Update from LCLS-II

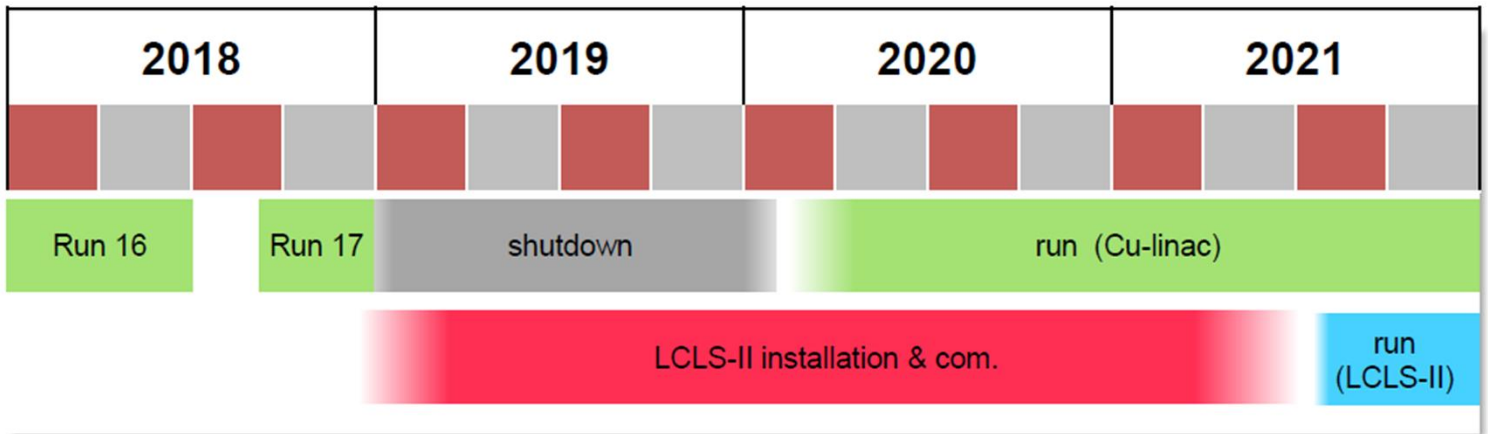
Workshop on Chemical Dynamics and Energy

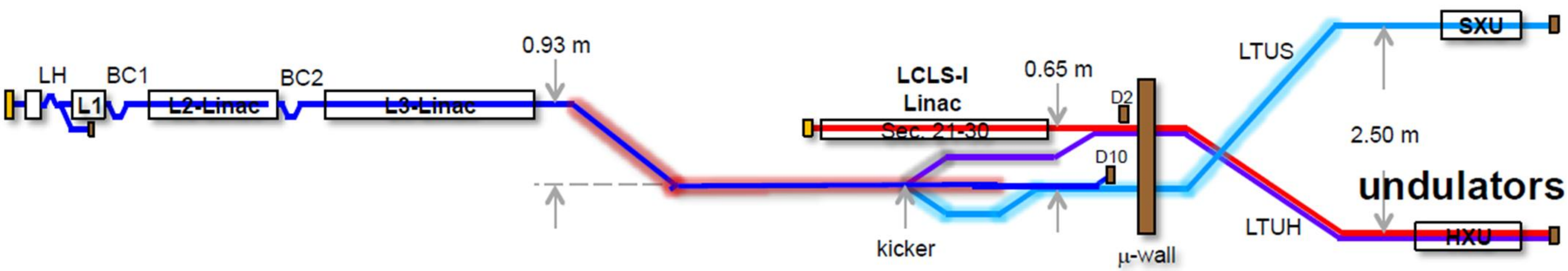
UK X-FEL Science Case

Newcastle, Dec. 11th, 2019

Georgi L. Dakovski
LCLS, SLAC

Status of LCLS II





Timeline

FEL Source	Inst.	Commissioning	Early Science (LCLS + users)
CuRF	XCS, MFX, CXI, MEC, XPP	N.A.	N.A.
CuRF	NEH 1.1 (LAMP)	4/2020	6/2020
CuRF	NEH 2.2 (chemRIXS)	6/2020	8/2020
SCRF	NEH 1.1 (LAMP)	12/2020	3/2021
SCRF	NEH 2.2 (chemRIXS)	6/2020	8/2021
SCRF	NEH 1.1 (DREAM)	3/2021	6/2021
SCRF	NEH 2.2 (qRIXS)	1/2022	5/2022
SCRF	NEH 1.2 - TXI	1/2023	5/2023

Requirements Flow-down

SLAC

FED — Released → **First Experiments Document**
A notional set of experiments of high scientific interest and importance, clearly establishing the need for LCLS-II

IRD & Scope — L2SI-PR-0005-R0, L2SI-SD-0040-R0 → **Instrument Requirements Document and Scope**
IRD establishes system-level physics and operational requirements. The Scope identifies the core components of NEH 2.2 necessary to carry out experiments

ConOps & Swimlane — Draft → **Concept of Operations and Swimlane Diagram**
The ConOps aims at capturing the lifecycle of an experiment at a high level. The Swimlane diagram establishes key tasks needed to perform successful experiments and identifies responsible sub-systems

ESB — Draft → **Experimental StoryBoard**
Breaks down individual tasks in a detailed description of hardware, controls, feedbacks, etc. (automation)

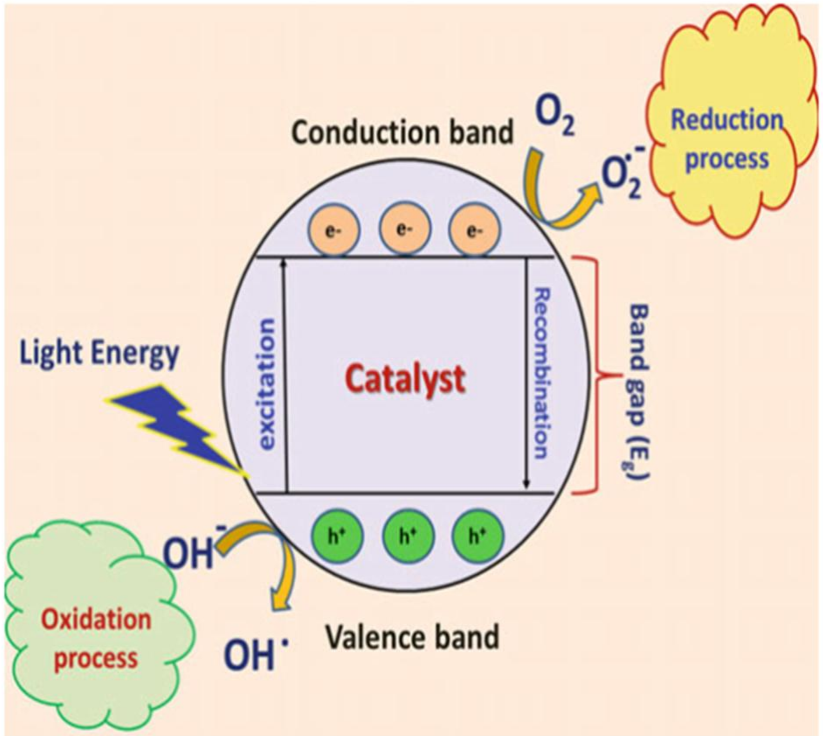
SRD — Released → **System Requirements Document**
Defines key instrument components and their physics requirements

ICD — Draft → **Interface Control Document**
Defines interface, boundaries and responsibilities with sub-systems

ESD — Released → **Engineering Requirements Document**
Provides a detailed description how the physics requirements set out in the SRD are met

