

Solution Phase Photochemistry in Run 21

LCLS Virtual Town Hall

Thomas Wolf, LCLS Chemical Sciences Department head
Roberto Alonso-Mori, Bio-Chemistry Group lead
03/03/2022

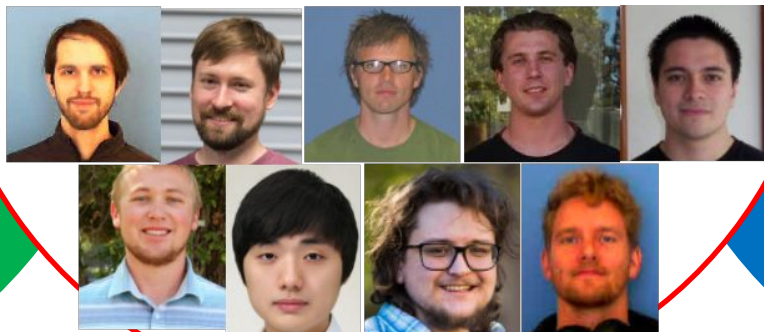


Solution Phase Photochemistry in the SRD Department Structure

Chemical Sciences
Department
Thomas Wolf



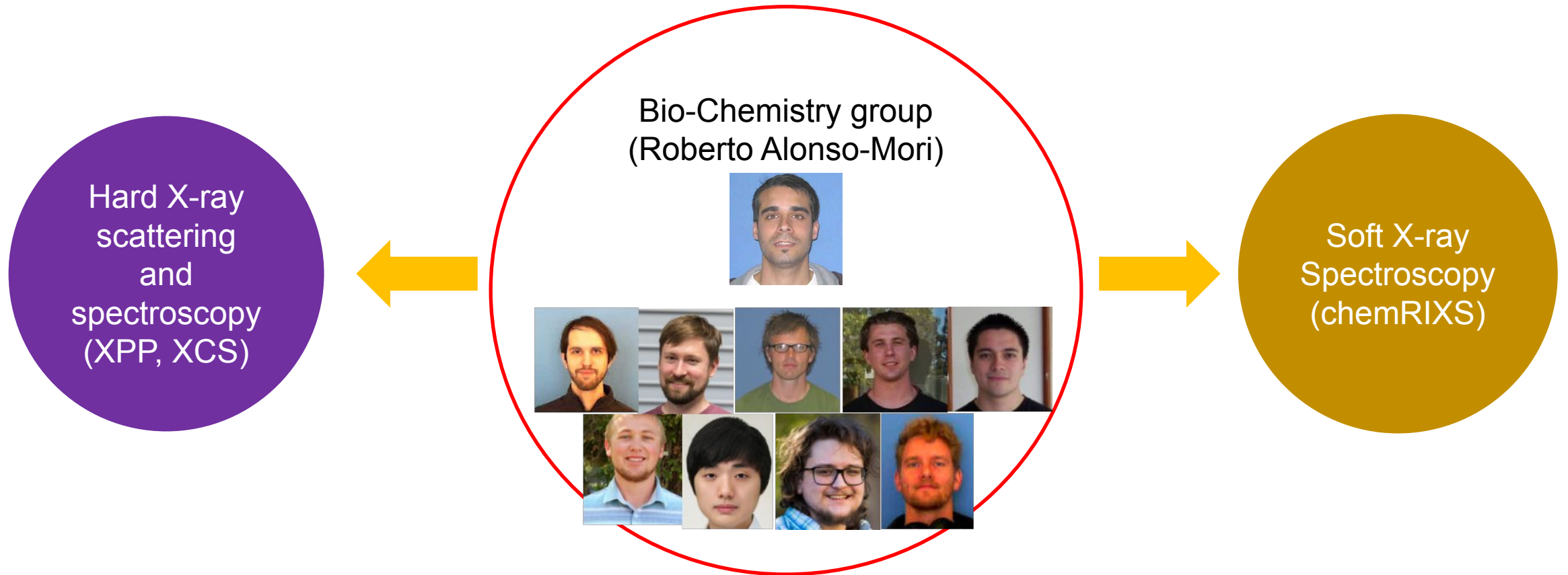
Bio-Chemistry group
(Roberto Alonso-Mori)



Biology Department
Mark Hunter



Techniques and Instruments Supported by the Group



Collaborate with Us

We are always open to and interested in collaborations!

Available fellowships from DOE and NIH:

- DOE Office of Science Graduate Student Research (SCGSR) Program:

<https://science.osti.gov/wdts/scgsr>

Applications due 05/04/2022

- NIH:

- NIH F31 graduate student fellowships:

<https://www.ninds.nih.gov/Funding/Training-Career-Development/Award/F31-Individual-NRSA-PhD-Students-MDPhD-Students-MSTP-0>

Deadlines: 04/08, 08/08, 12/08

- NIH F32 Postdoctoral fellowships:

<https://www.niehs.nih.gov/research/supported/training/fellowships/f32/index.cfm>



