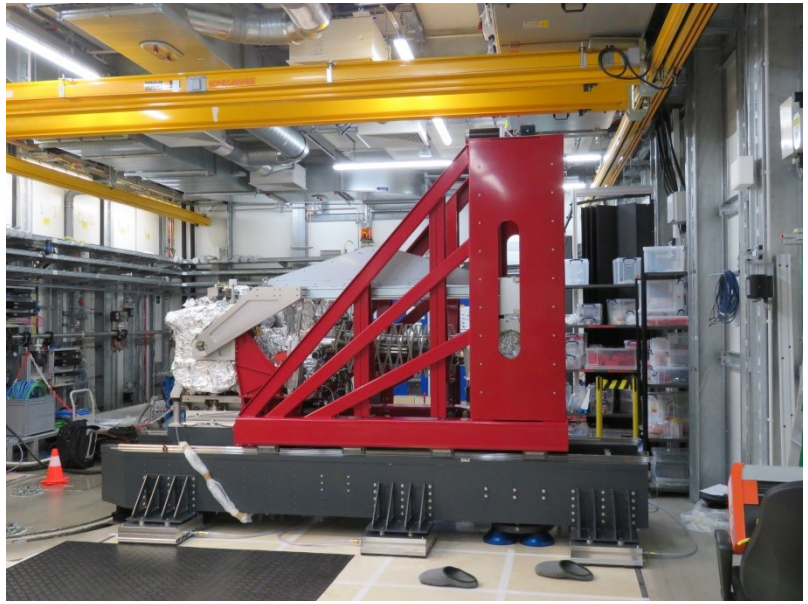
hRIXS@SCS Instrument of European XFEL
Virtual Town Hall Meeting

October 28, 2020



Agenda:

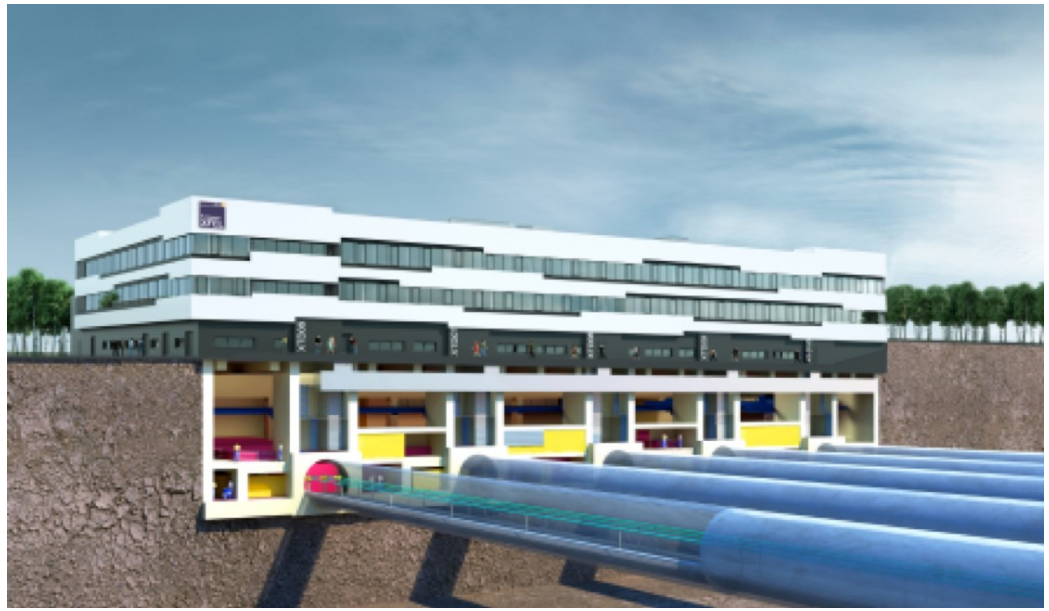
- Status of hRIXS instrumentation (J. Schlappa)
- Commissioning and proposal schedule (A. Scherz)
- Plan for user-assisted commissioning (B. van Kuiken)
- Q-A Session