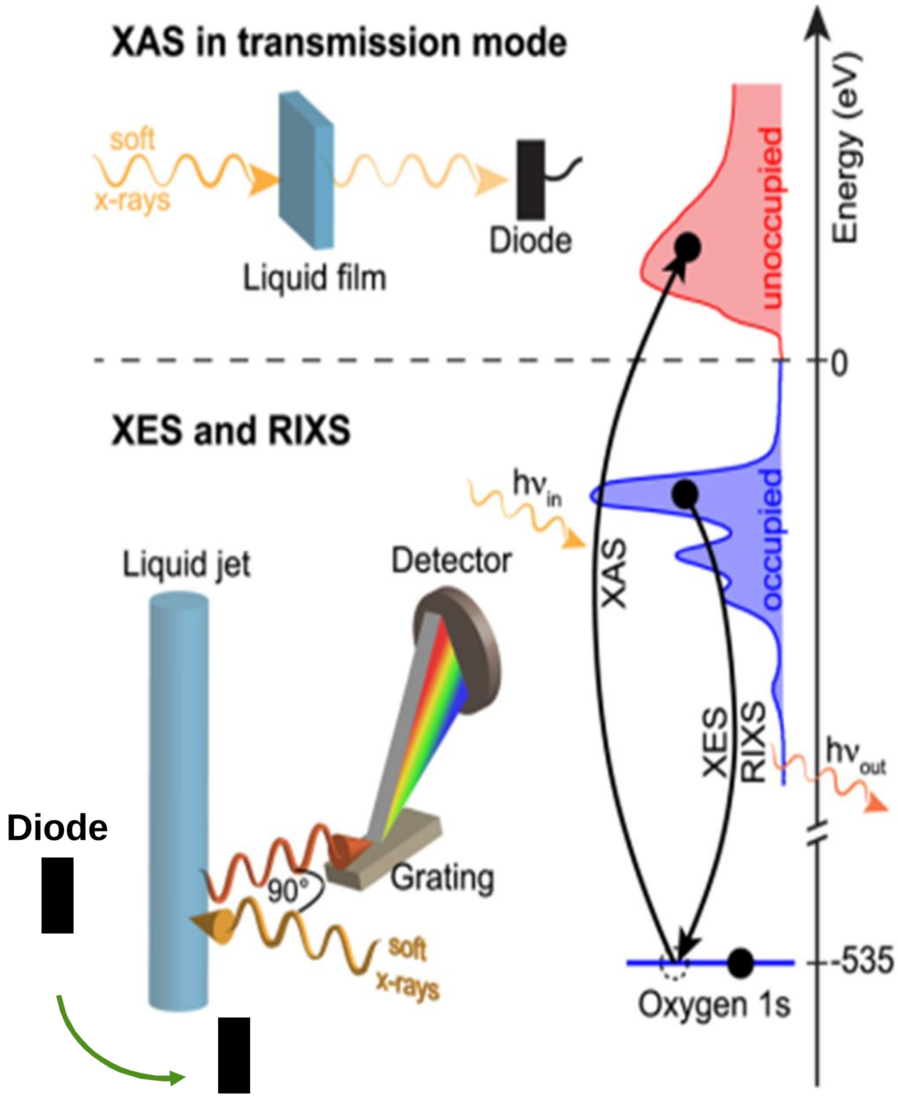
Science motivation: Photocatalysis

- **Key questions**:
  - How do photogenerated carriers catalyze chemical reactions?
  - How does charge separation, transport and localization occur on ultrafast time scales?
  - For systems in a photoexcited state, how does the nuclear structure and local defects influence the catalytic process?



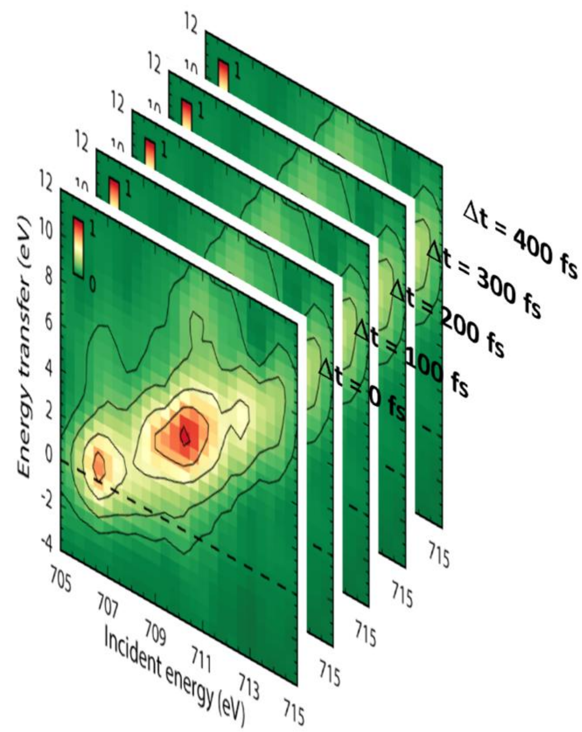
R. Saravanan, Francisco Gracia and A. Stephen, Springer, *Nanocomposites for Visible Light-induced Photocatalysis*

Techniques of choice



S. Schreck, *et al.*, Struct. Dyn., **1**, 054901, 2014

XAS: X-ray Absorption Spectroscopy
XES: X-ray Emission Spectroscopy
RIXS: Resonant Inelastic X-ray Scattering

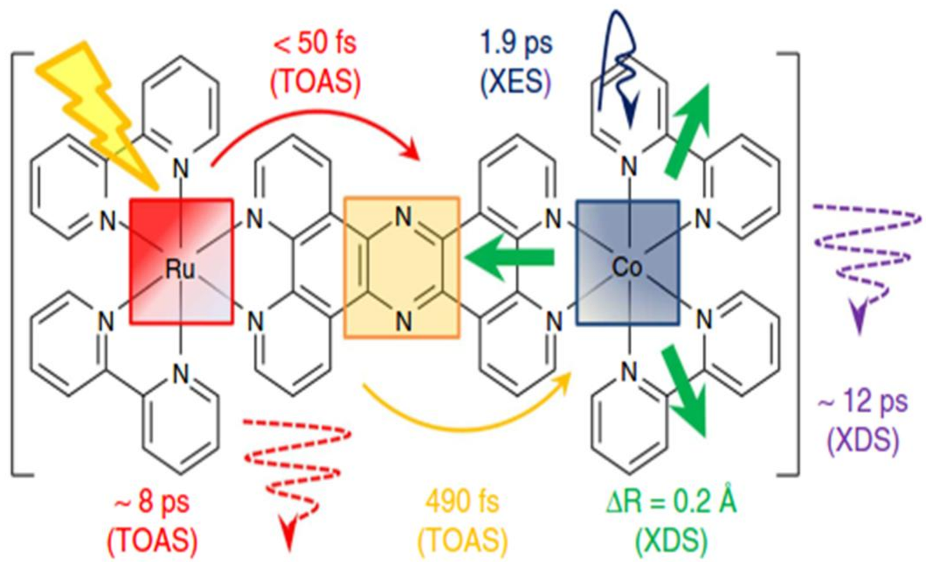


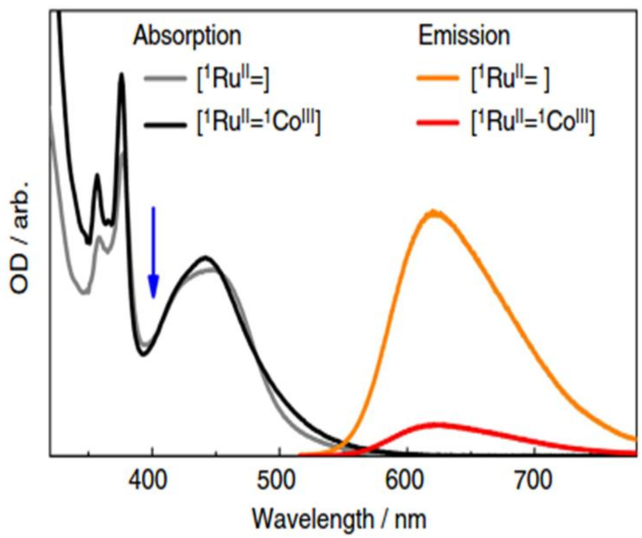
Wernet *et al*, *Nature* **520**, 78 (2015)

Deciphering the intramolecular electron transport on the femtosecond timescale

- **Key steps**:

1. Selective photoexcitation at the Ru site
2. XAS, XES and RIXS at Ru, N and Co to map (un)occupied DOS





- **Key requirements**:

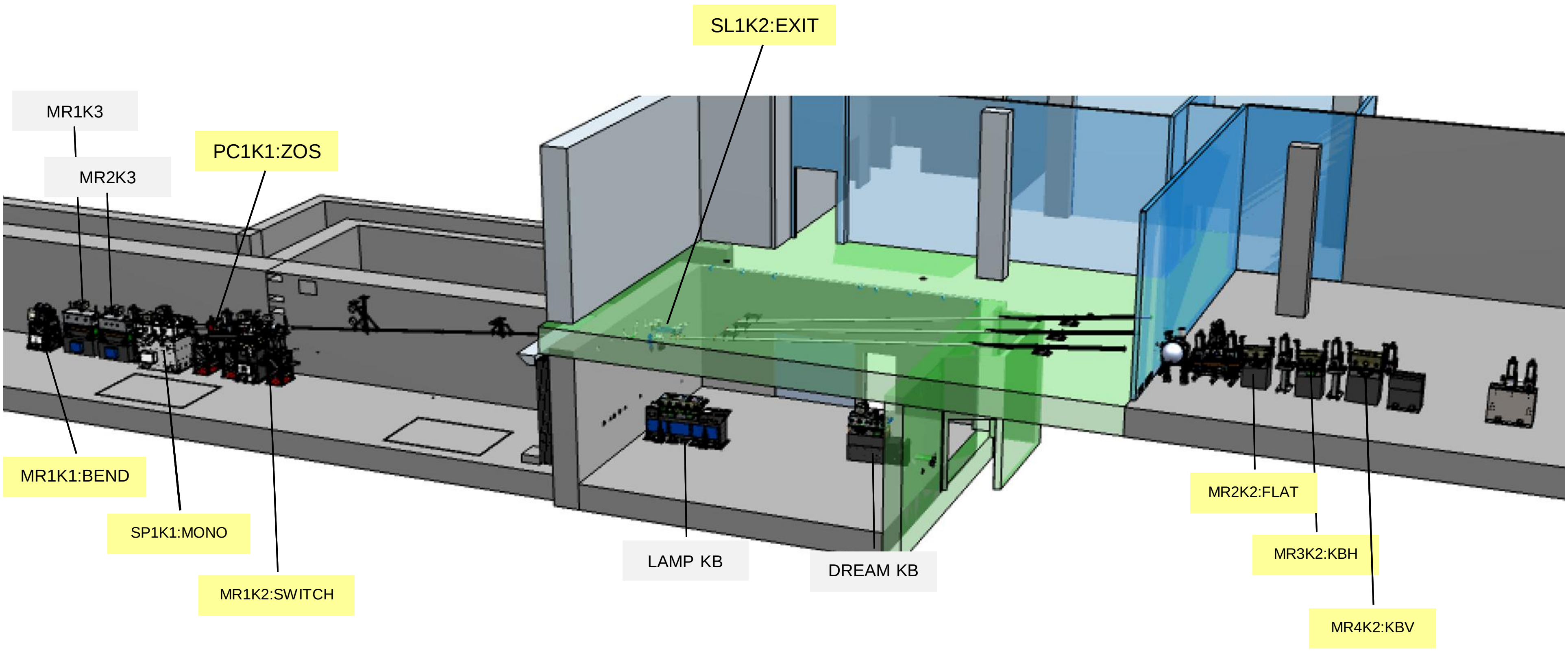
1. High throughput moderate resolution RIXS spectrometer
2. Tunable visible excitation
3. Fourier-transform-limited optical and x-ray pulses

S. Canton, *et. al* Nat. Comm. 6:6359, 2015

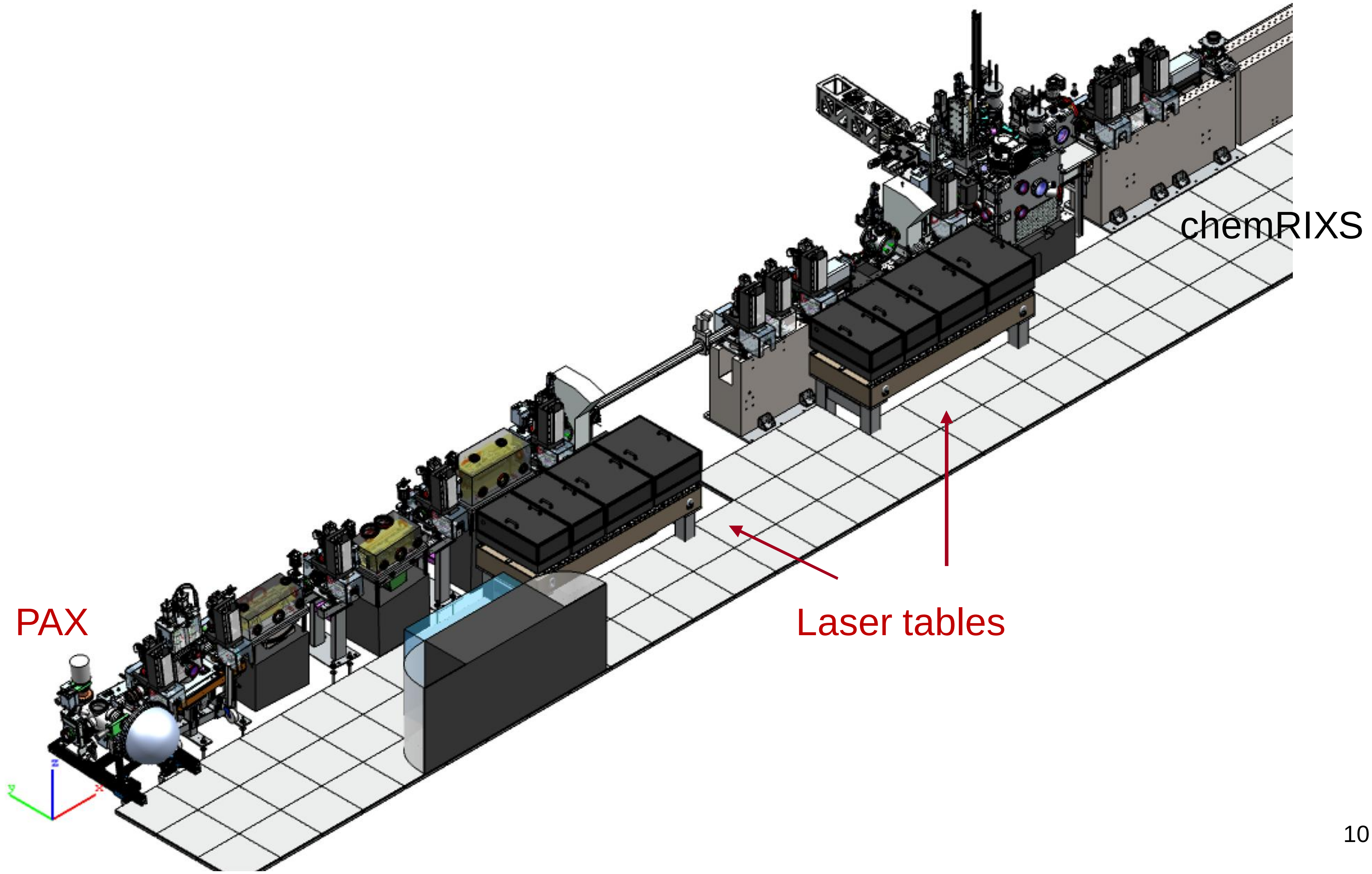
Key Beamline Performance Requirements

Parameter	Range	Comment
Photon Energy Range SXU [eV]	250-1600	Cover the C, N, O *K*-edge, L-edge of 3*d* transition metals, *M*-edge of rare earths
Bandwidth Control [RP, resolving power]	50,000; 10,000 5,000	Required for RIXS: 2 x FT limit Required for all other techniques: < 2 x FT limit
Experimental Spot Size Range a. Horizontal [µm] b. Vertical [µm]	3-1000 3-1000	Spot size adjustable to the interaction point at each endstation
Lasers	Visible to THz Visible to 2.4 µm	For correlated materials For chemistry