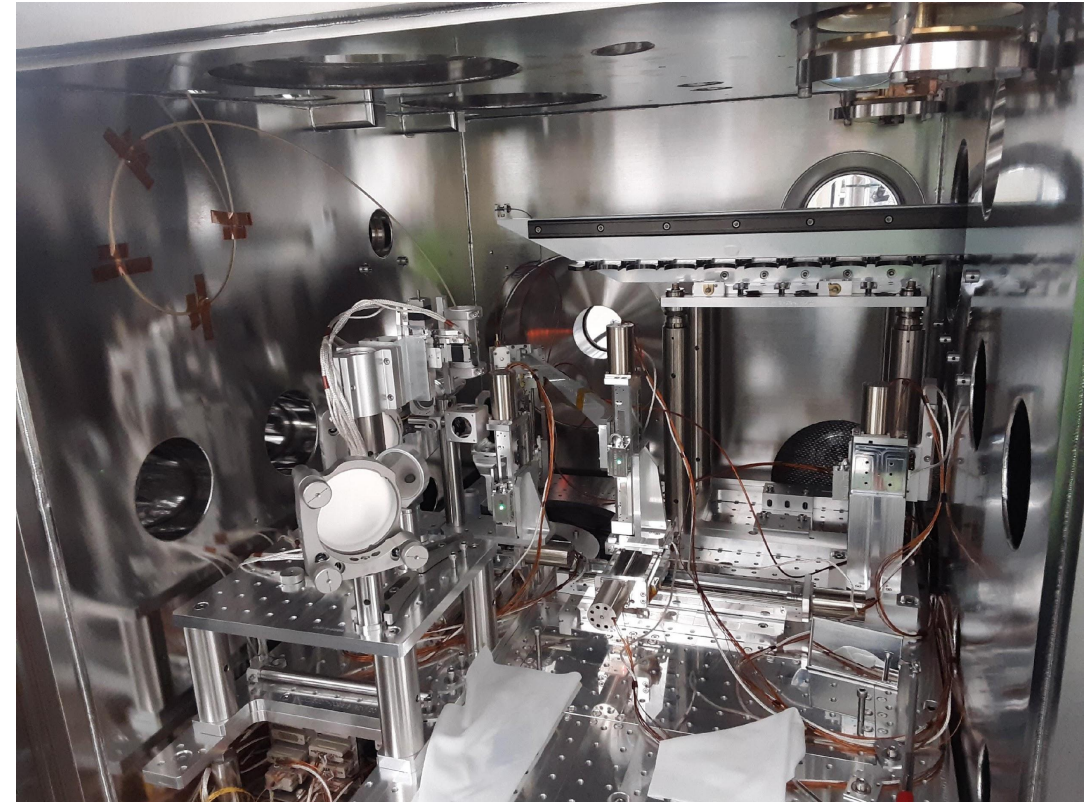
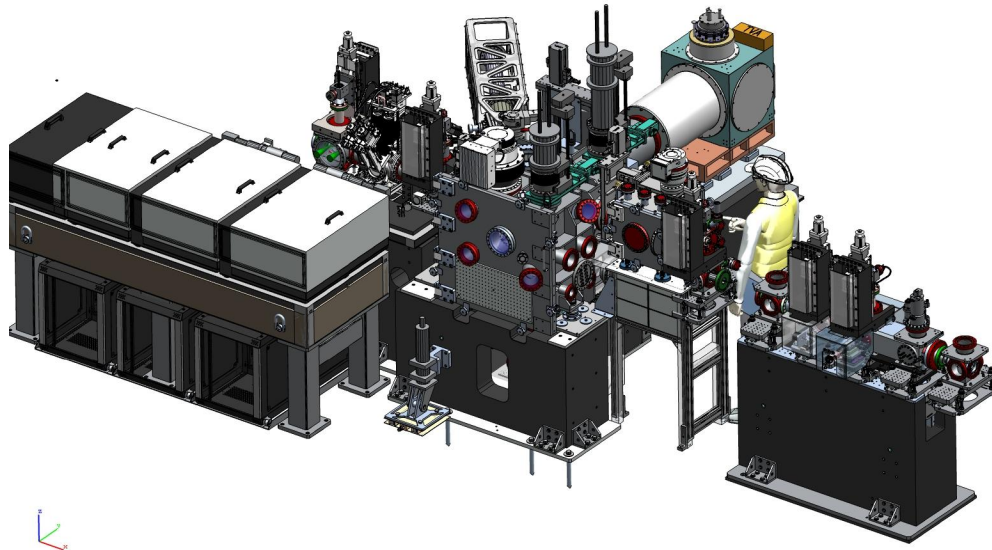
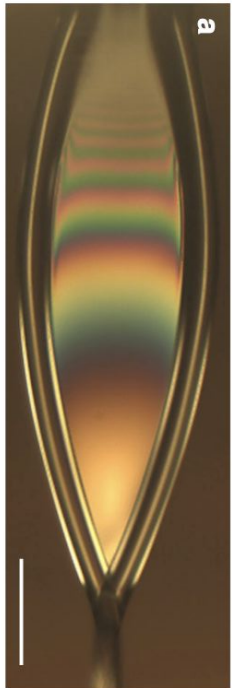
Soft X-ray
Spectroscopy
(chemRIXS)

The chemRIXS Endstation

Endstation for in-vacuum liquid sheet jets

Available detectors:

- APDs for Total fluorescence yield detection
- Andor camera
- Variable line spacing spectrometer