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

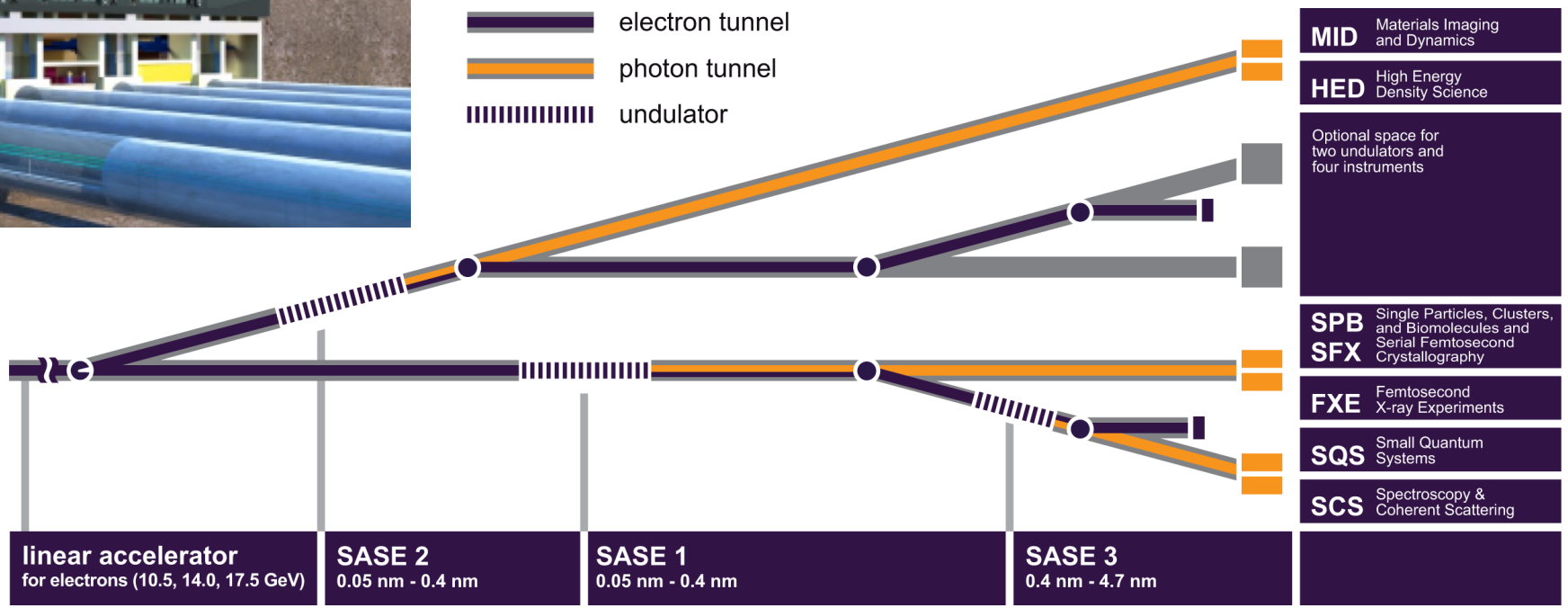
Status of hRIXS instrumentation

Justine Schlappa
SCS instrument, European XFEL

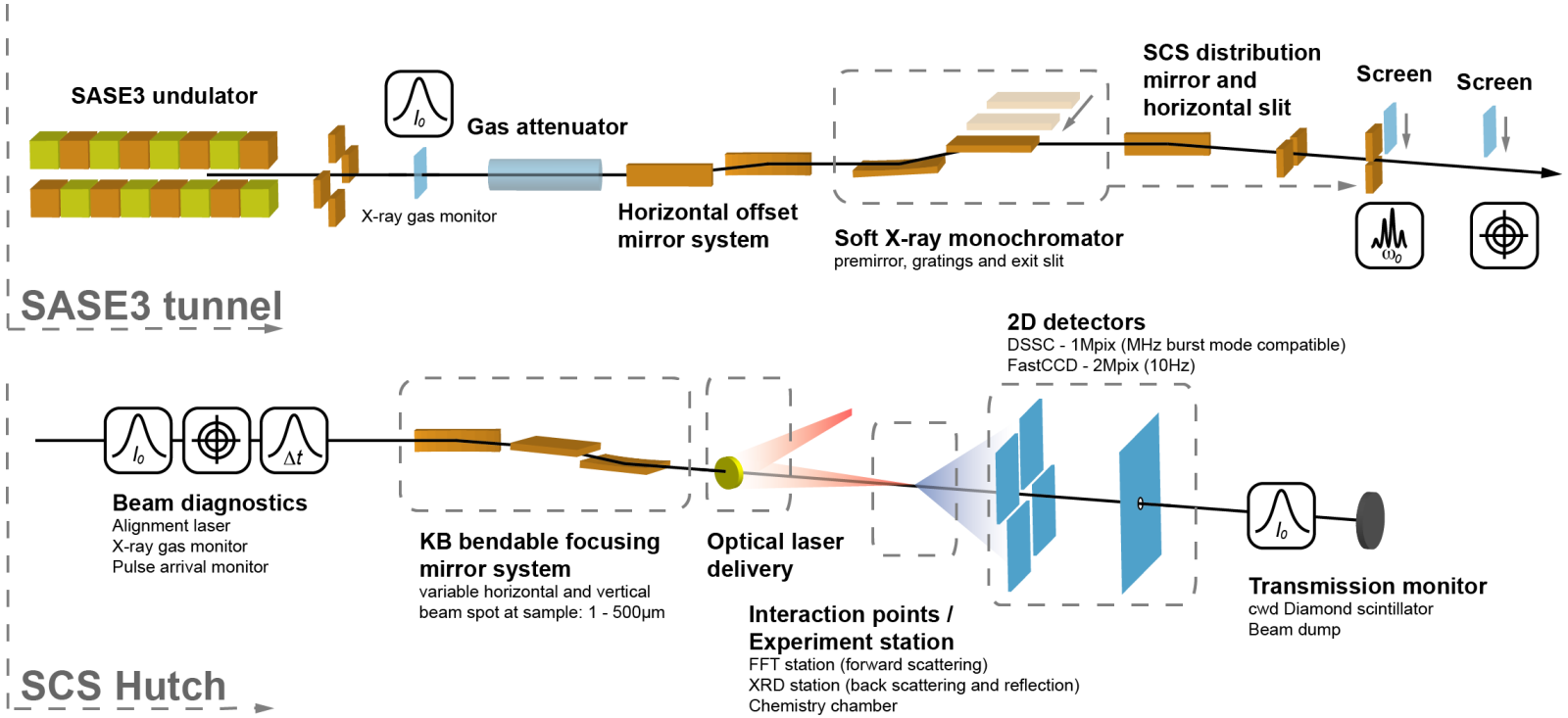
SCS Instrument & SASE3



XFEL beam parameters	
Photon energy	0.49 – 3.0 keV
Bandwidth	0.5 – 1.0 %
X-ray pulse energy	Up to 8 mJ
X-ray pulse duration	25 fs
SA1 / SA3 mode	Interleaved @ 2.2 MHz

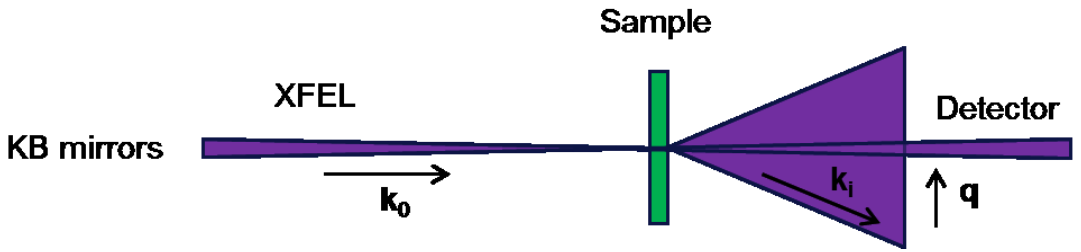


SCS Instrument: Spectroscopy & Coherent Scattering



Beamline settings:

Mono resolving power:	2500-5000 (currently)
Beam size:	1 µm – 1 mm
PP laser wavelength:	800 nm 400 nm 266 nm OPA
PP laser rep. rate	113kHz – 1.1MHz

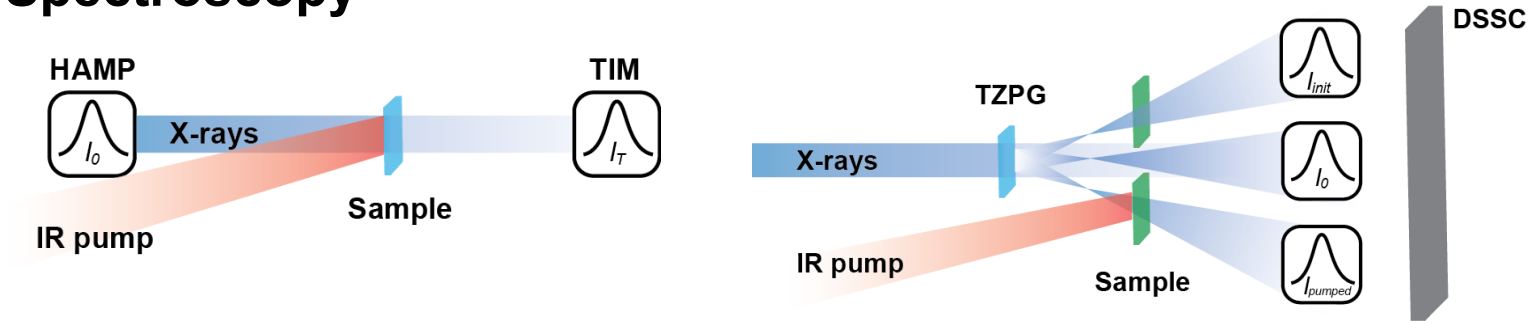


Forward-scattering fixed-target setup (FFT)

