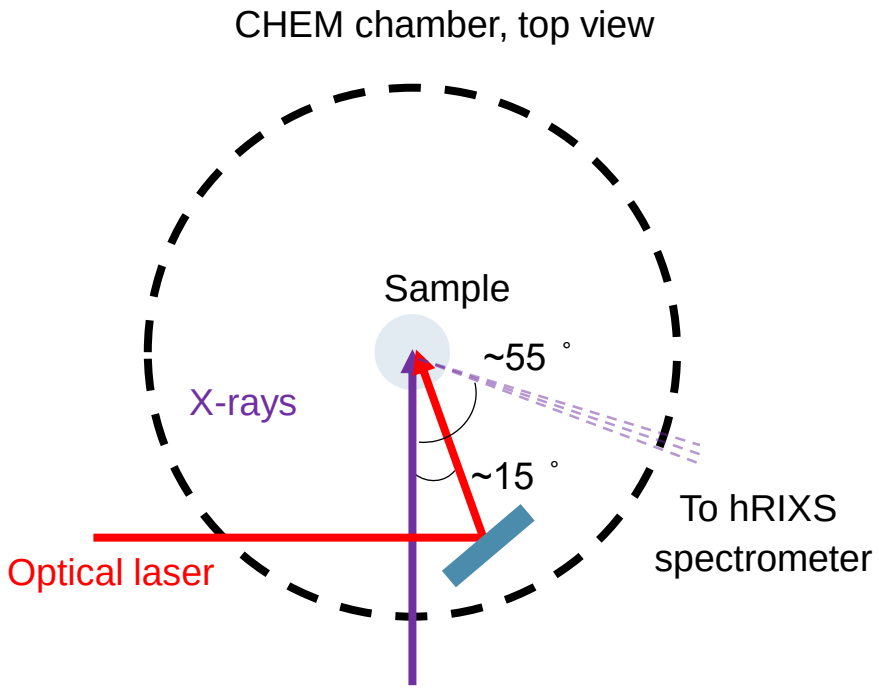
- **Optimized Chem chamber for high resolution time resolved RIXS studies of chemical samples in the liquid phase:**
  - **jet with diameter ranging from 15 µm till 50 µm**
  - **running jet for bio-chemical relevant solvents, i.e. liquid water, ethanol, iso-propanol**
  - **a high spatial resolution microscope**
  - **Switching channel device for up to 6 samples**
  - **Renewable sample, up to MHz repetition rate**

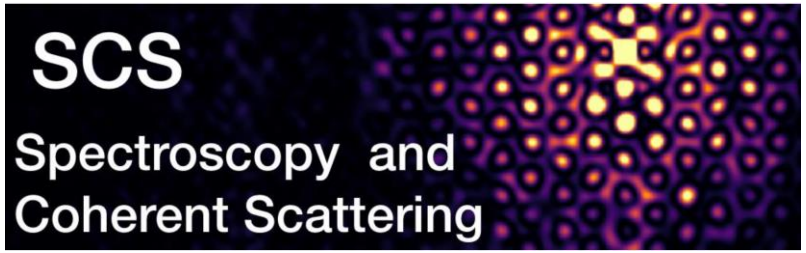
# Optical laser parameters

* Central wavelength: 800 nm, 2 mJ/pulse @ 113 kHz
* Wavelength conversion: SGH – 0.56 mJ/pulse, THG – 0.14 mJ/pulse
  Conversion with OPA: 380 nm – 2500 nm.
  Contact sergii.parchenko@xfel.eu, robert.carley@xfel.eu for details
* Polarization: linear, circular
* Repetition rate: 113 kHz (default), 1.1 MHz – 113 kHz (0.2 - 2 mJ/pulse)

Laser in-coupling geometry.






Website:

https://www.xfel.eu/facility/instruments/scs/index_eng.html

## 8th-Call-for-Proposals: RIXS@SCS

SCS instrument and beam parameters
8th Call-for-Proposals, scheduled for the second half of 2022

DOWNLOAD

**Subscribe to SCS newsletter in order to be informed about proposal calls:**

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# PostDoc position at hRIXS, SCS:

https://www.xfel.eu/careers/open_positions/index_eng.html

## Post Doc / Instrument Scientist (f/m/d)

### The position

- research in ultrafast spectroscopy, particularly time-resolved RIXS, in collaboration with the SCS group and the Heisenberg-RIXS user consortium
- active role in user-assisted commissioning, in-house proposals and development of hRIXS
- user support at the hRIXS spectrometer, CHEM and XRD setup, including shift-work periods (partially nights and during weekends)

### Reference number

S-400

Deadline: 02 November 2021

# Q & A Session

*Please Type your Questions in the Q&A Chat*

## Important Contacts:

Chem Chamber Experiments: Zhong Yin (zhong.yin@xfel.eu)
Ben Van Kuiken (benjamin.van.kuiken@xfel.eu)

XRD Chamber Experiments: Sergii Parchenko (sergii.parchenko@xfel.eu)
Justine Schlappa (justine.schlappa@xfel.eu)

SCS group (scs@xfel.eu)

XFEL User Office (useroffice@xfel.eu)