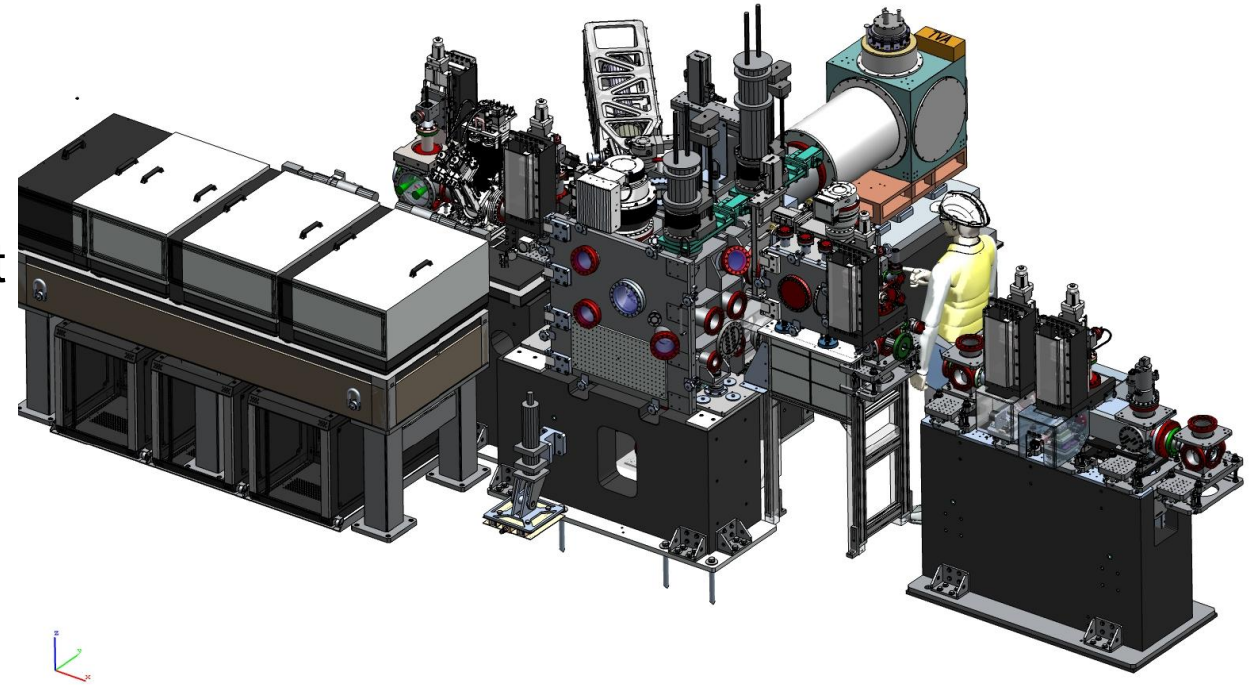
X-ray and Laser Parameters for chemRIXS in Run 21

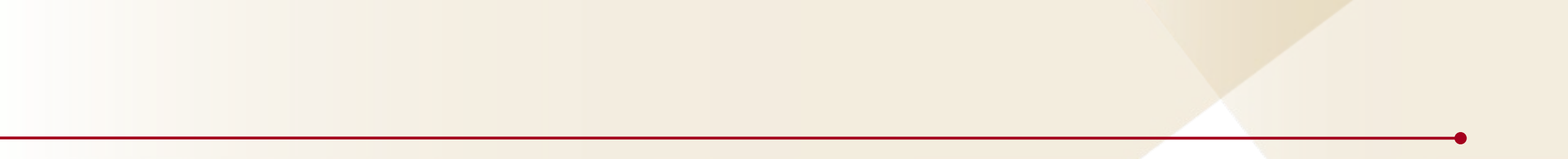
X-ray Parameters	
Repetition rate (Hz)	Up to 50 kHz
Energy Range (eV)	250 - 1100
Pulse Duration	20 fs (nominal)
Energy per pulse (downstream of mono)	>100 nJ
Beamline resolving power	> 2000
Spot Size, FWHM (range)	10 - 1000 (um) diameter
Polarization	Linear, Horizontal

Laser Parameters			
Repetition rate (Hz)	Synchronized up to 33 kHz		
Wavelength	800 nm	400 nm	High Risk 266 nm
Pulse Duration	< 25 fs	< 50 fs	< 50 fs
Energy per pulse (on target)	300 μ J	> 30 μ J	~ 3 μ J
Spot Size, FWHM (800 nm)	50 to 100 um		
Polarization	Variable: linear, circular		
Angle	~0.5 deg angle with x-ray beam		
Arrival Time Monitor	< 20 fs accuracy in x-ray/laser arrival time tagging.		

User Involvement in Early Science

- Interested groups should contact Thomas (thomas.wolf@slac.stanford.edu)
- Department head collects experiment ideas and prioritize together with the chemRIXS instrument team and the instrument advisory panel.
- LCLS communicates consolidated early science plan with user community and broadly advertise participation.
- LCLS updates interested user groups on adjustments to the early science plan.