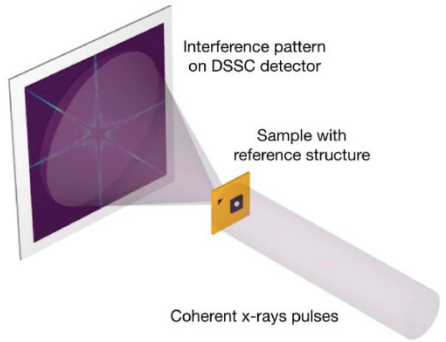
In operation since Dec 2018

SCS Instrument: x-ray scattering in transmission geometry

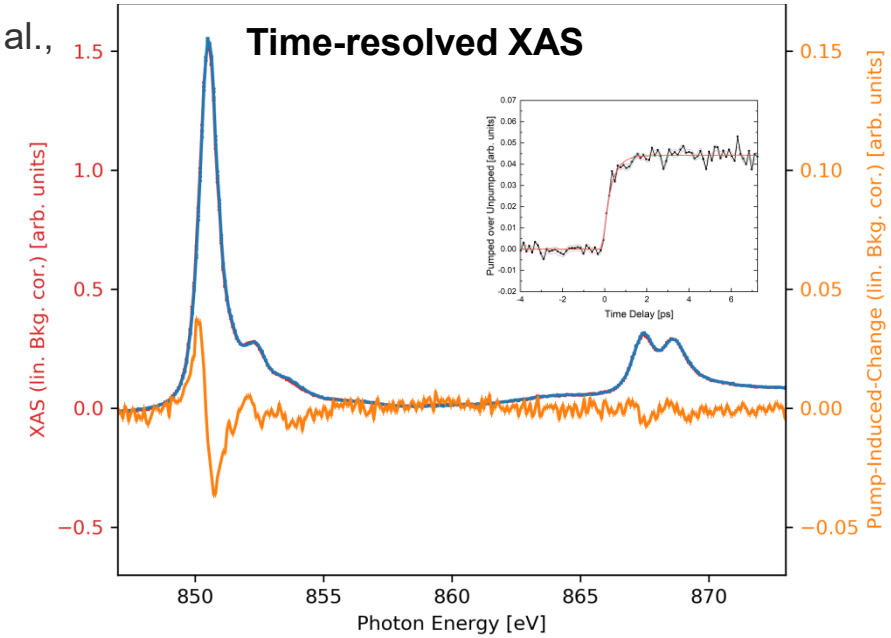
Spectroscopy



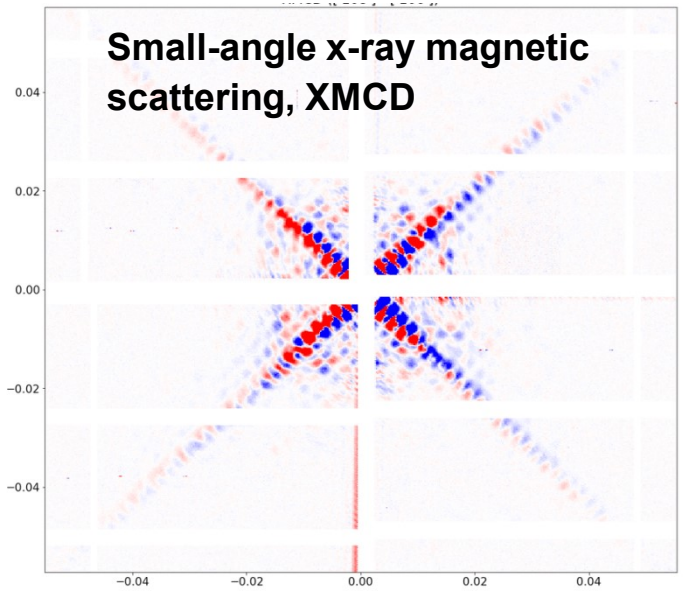
Holography



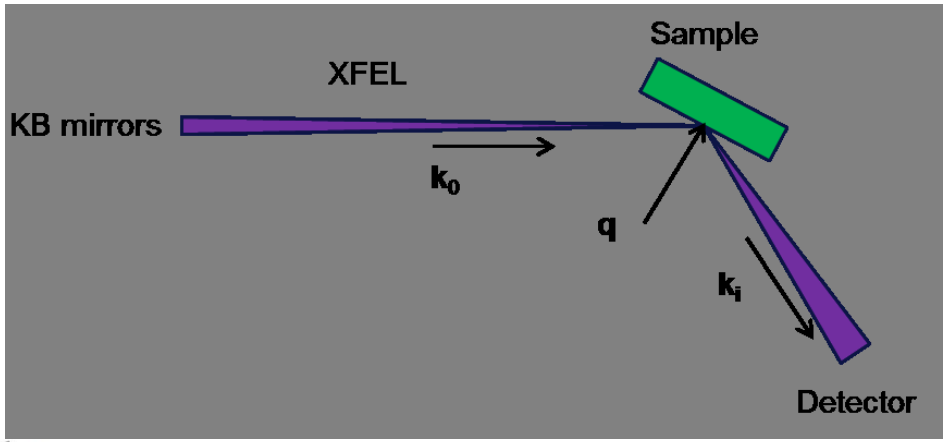
Eschenlohr et al., community proposal

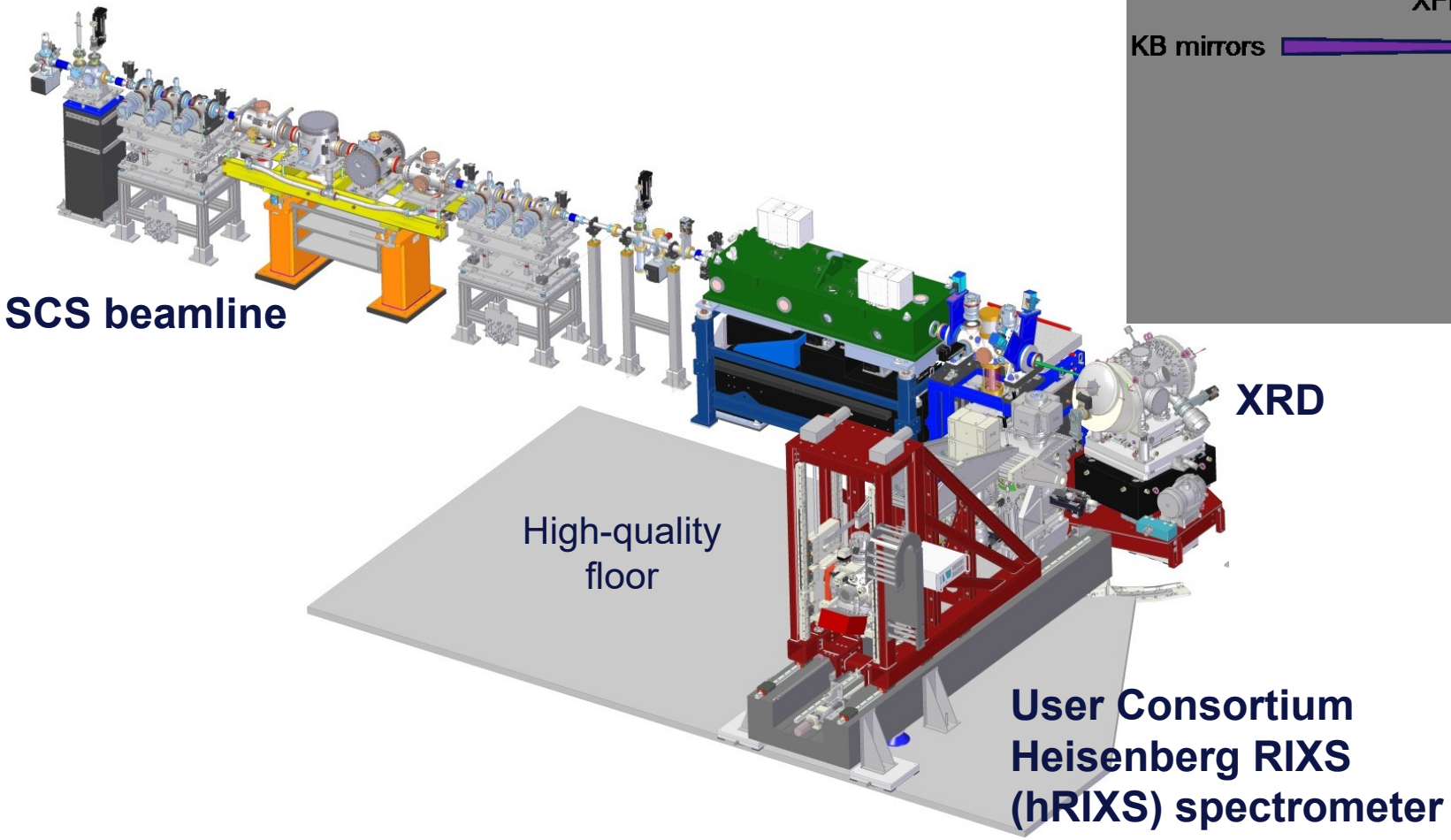


Bonetti et al., community proposal



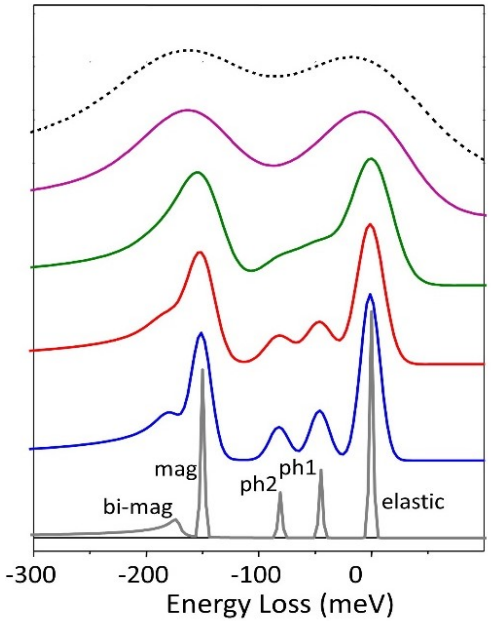
Elastic and inelastic x-ray scattering in reflection geometry at SCS





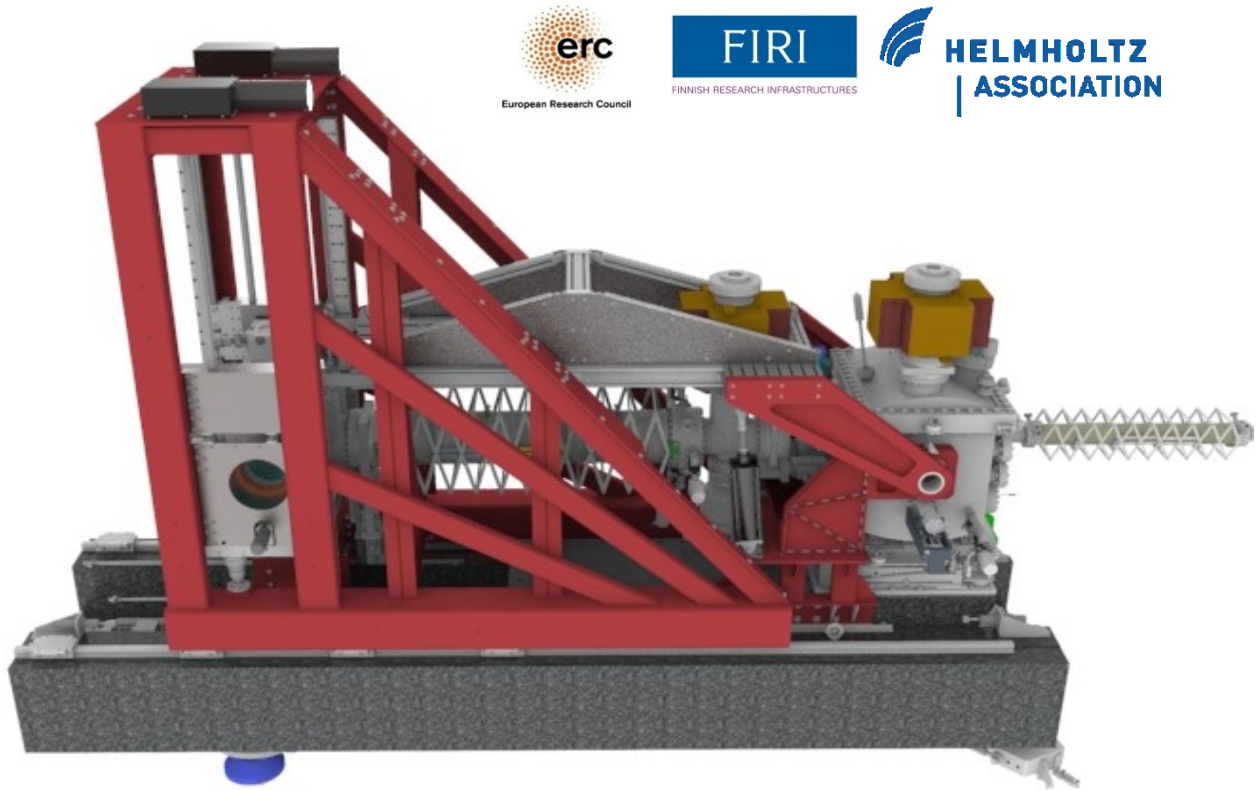
hRIXS: Heisenberg RIXS User Consortium instrumentation