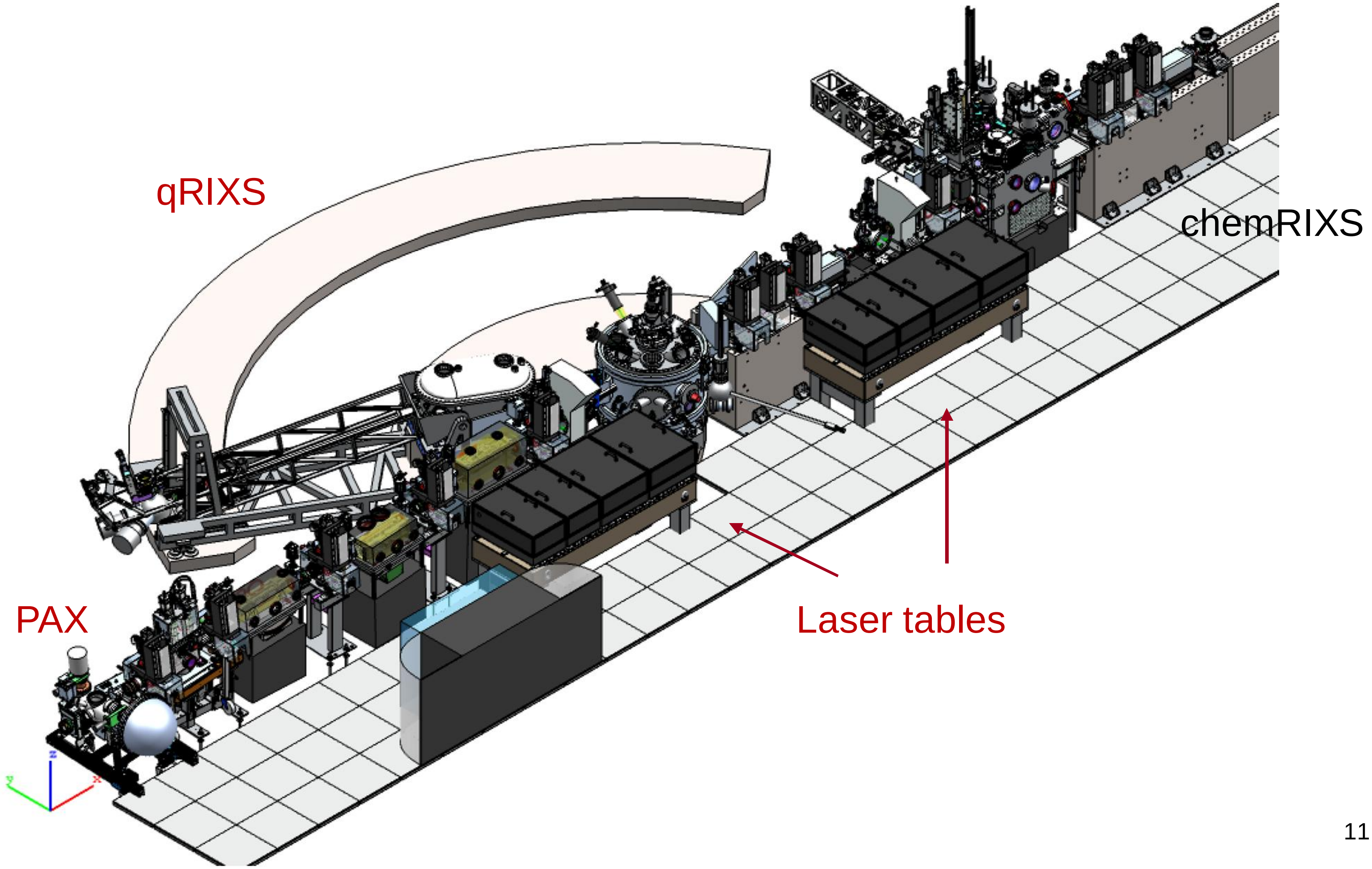
NEH 2.2 Optical Layout



NEH 2.2 Instrument Layout – Phase 1



NEH 2.2 Instrument Layout – Phase 2



What is NEH 2.2 all about?

- <u>X-ray beam with well-defined</u>:
  - Photon energy
  - Bandwidth
  - Pulse duration
  - Spot size
  - # of photons/pulse
  - Trajectory
  - Polarization

- <u>Laser beam with well-defined</u>:
  - Photon energy
  - Bandwidth
  - Pulse duration
  - Spot size
  - # of photons/pulse
  - Trajectory
  - Polarization

Stability

- Temporal overlap
- Spatial overlap

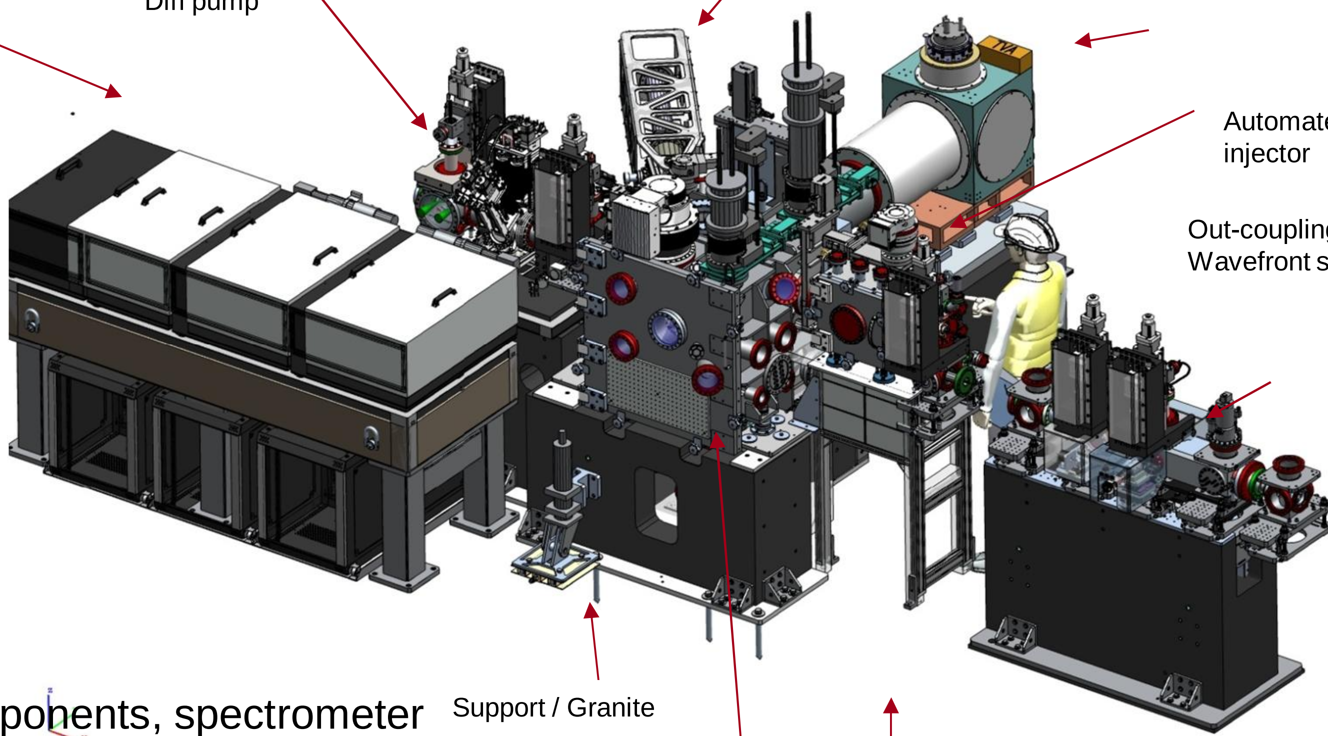
Diagnostics

Diagnostics

<u>Measurement</u>

- High SNR: normalization, photon counting
- Photon energy scanning: undulator + mono, laser
- Timing: PFTS, ATM
- Goal:
  - high-quality well-understood static spectra
  - Ability to detect small changes to controlled excitation

Integrated view



Design:

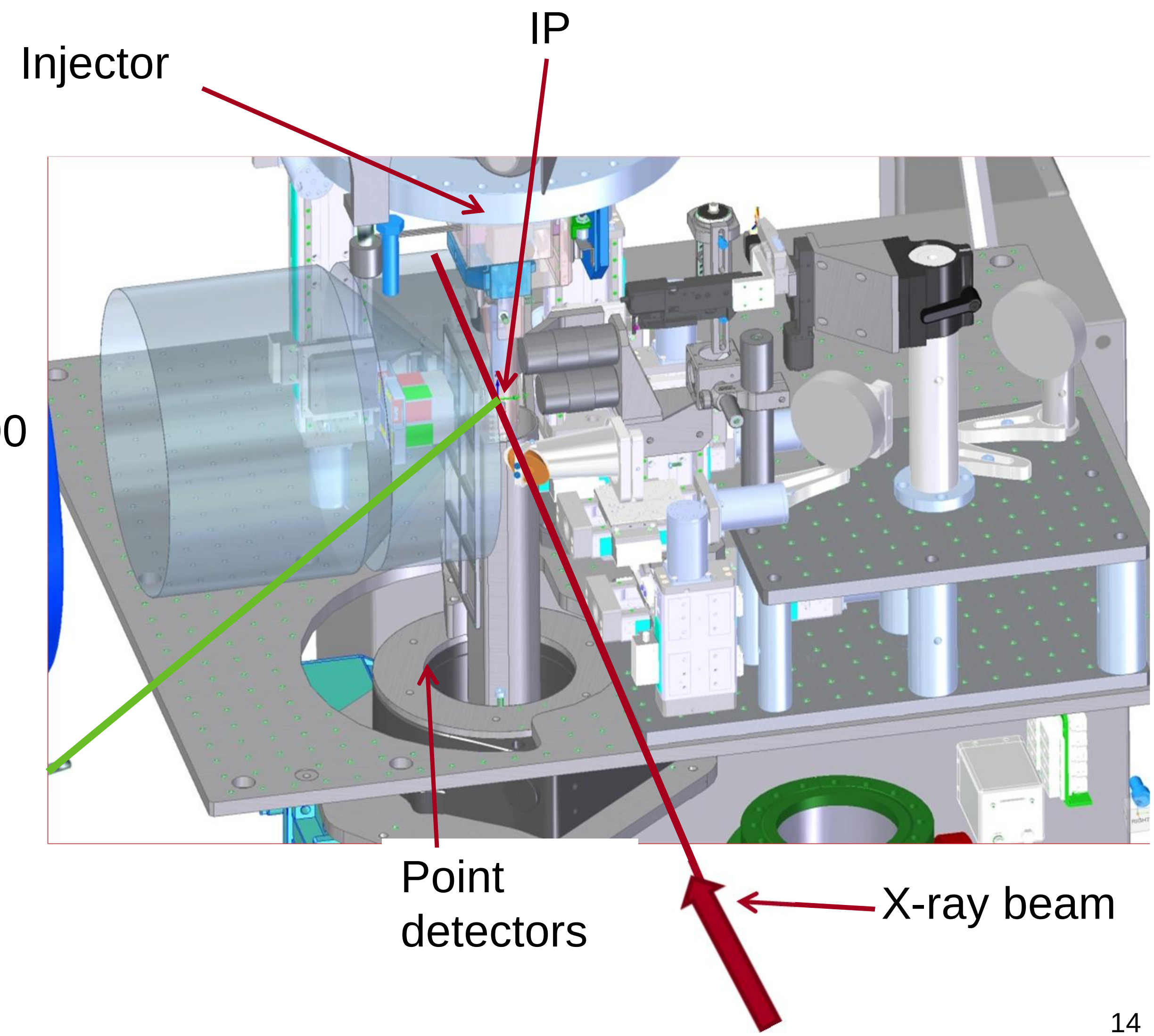
Advantages**:**
- Chamber, key components, spectrometer

Challenges:
- New sample delivery system, integration of multiple components, sub-system coordination

chemRIXS requirements: sample environment

Capabilities:

- Vacuum: 10^{-4} Torr (jets) to $<10^{-8}$ Torr (solids)
- Spectrometers: grating and transition-edge sensor, 2000 RP
- Point detectors: avalanche photodiode and microchannel plate: 1 MHz readout rate
- Sample Viewing: on-axis & perpendicular; infrared illumination