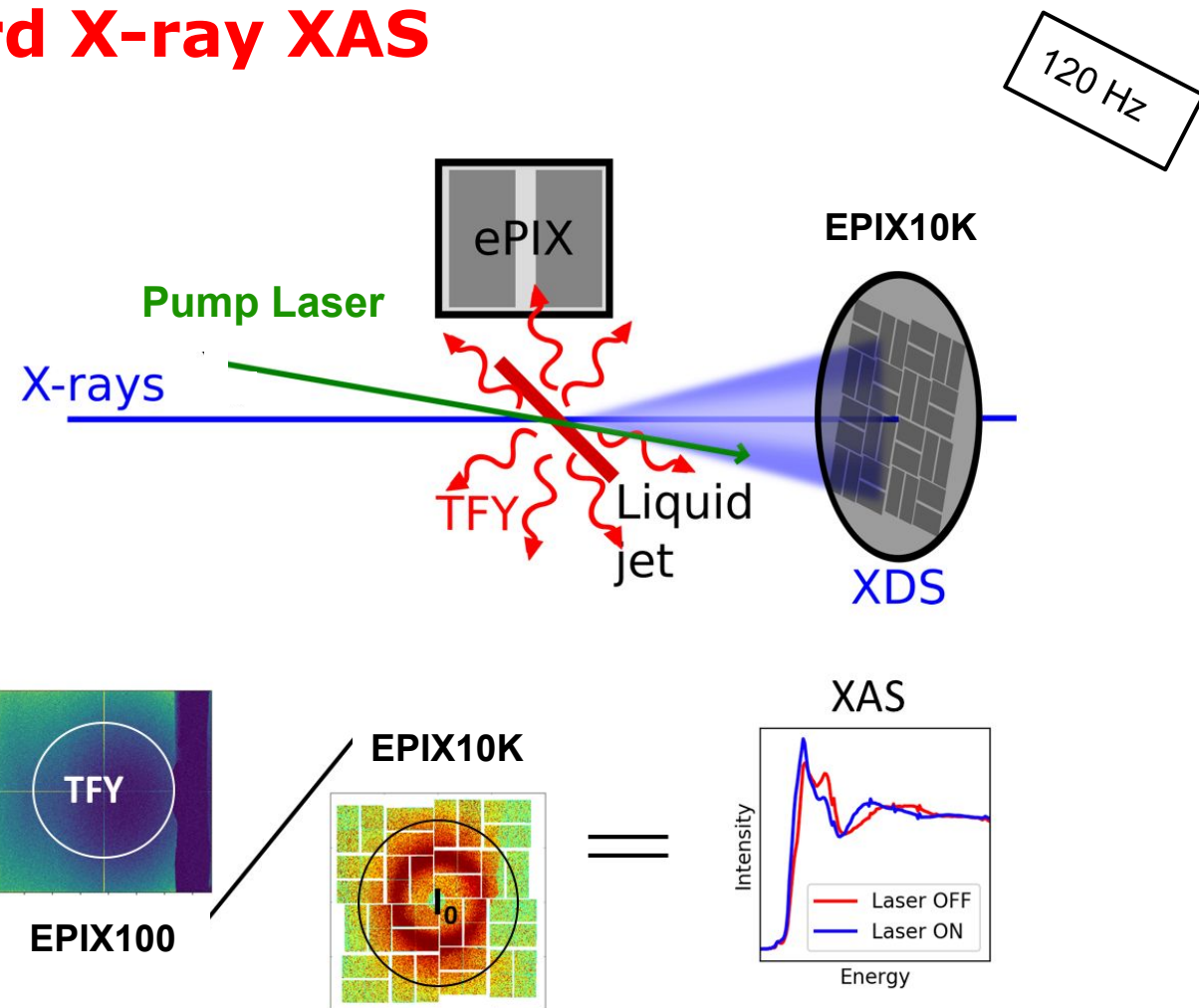
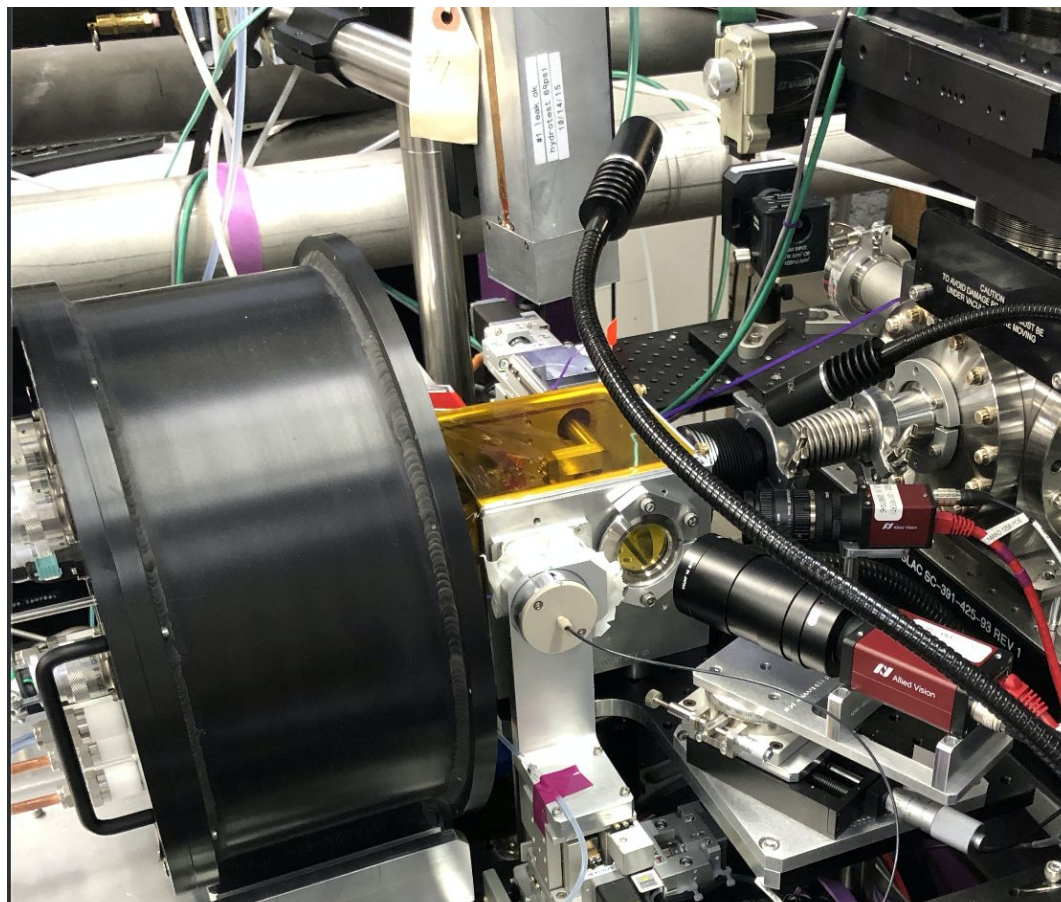