Aim:
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
∞		

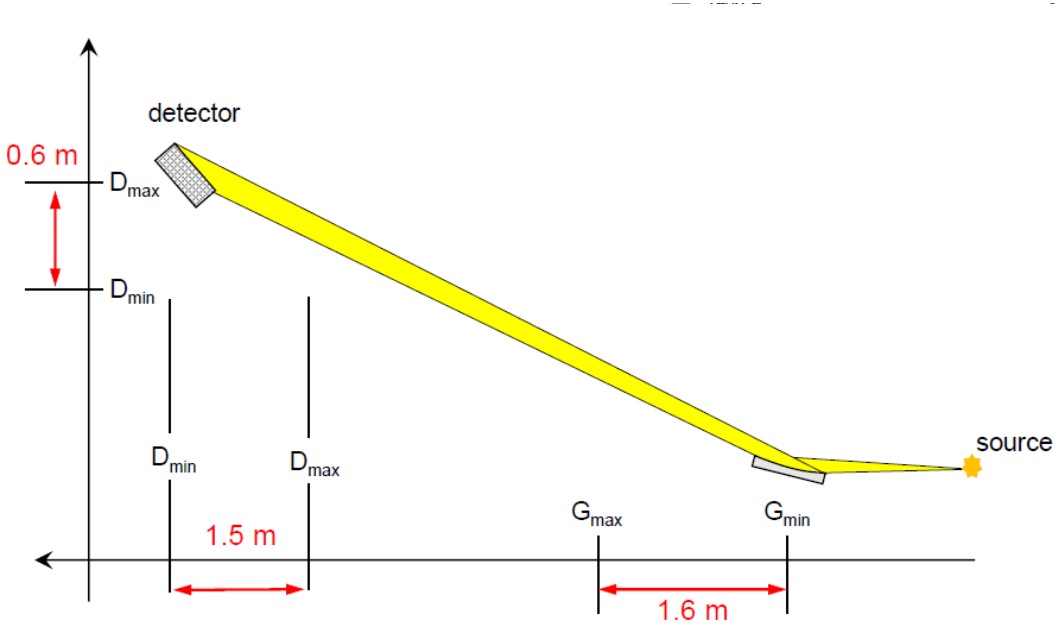
$\Delta t = h/\Delta E$

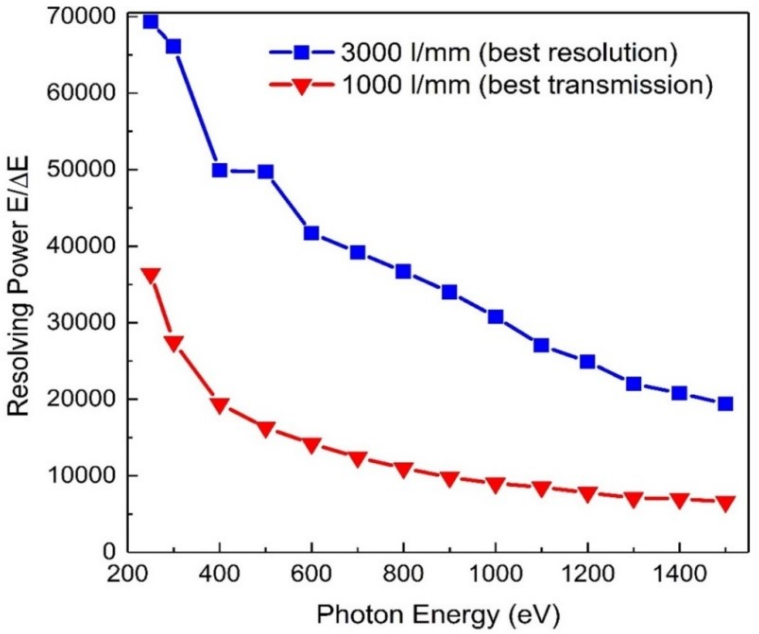


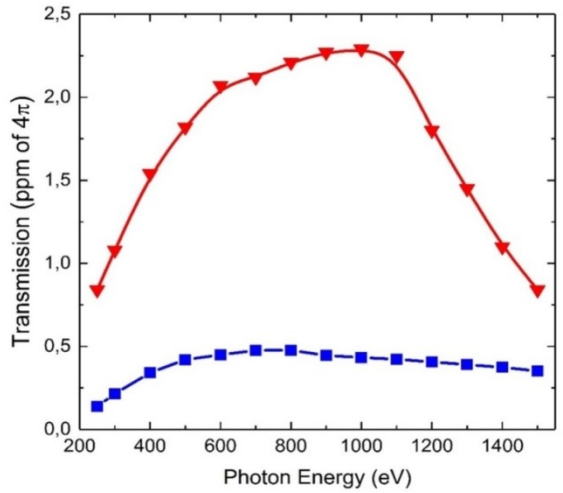
hRIXS Proposal, User Consortium

J. Schlappa, B. van Kuiken, J. T. Delitz, A. Scherz,
S. Neppl, F. Senf, C. Weniger, A. Föhlisch,
T. Reuss, S. Techert, T. Laarmann, G. Ghirinhelli, S. Huotari.

hRIXS spectrometer: design & performance







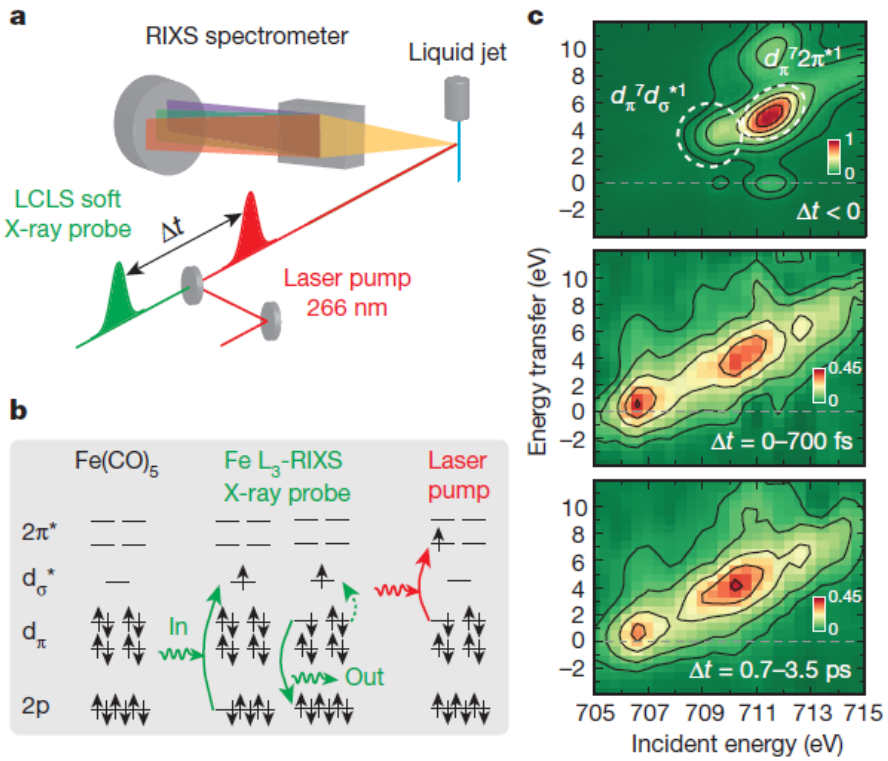
- Spherical VLS
- Single optical element -> ease of alignment and operation
- optimisation for working range: 270 – 1500 eV with one grating
- Slots for 3 gratings

G. Ghiringhelli, Y.Y. Peng, F. Senf, S. Neppl (2016)

Scientific Motivation for Time-Resolved RIXS

Photochemical dynamics in transition metal complexes:

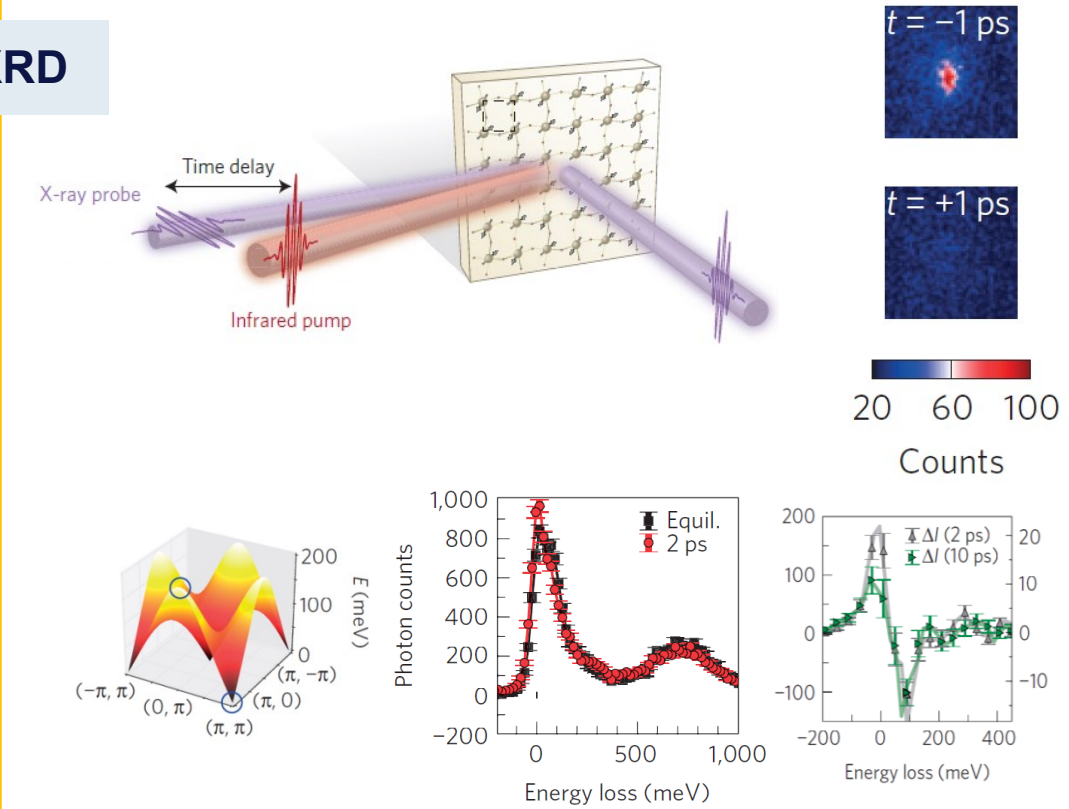
CHEM



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

Magnetic correlation dynamics in 3D and 2D:

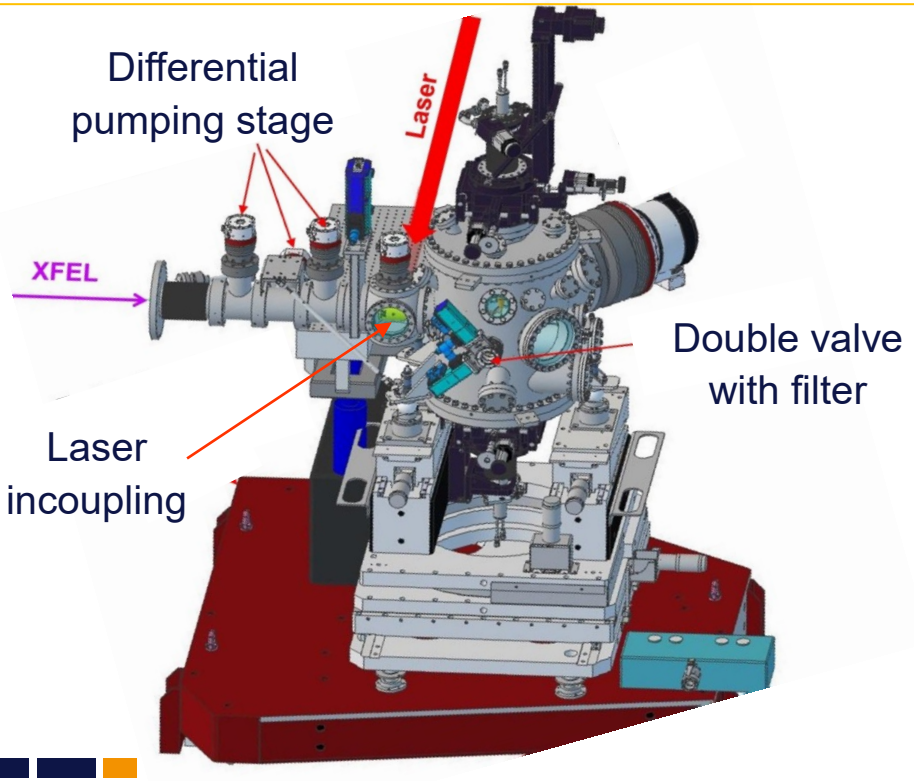
XRD

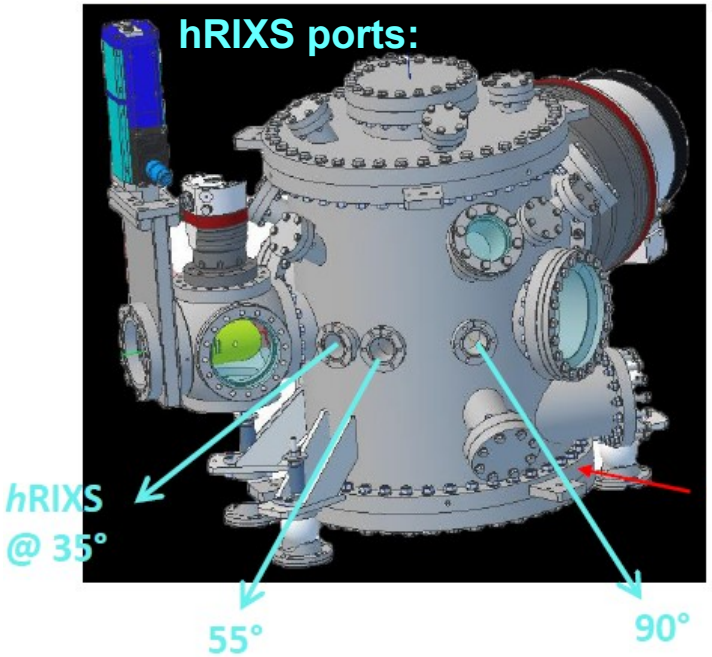


M. Dean et al., Nature Mat 15, 601 (2016).

Heisenberg RIXS UC setup for chemical environment (CHEM)

- Time-resolved spectroscopy from a liquid-jet:
  - Resonant inelastic x-ray scattering
  - X-ray absorption
- Time-resolved spectroscopy from chemical solid samples

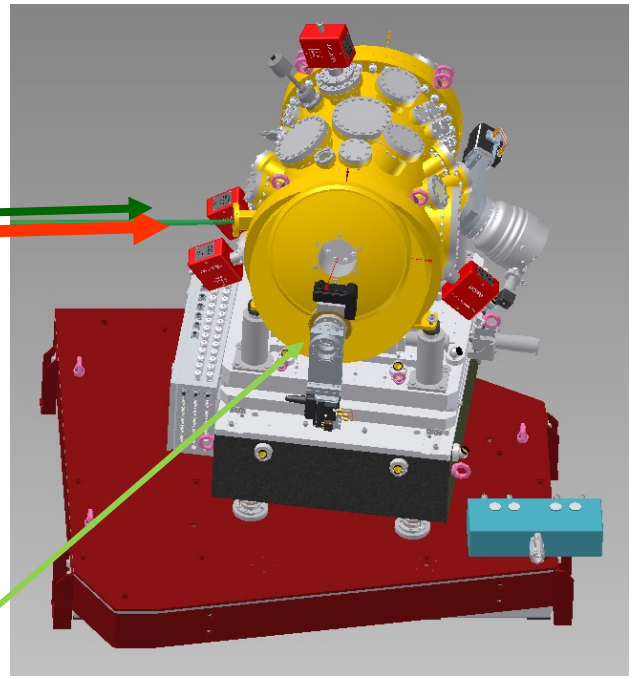




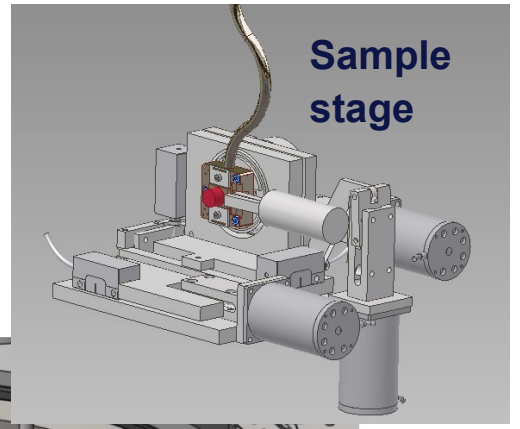
- Base pressure: 10^{-3} - 10^{-9} mbar
- Cylindrical liquid jet system + cryotrap
- Sample holder for solid samples
- Three fixed scattering angles: 90, 125 and 145 deg