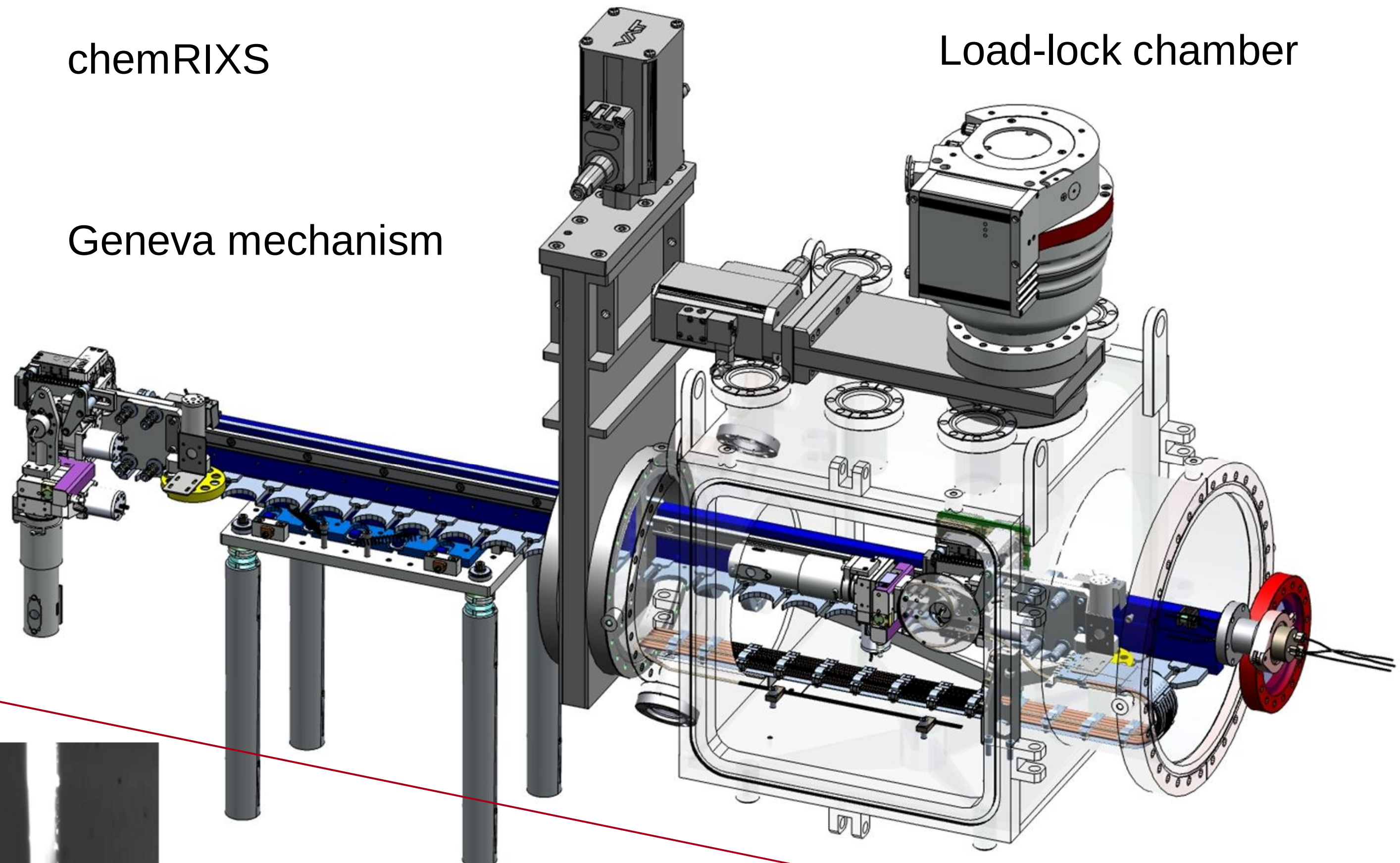


New development of sample delivery

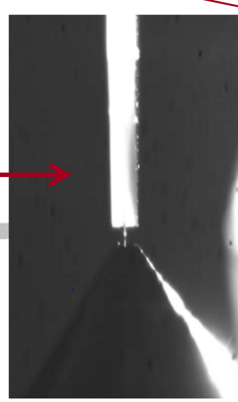
chemRIXS

Load-lock chamber

Geneva mechanism



Microfluidic chip

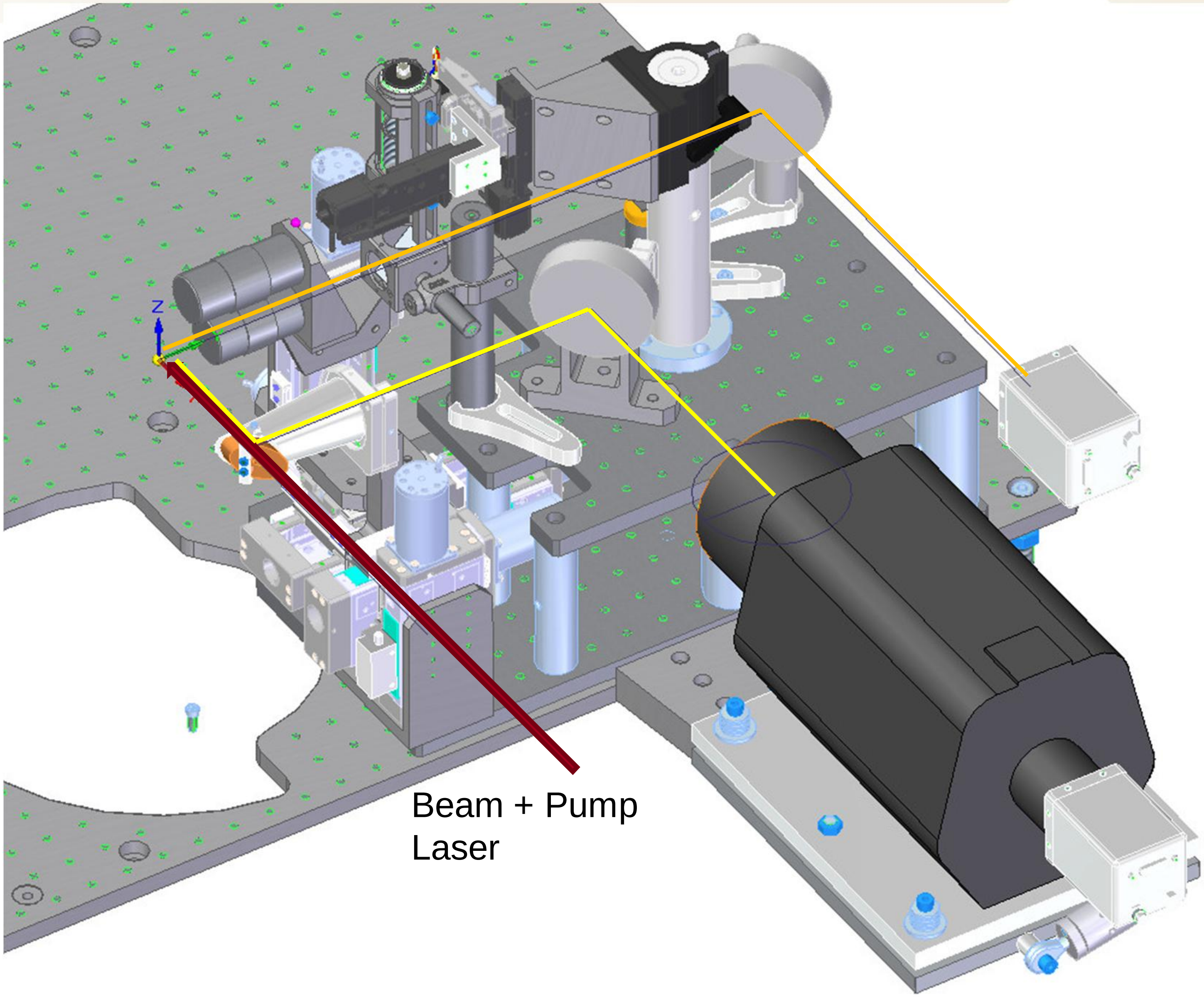


X-ray beam

Recirculating catcher

Viewing

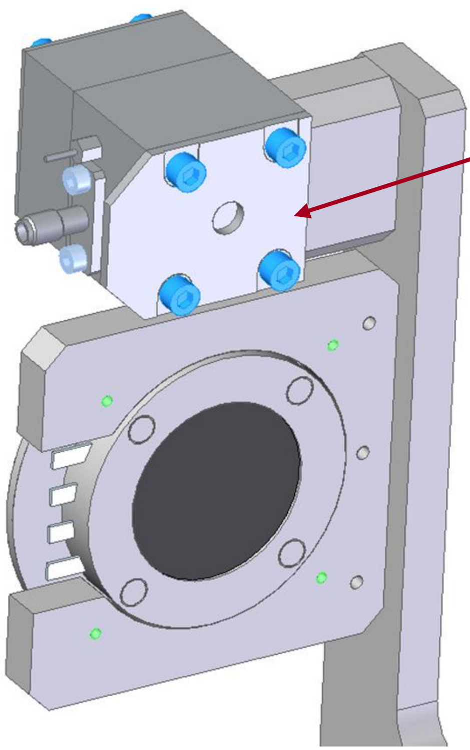
SLAC



Point Detectors

Motion	Range		Resolution		Repeatability	
	Req	Stages	Req	Stage	Req	Stage
Yaw	-10 + 155 deg	360 deg	0.001	0.000029	0.005	0.0005
T_Y	±20 mm	±25mm	0.5 µm	0.05 um	2 µm	±0.1 um

Point detector: APD + MCP



Alignment plate for Yaw

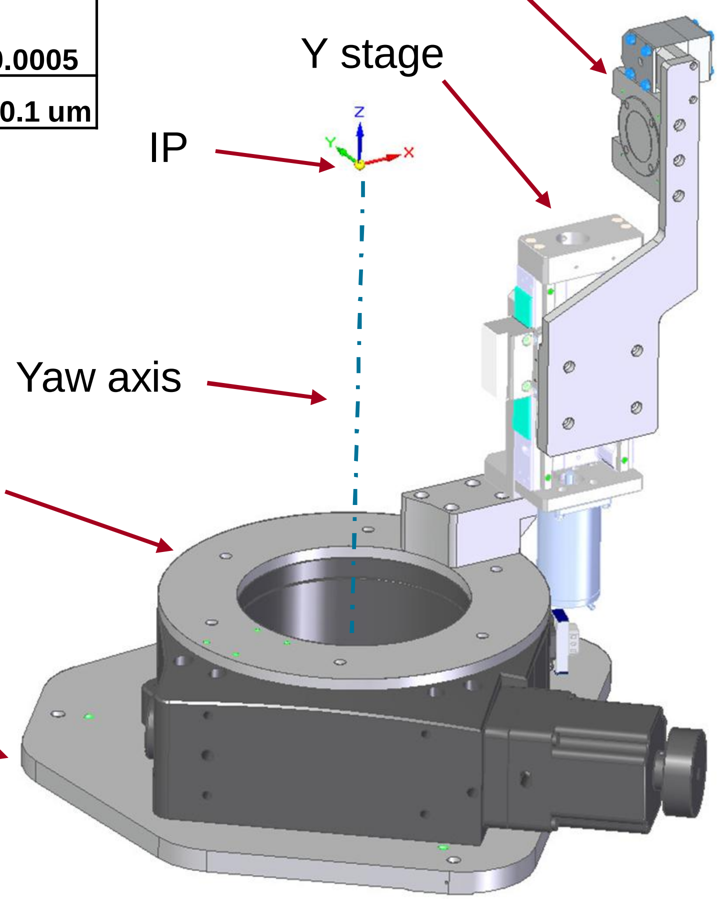
Point detectors, MCP + APD

Y stage

IP

Yaw axis

PI PRS-200



Run 18 call

The ChemRIXS instrument is a new endstation targeting studies of samples in solution using monochromatic soft x-ray pulses and a tunable optical laser pump. It is designed with emphasis on soft X-ray spectroscopy experiments on liquid samples, measured with a Varied Line Spacing (VLS) portable spectrometer. For rapid XAS measurements and direct beam detection (in the case of transmissive samples), a suite of in-vacuum detectors will be implemented on a rotating arm. The chamber will be equipped with the following:

- Liquid jet delivery via a microfluidic chip
- A load-lock chamber that allows chip exchange
- Catcher for capturing and/or re-circulating sample
- Viewing and illumination
- Diagnostic paddle for calibration targets, spatio-temporal overlap, etc.
- Laser in- and out- coupling
- Detectors optimized for x-ray absorption and emission spectroscopies
- Arrival time monitor located ~1 m from the interaction point

Key Performance Parameters for Run 18:

X-ray Parameters			Laser Parameters	
Repetition rate (Hz)	Up to 120		Repetition rate (Hz)	120
Energy Range (eV)	400 - 1200		Wavelength (nm)	400, 800, 480 - 900 (tunable)
Spot Size (um), H x V	10 x 10, min 1000 max		Pulse Duration (fs)	<40 @ 800 nm
Energy per pulse (uJ)	>2		Fluence (mJ/cm^2)	>50
Pulse Duration (fs)	<40		Spot size (um)	Min <50 X 50, option for 1:4 aspect ratio with <50 minor axis
Beamline Resolving Power	>2,000		Polarization control	Horizontal and vertical, circular at select wavelengths
Temporal resolution (fs)	<60		Arrival time monitor precision (fs)	<20
Polarization	Linear horiz.			
Wavelength scanning	Yes			

ChemRIXS will be optimized for studying systems with C, N, O and transition metal elements using various spectroscopy methods. Spectroscopic studies of rare earth elements will also be relevant so the beamline reach will extend to 1600 eV.