Hard X-ray
scattering and
spectroscopy
(XPP, XCS)

XPP Standard Configuration #2: Liquid Phase XAS

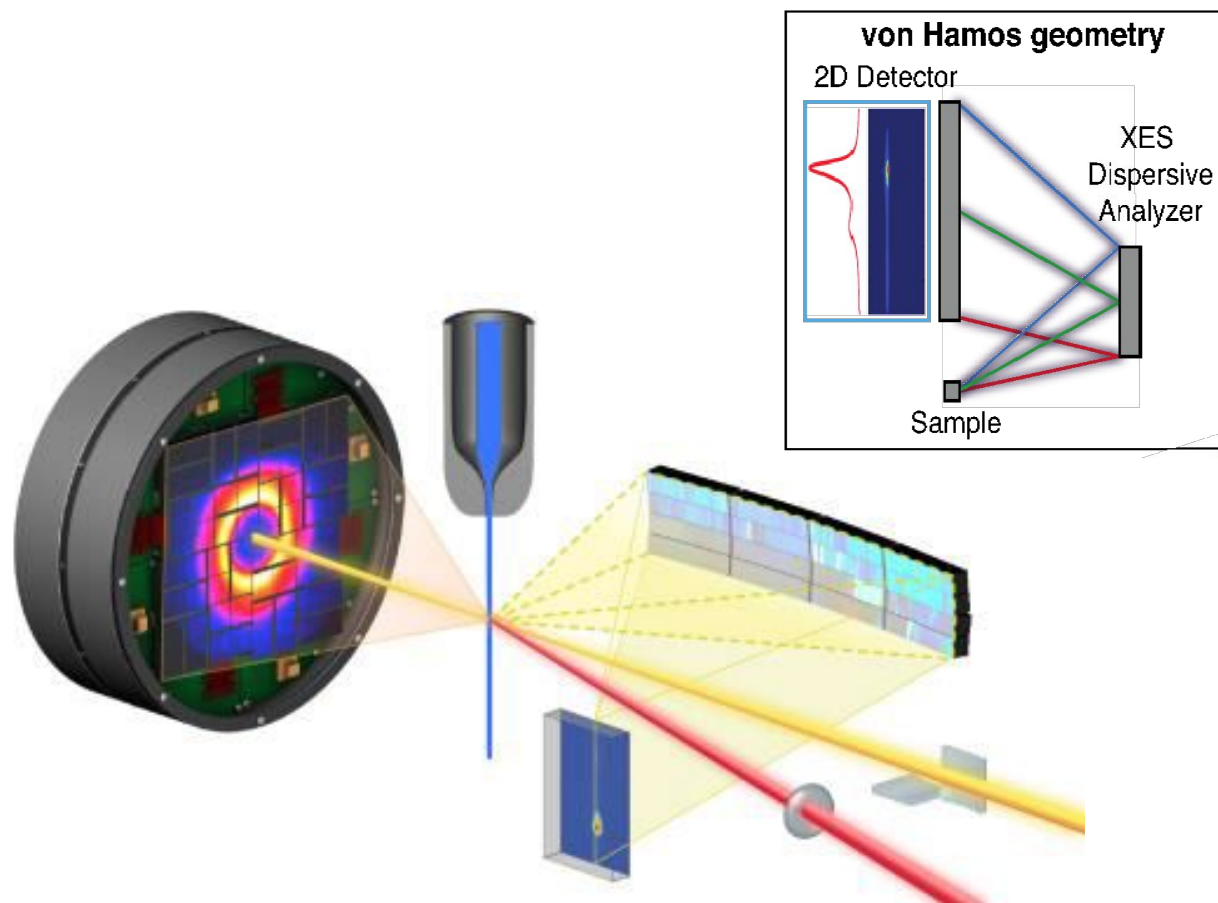
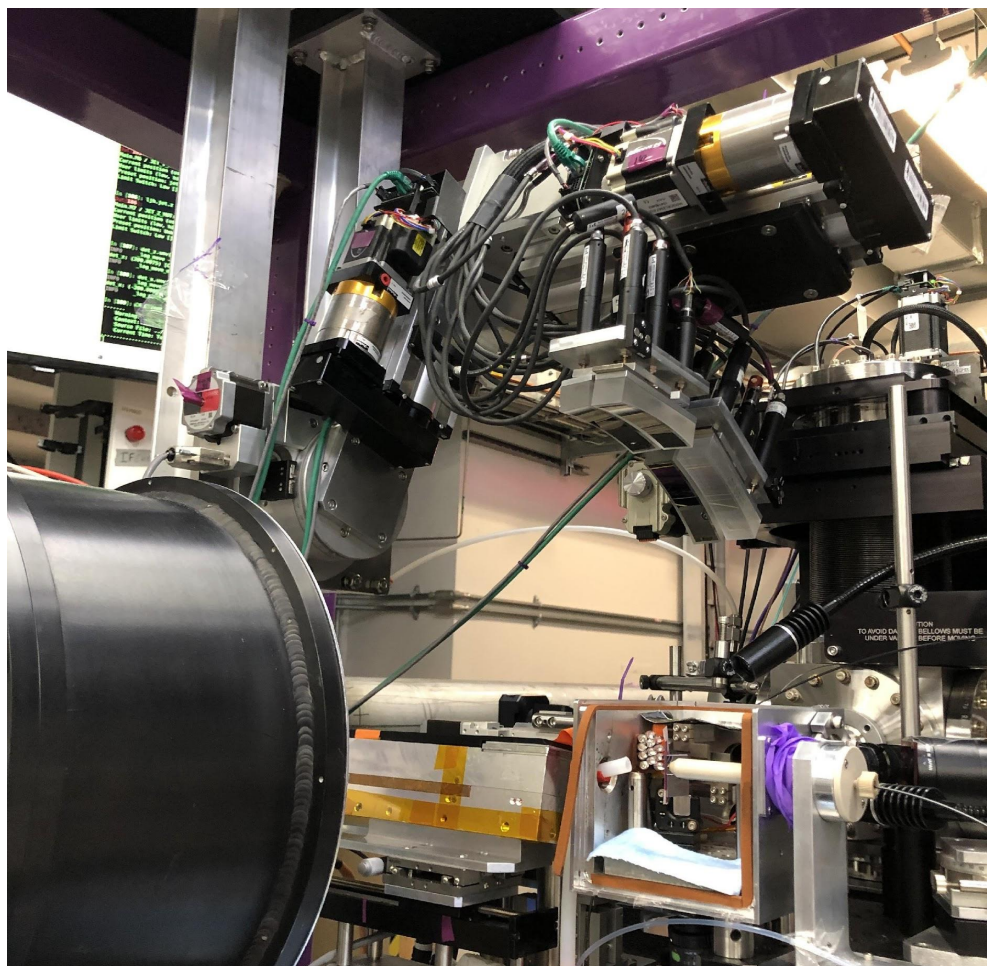
Time Resolved Hard X-ray XAS