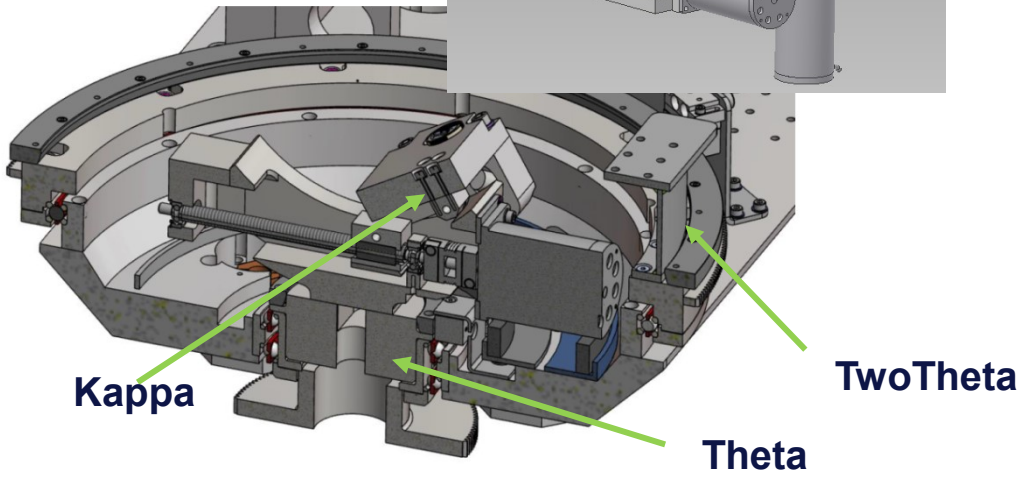
Baseline SCS setup for X-ray Resonant Diffraction (XRD)

- Time-resolved spectroscopy from solid samples:
  - Resonant inelastic x-ray scattering
  - Resonant x-ray diffraction / x-ray reflectivity
  - X-ray absorption
- Nonlinear scattering



Sample environment:

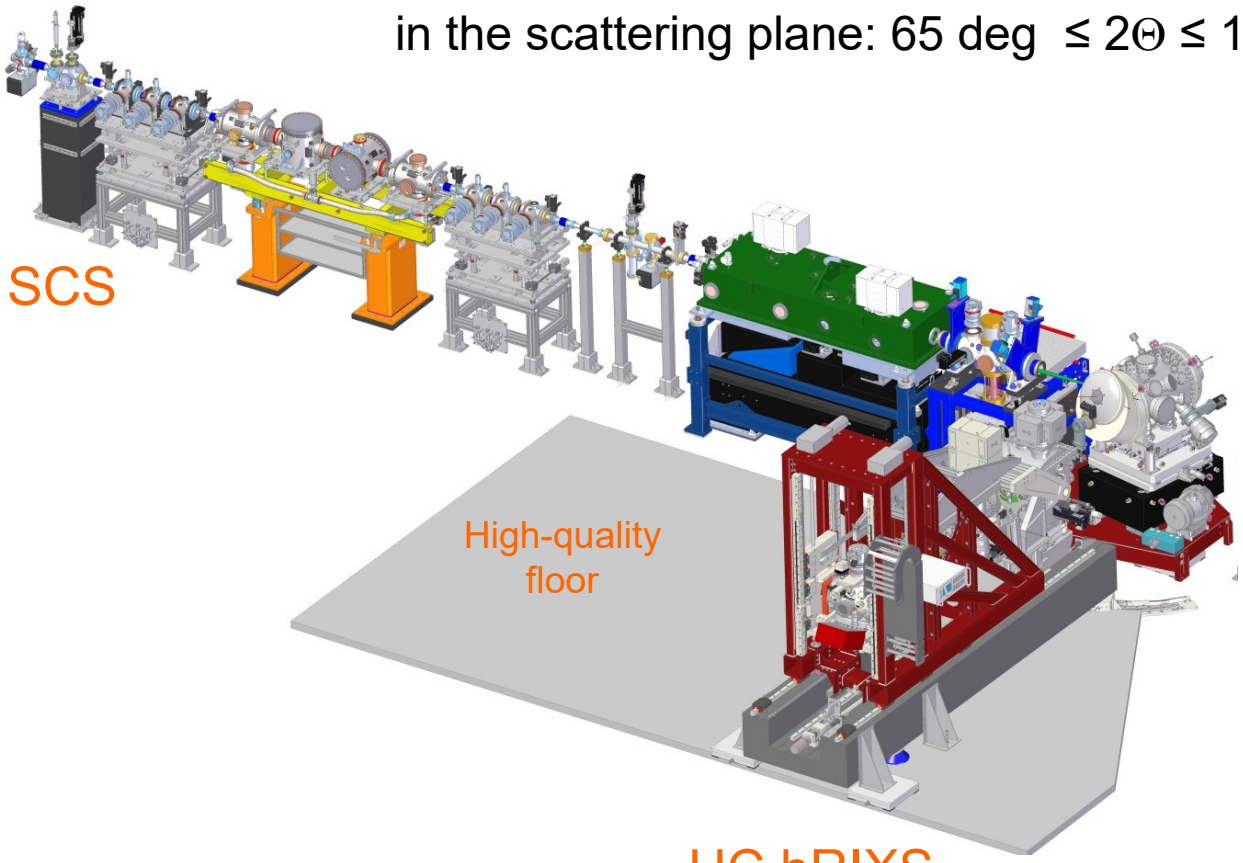


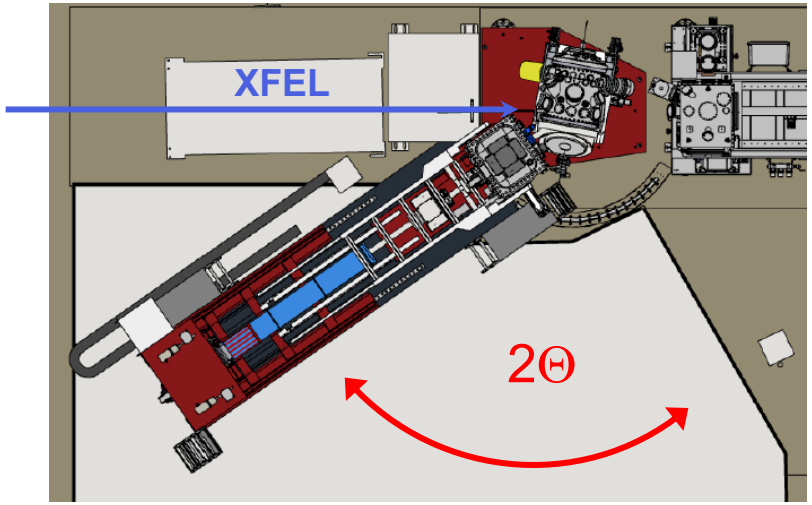


- UHV ($p < 10^{-9}$ mbar)
- Cryogenic temperatures
- 3-circle diffractometer, 6 DOF of motion for sample
- Detectors: APDs and MCP
- Triple rotating flange: 60 deg ≤ 2Θ ≤ 150 deg

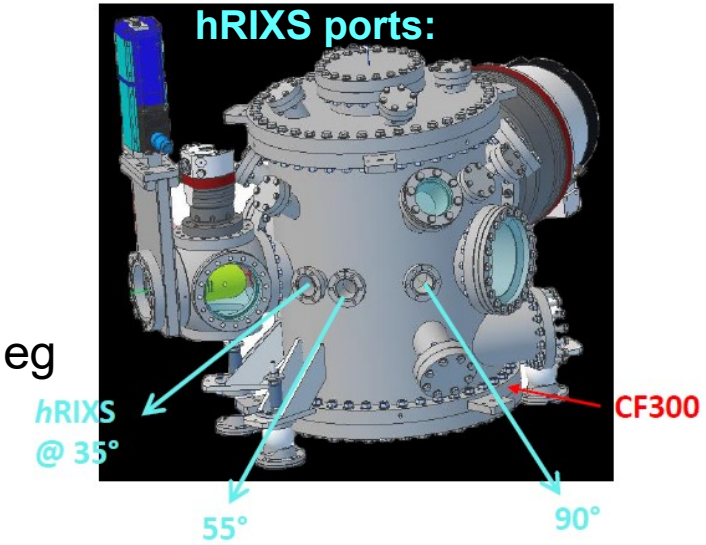
Momentum-resolved RIXS at SCS instrument:

- XRD + hRIXS: combined continuous rotation in the scattering plane: 65 deg ≤ 2Θ ≤ 145 deg



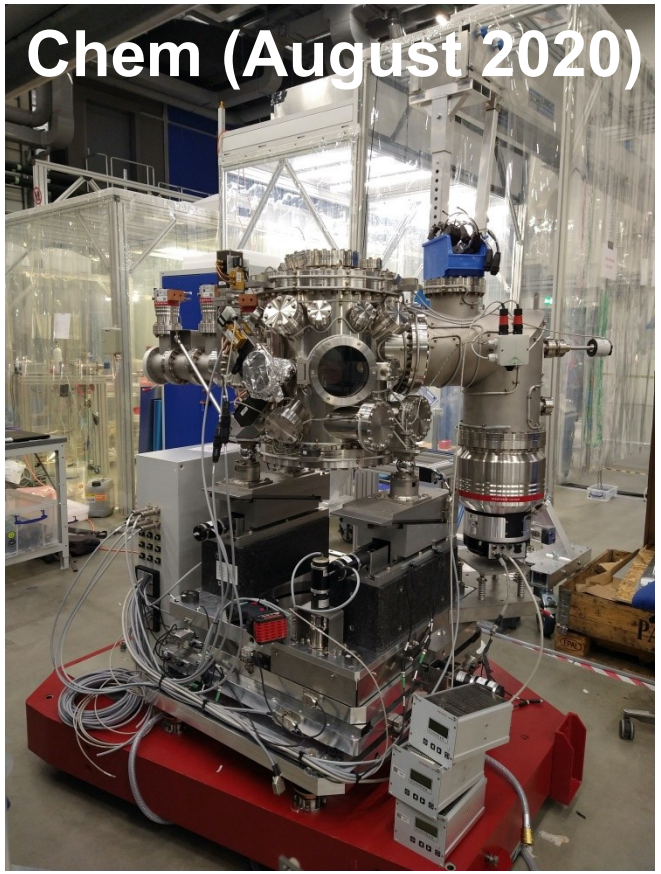


- CHEM + hRIXS: fixed geometry. Three 2Θ angles: 2Θ = 90, 125, 145 deg



Outlook for the winter shutdown:

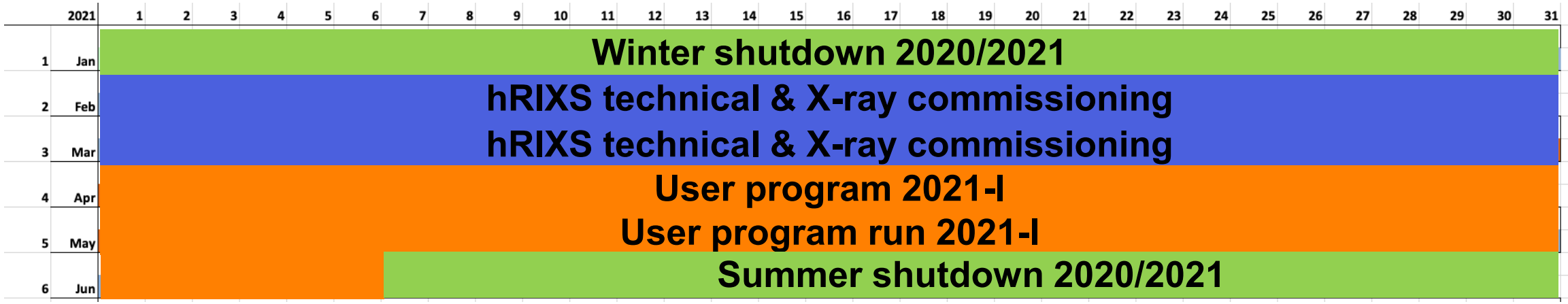
- Installation of hRIXS and CHEM at SCS
- Start of technical commissioning
- Installation of new SCS monochromator grating



Schedule of hRIXS Commissioning

Andreas Scherz
SCS instrument, European XFEL

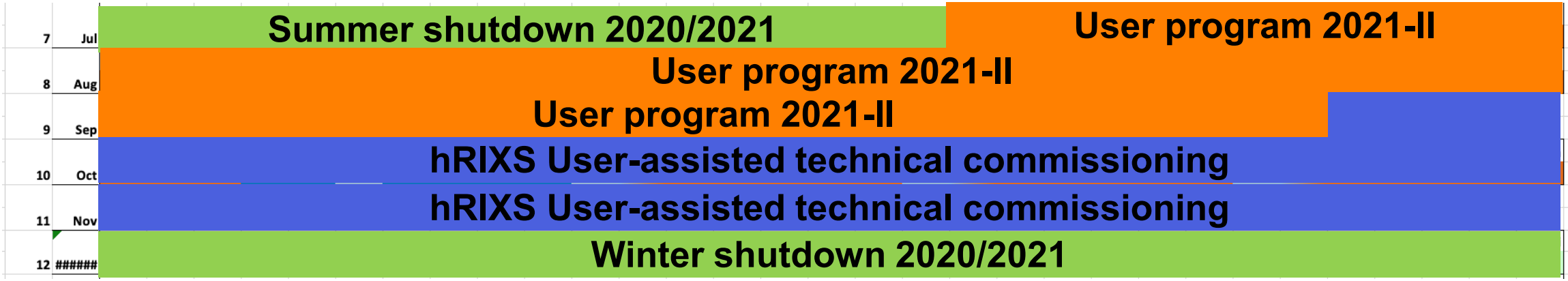
SCS operation schedule for the first half of 2021 (2021-I)



hRIXS Program: **February – March 2021**

- Soft X-ray Monochomator and hRIXS Spectrometer commissioning at few working points
- Commissioning of Chemistry chamber
  - Solid sample environment
  - X-ray diagnostics
  - Liquid jet environment

SCS operation schedule for the second half of 2021 (2021-II)



hRIXS Program: **end of September – November 2021**

- User-assisted technical commissioning:
  - Enabling methodologies for the start of user program in 2022
- Proposals for 2021-II:
  - the proposals will be coordinated and submitted by SCS **outside of the normal user proposal call**

Preparation of hRIXS proposal calls for the operation schedules 2021 and beyond

Call for proposals:

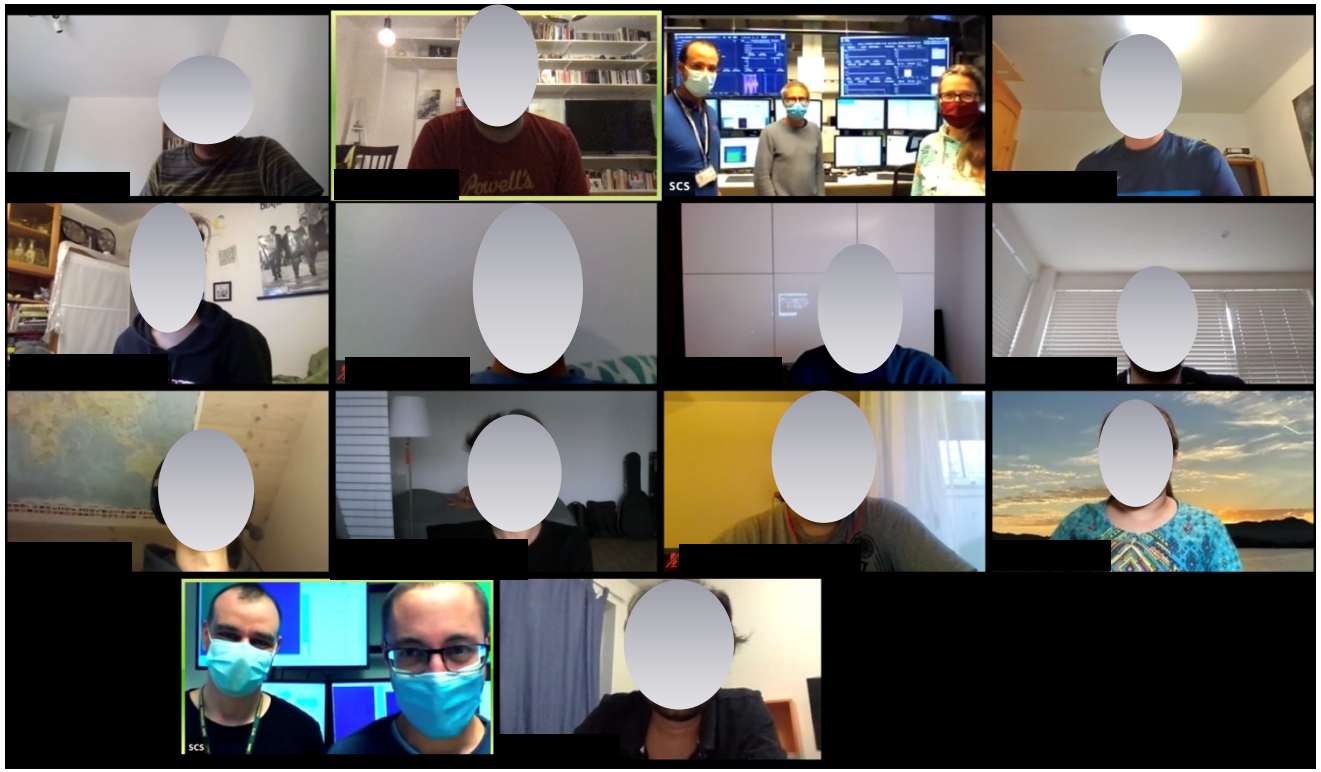
- 2021-II **deadline Dec 2020**
  user-assisted technical commissioning proposals for hRIXS (**coordinated by SCS**)
  (information today in the virtual town hall meeting)
- 2022-I **deadline June 2021**
  open for community and individual user proposals for hRIXS