The following detectors will be provided to the users:

- Avalanche PhotoDiode (APD) and MicroChanel Plate (MCP). These are single-photon sensitive fast detectors suitable for X-ray Absorption Spectroscopy (XAS) in Total Fluorescence Yield (TFY) mode. These detectors will be mounted on an in-vacuum rotatable stage and can be placed in the horizontal scattering plane.
- Andor Newton_SO, 512 X 2048 pixels, 13.5 microns pixel size, capable of full frame read-out at 120Hz when operated in Full Vertical Binning mode. This CCD detector will be placed outside chemRIXS in the direct beam and will allow for measuring XAS in transmission when using thin sheet jets
- Portable Varied-Line Spacing (VLS) X-ray Emission Spectrometer (XES). This is an existing XES spectrometer with resolving power of ~2000, that will nominally be equipped with the abovementioned Andor Newton_SO CCD. Plans to incorporate a flange mounted MCP assembly, providing a factor 5 increase in horizontal acceptance (higher throughput), are underway and are expected to be delivered early on in Run 18. The spectrometer will be mounted in the horizontal plane at 90 degrees with respect to the X-ray beam.

The community is encouraged to propose experiments focusing on the following techniques

- Time-resolved XAS, which can be implemented in three modes:
  - Direct transmission (for samples delivered in the form of a thin sheet)
  - TFY mode, using the in-vacuum APD or MCP
  - Partial Fluorescence Yield (PFY) mode, using the VLS spectrometer
- Time-resolved XES, using the VLS with non-resonant excitation

Resonant Inelastic X-ray Scattering (RIXS)measurements, while possible as demonstrated during LCLS-I operation, are expected to remain quite challenging given the similar average flux expected during early operation with the Cu linac. Unless a compelling case is made, we discourage users from submitting proposals for experiments targeting time-resolved RIXS, as these will be much more efficient when the superconducting linac is operational.

Operation at 120 Hz (CuRF, Runs 18 & 19)

Limitations

- Energy per pulse will be limited to ~1 mJ to avoid possible grating damage; this is only an issue for CuRF, not for SCRF operation
- Average flux on the sample is expected to be similar to LCLS-I

- TES spectrometer is delayed to better align with SCRF and to assure performance of RP 2,000, currently an R&D effort
- An on-going effort to develop a high-throughput, dedicated grating spectrometer is underway

- Lasers will be based on Ti:Sapphire system: known performance, high energy per pulse, pulse duration ~40 fs
- Same CuRF infrastructure, jitter

chemRIXS objectives (for Cu-linac operation)

Main objectives:

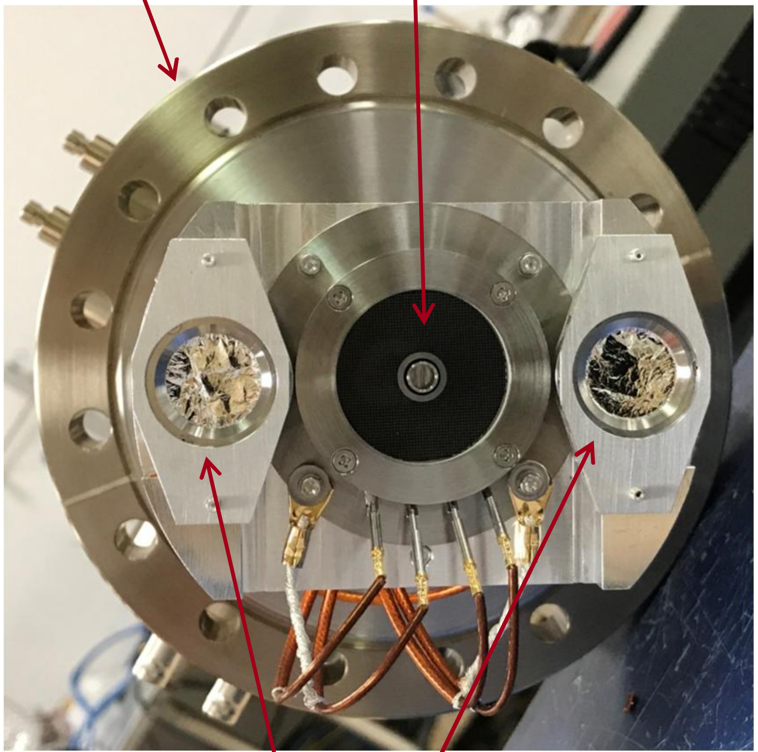
- Demonstrate scientific impact
- Demonstrate acquisition of high-quality XAS spectra
  - In transmission mode optimize counts on detector (size and attenuation of beam)
  - In TFY mode optimize solid angle acceptance and vacuum conditions (APD & MCP)
  - In PFY mode optimize collection efficiency with existing spectrometer
- Improve signal normalization
  - Characterize optimal FIM performance for specific experimental conditions
- Improve timing synchronization
  - Characterize ATM under experimental conditions, better understanding of long-term drifts
- Sample delivery improvement
  - Stability, visualization, exchange
- This information has been communicated to the users community with the call for Run 18

Fluorescence Intensity Monitor Prototype

- Heimann *et al.*, *J. Synchrotron Radiat.* **26**, 358 (2019)

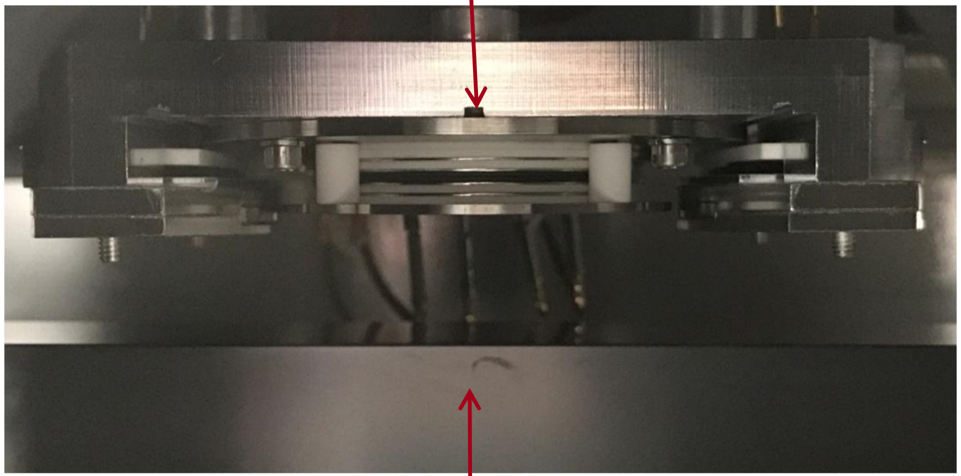
Multi-Channel Plate (MCP)
Hamamatsu F2223-21SH