XCS Standard Configuration #1: Liquid Phase XES/XDS

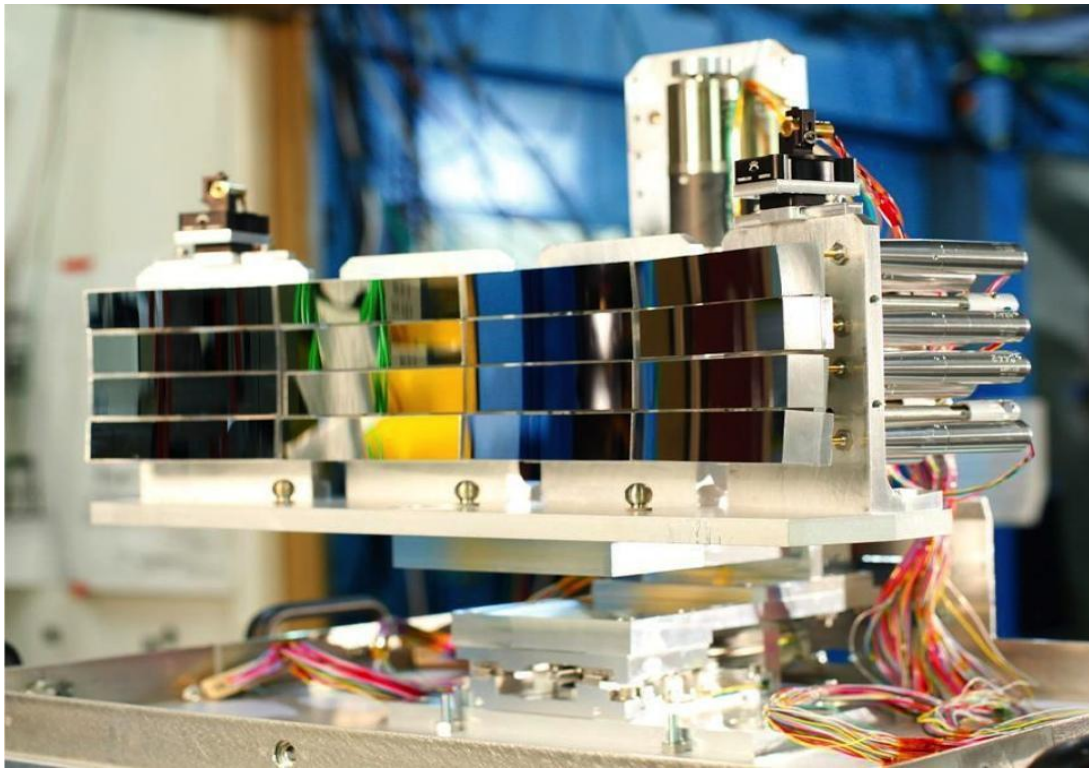
Time Resolved Hard X-ray XES + XDS

120 Hz

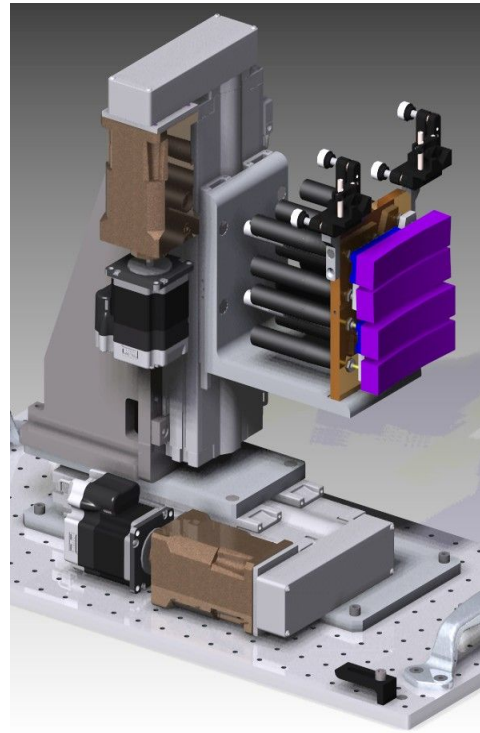


Hard X-ray Spectroscopy at LCLS: XES

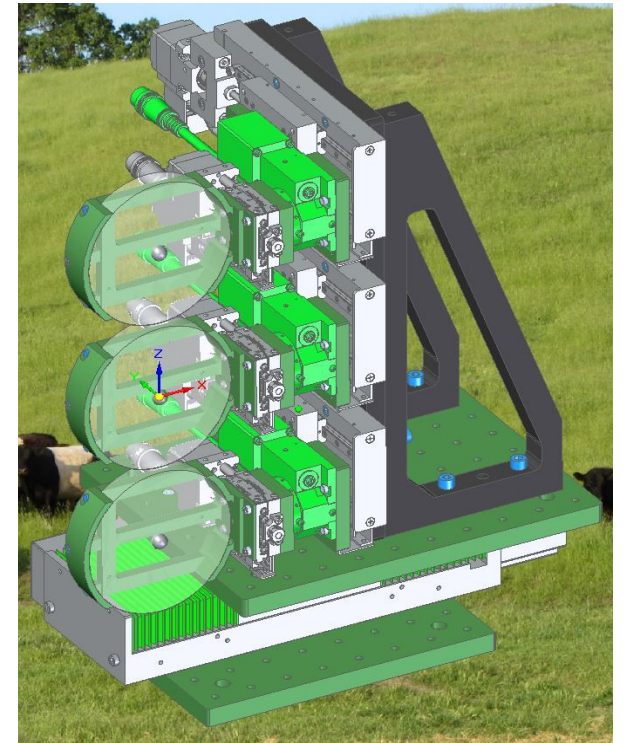
Existing LCLS multi-crystal X-ray Emission Spectrometers