Allocation period

- 2021-I
  Start of hRIXS x-ray commissioning
- 2021-II
  User-assisted technical hRIXS x-ray commissioning
- 2022-I
  First hRIXS user program

Remote User operation:

- Zoom channel to the control room of the instrument
- exchange of information via e.g. SLACK
- elog / myMDC for documentation
- document sharing and editing on XFEL/desycloud



User-assisted commissioning proposals for 2021-2

Ben Van Kuiken
SCS Instrument, European XFEL

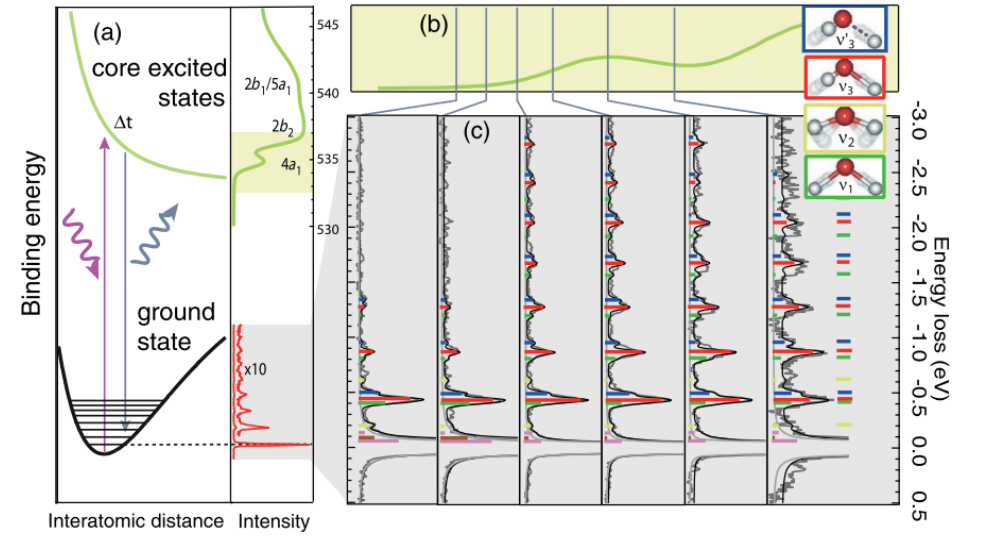
Goals:

- Technically-driven proposals targeting the base functionalities of the instrumentation
- SCS has identified two liquid phase (Chem chamber) and two solid state projects (XRD Chamber)
- Measurements shall be done on scientific samples from users, in collaboration with users

Chem Proposal 1: High-Resolution RIXS Spectroscopy of Liquids

Scientific Purpose: Probing vibrational dynamics in liquids

Technical goal: Commissioning of combine hRIXS + Chem chamber for high-resolution studies on pure liquid samples



Pietzsch, *et al.* PRL 114, 088302 (2015)

- Potential Samples: water, organic solvents.
- Photon energies: from 530 eV (O K-edge). Optimize X-ray resolving power for measuring vibrations.
- Instrumentation
  - Liquid jet system
  - X-ray Beam: Focusing conditions, pulse energies, rep. rates

Chem Proposal 2: Solution-Phase Time-resolved RIXS of Coordination Complexes

Scientific Purpose: Examining photochemical reaction with RIXS to measure d-d excitations in ground and excited states.

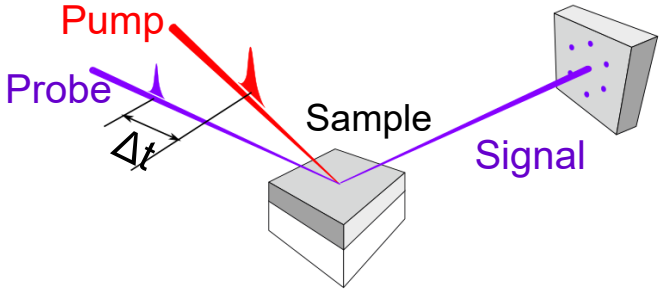
Technical goal: Commissioning of combine hRIXS + Chem chamber for optical pump/x-ray probe experiments

- Samples: solutions of transition metal complexes: high solubility, easily obtained, balanced cross-sections
- Photon energies: 700 eV – 1000 eV (Fe, Co, Ni, Cu L-edges)
- Instrumentation
  - PP laser in-coupling via breadboard at Chem and the Chem LIN chamber with possible laser wavelengths of 400 nm, 800 nm, 266 nm, or outputs from the OPA.
  - Timing measurements

XRD Proposal 1: Pulse-resolved x-ray resonant diffraction (or reflectivity)

Scientific purpose: Pulse-resolved diffraction from a photo-excited correlated system, after excitation inside and above the band gap

Technical goal: X-ray commissioning of XRD chamber, commissioning of optical-pump/ x-ray-probe setup starting with 800 nm (fundamental)



- XRD: solid samples, stable on air, UHV compatible, stable upon x-ray irradiation.
- Photon energies: from 700 eV – 3000 eV. Band width ~3.000. No of photons: 10^{10}/pulse.
- Instrumental:
  - Detectors: APDs (@ TwoTheta circle) + MCP (@ fixed geometry)
  - PP laser: co-linear through LIN, **800nm** and 400nm or 266nm. Repetition rate: up to 113 kHz
  - Temperature: Preferred RT, LN2 or LHe might be available

XRD Proposal 2: High-resolution pump-probe RIXS from solid samples

Scientific purpose: high resolution RIXS from a photo-excited correlated system

Technical goal: optimization of hRIXS spectrometer for high-resolution RIXS, commissioning of optical-pump/x-ray probe RIXS in the combination XRD/hRIXS

- XRD: solid samples, stable on air, UHV compatible, reasonably stable upon x-ray irradiation.
- Photon energies: from 700 eV – 900 eV. Resolving power >5.000.
- Instrumental:
  - hRIXS Detectors: Princeton CCD. Signal integrated over several trains
  - hRIXS spectrometer at fixed geometry (preferably between 125 – 145 deg)
  - PP laser: co-linear through LIN, 800nm, 400nm or 266nm.
  - Temperature: Preferred RT, LN2 or LHe might be available

User-Assisted Commissioning Participation

- Those with suggestions of samples and/or strategies relevant to the technical commissioning projects should contact us by November 11

Chemistry proposals: benjamin.van.kuiken@xfel.eu
XRD Proposals: justine.schlappa@xfel.eu

- SCS will shortlist the most practical and ideal projects for technical commissioning
- A small group zoom meeting will be had between SCS and users that would like to participate for each of the projects (Week of November 16th)
- Finally, SCS will submit these user-assisted commissioning projects to the PRP

Ideal Experimental Parameters

Proposal	Photon Energies	Laser Wavelengths	Scattering Angle (2θ)
Chem 1: High-Res RIXS of Liquids	530 eV (O K-edge)	N/A	125°, 145°
Chem 2: Time-resolved RIXS in Solution	700 – 1000 eV (Fe, Co, Ni, Cu L-edges)	800, 400, 266 nm	125°, 145°
XRD 1: Pulse-resolved diffraction	700 – 3000 eV	800 and 400 or 266 nm	125°-145°
XRD 2: Time-resolved RIXS in Solids	700 – 1000 eV (Fe, Co, Ni, Cu L-edges)	800, 400, 266 nm	125°-145°

Slides available for download on indico site: https://indico.desy.de/event/27658/

Q & A Session

Please Type your Questions in the Q&A Chat

Important Contacts:

Chem Chamber Experiments: Ben Van Kuiken (benjamin.van.kuiken@xfel.eu)
XRD Chamber Experiments: Justine Schlappa (justine.schlappa@xfel.eu)
XFEL User Office (useroffice@xfel.eu)