16 crystal energy dispersive von Hamos



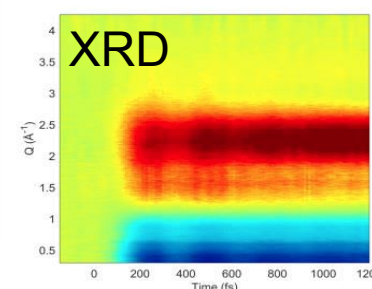
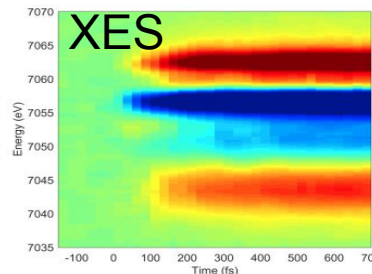
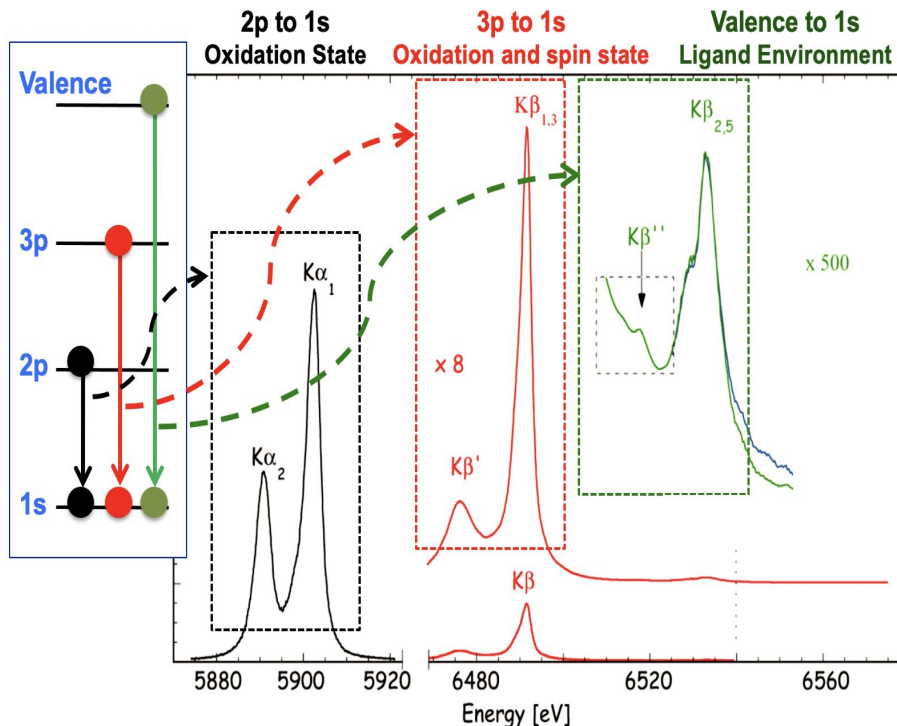
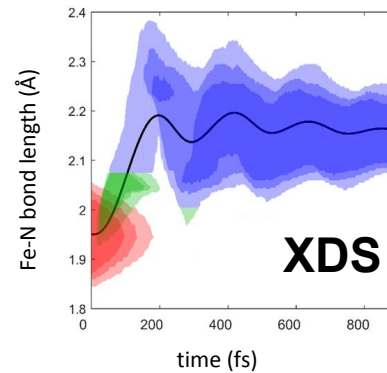
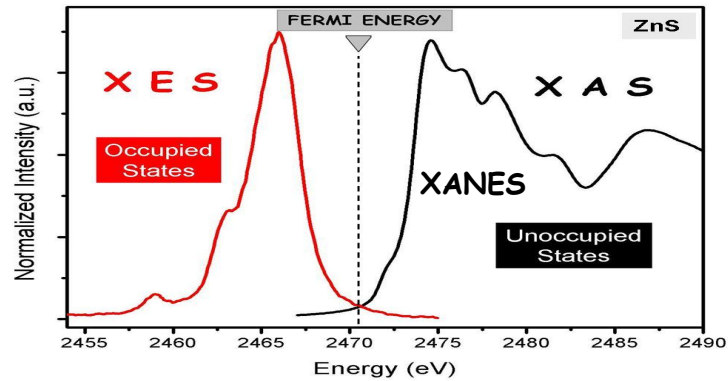
4 crystal E. dispersive von Hamos



3 crystal scanning Rowland

Alonso-Mori et al. RSI, 83 (2012)

Spectroscopy/XDS Measurements:



Standard:

- XAS (XANES)
- XDS (0.2 to 5 q-range)
- HighEnergy XDS expand q (<25keV)
- $K\alpha$, $K\beta_{1,3}$ and $K\beta_{2,5}$ XES of 3d TM
- L XES of 5d TM

Not so Standard:

- Resonant XES measurements
- RIXS (von Hamos)
- HERFD (Rowland)
- EXAFS

Standard Configuration Parameters Table:

Sample Delivery:

Standard:

- Round jets (30-100um)
- Sheet jets

Not so Standard:

- Thinner jets
- Drop on demand
- Solid targets

Pump Laser:

Standard:

- Collinear (2 deg)
- Fundam&Harm 800,400,266nm
- OPA (480-2400 nm)

Not so Standard:

- Not collinear
- THz
- 8 ns laser (410-2200 nm)

Resolution (Instrument Response):

Standard: 65 to 100 fs

Not so Standard: <65

Parameter Table for the XPP Standard Configuration

Sample	Sample(S) description Temperature range [C]	
X-ray Parameters	X-ray Energy	Fixed to 9(Cu k-edge)-13 keV
	X-ray Pulse Duration Mono bandwidth [meV] (default 600 meV with Diamond(111)) X-ray Focal spot size within 10 to 200 μm X-ray polarization Vertical(default), horizontal or Circular (including switching capability)	Fixed to ~50fs
Detector	Detector positioning range, List of Bragg reflections and typical scattering angles.	
Optical beam parameters	Wavelength [nm] Pulse duration [fs] Maximum Pulse Energy [μJ] Focal size (FWHM) [μm] Polarization requirements? Minimum fluence on sample [mJ/cm^2] Geometry	Collinear or Non-collinear up to 7 degree
X-ray Beam Time	Number of shifts shift = 12 hr	[1]
Any additional comments		

Parameter Table for the XCS Standard Configuration

Sample & sample delivery	Sample(S) description Round jet diameters [20, 30, 40, 50, 75, 100, 125, 150, 175, 200, 250, 300, 500] μm Flat sheet jet thickness [19, 25, 38, 50, 75, 100, 125, 175, 188, 250] μm	
Scattering	[yes/no] Maximum Q [\AA^{-1}]	
X-ray Emission Spectroscopy	[yes/no] Which Emission line(S) : Mn : $\text{K}\beta_{1,3}$, $\text{K}\beta_{2,5}$ and K Fe : $\text{K}\beta_{1,3}$ and $\text{K}\beta_{2,5}$ Co : $\text{K}\beta_{1,3}$ and $\text{K}\beta_{2,5}$ Ni : $\text{K}\beta_{1,3}$ and $\text{K}\beta_{2,5}$ Ti : $\text{K}\beta_{1,3}$ and $\text{K}\beta_{2,5}$ V : $\text{K}\alpha$.	
X-ray Parameters	X-ray Energy	Fixed to 9.5keV
	X-ray Pulse Duration Monochromatic or Pink X-ray Focal spot size within 2 to 100 μm	Fixed to ~50fs
Optical beam parameters	Wavelength [nm] Pulse duration [fs] Maximum Pulse Energy [μJ] Focal size (FWHM) [μm] Polarization requirements? Minimum fluence on sample [mJ/cm^2] Geometry	Collinear
X-ray Beam Time	Number of shifts shift = 12 hrs	[1]
Any additional comments		