6” Flange



0.1 μm Al filter / Photodiode
Optodiode AXUV63HS1

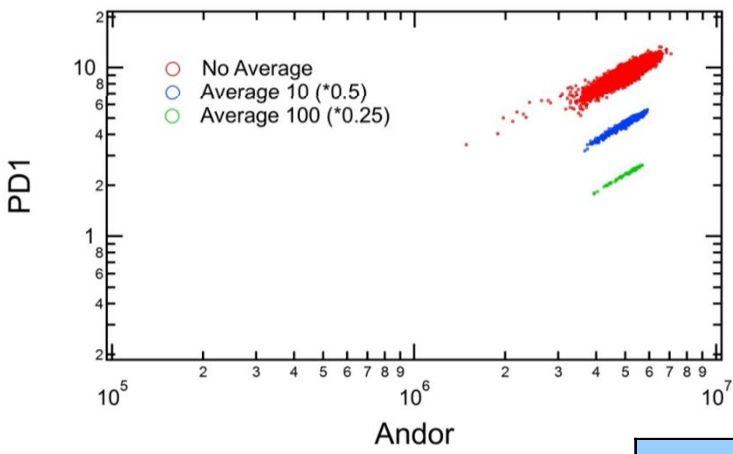
FIM

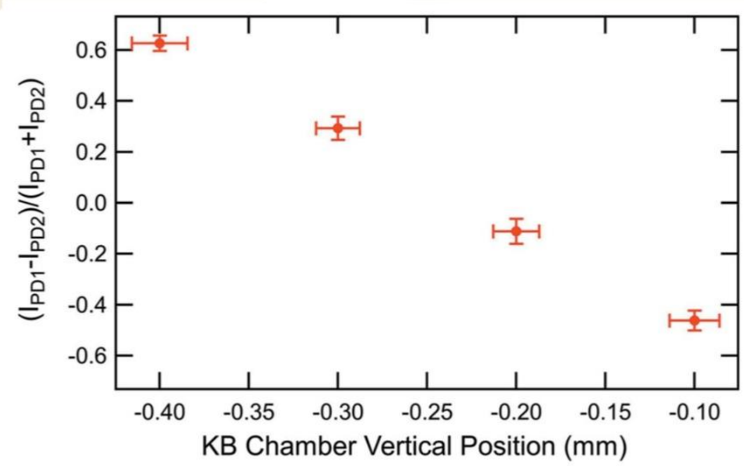


SXR Vertical KB Mirror

- Performed bakeouts and RGA scans on individual components for meeting the LCLS vacuum qualification.
- P(KB chamber) = 3 x 10^{-9} Torr two months after installation.

Sensitivity to X-ray Beam Position





Average	σ
1	0.051
10	0.019
100	0.0084

- σ improves with averaging and reaches <1% when averaging 100 pulses.

$$f(y) = \frac{I_{PD1} - I_{PD2}}{I_{PD1} + I_{PD2}}$$

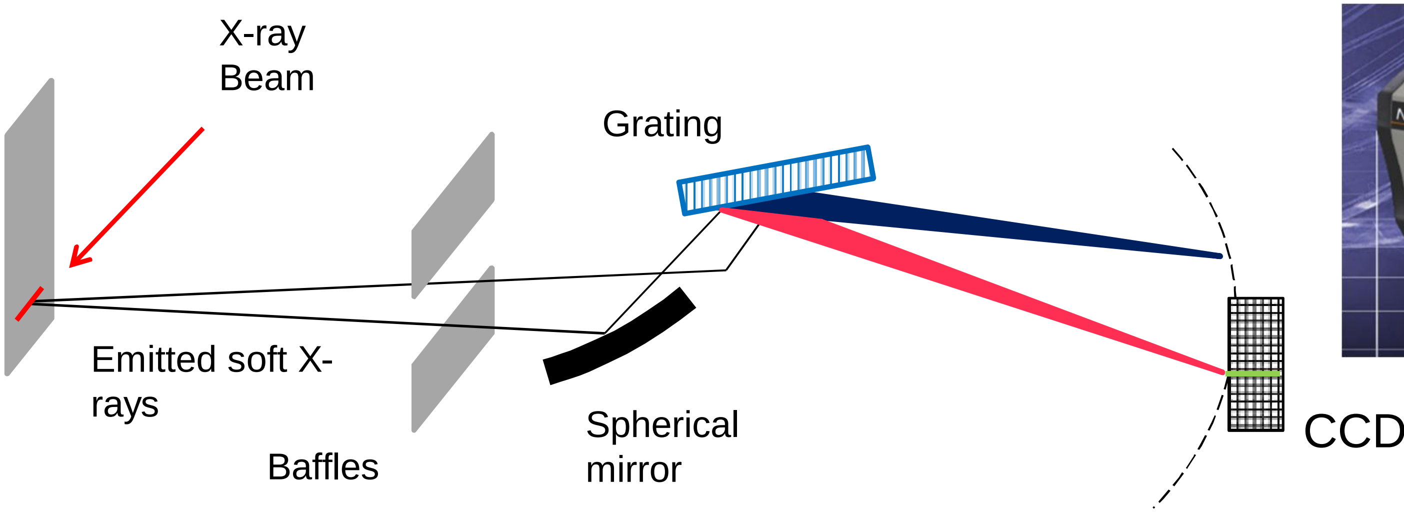
- An uncertainty of 2 μm in the vertical beam position ($\frac{1}{400}$ of the beam width) is calculated.
- It is possible to use the FIM to measure the X-ray beam position and for feedback correction of thermal drift.

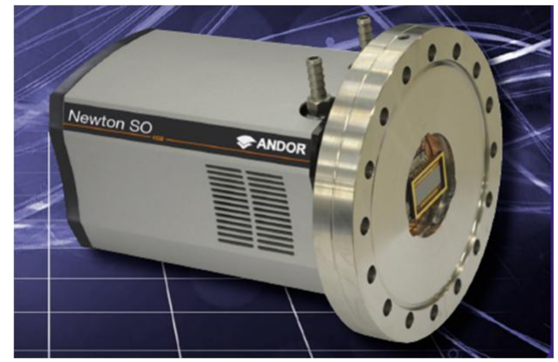
Near-term upgrade to our VLS spectrometer

SLAC

1200 l/mm VLS

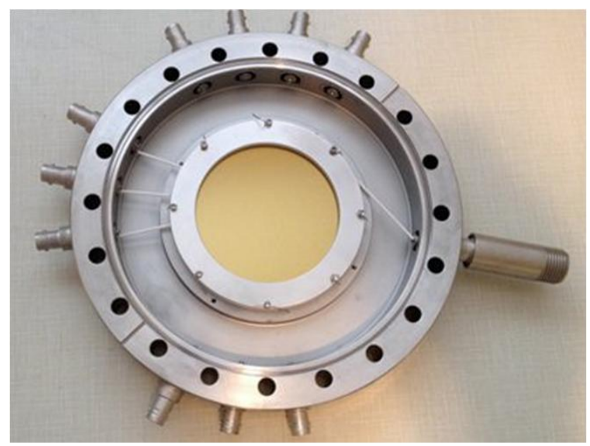
Resolving power ~2000





Acknowledgments:

- Project lead: Bill Schlotter
- Design: LBNL -> Yi-De Chuang, Zahid Hussain
- Design SLAC -> Daniele Cocco, Michael Holmes (CAM)
- Funding**: Nora Berrah**

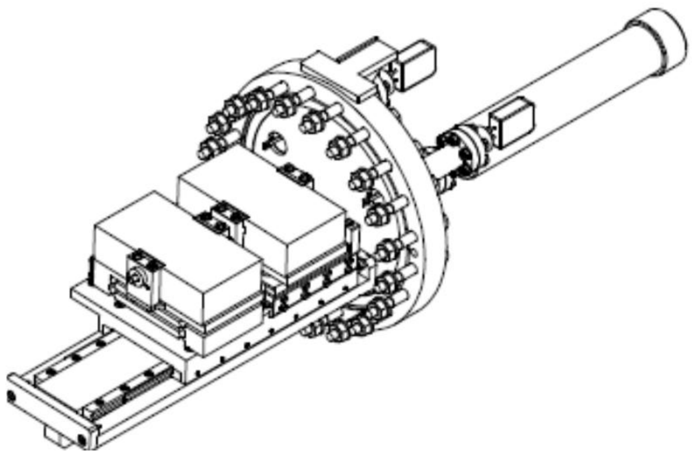


Large MCP + Phosphor screen + optical camera

Long-term upgrade to a new grating spectrometer

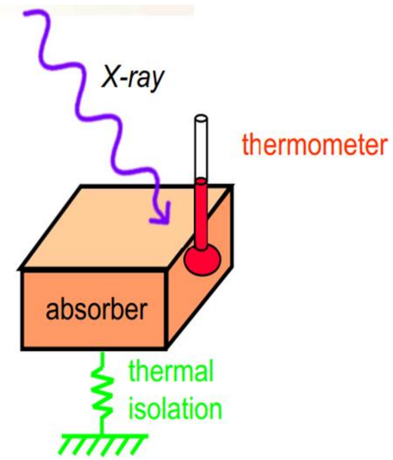
We plan to develop a new grating spectrometer, optimized for chemRIXS, with a target delivery date coinciding with the turn-on of the SC linac.

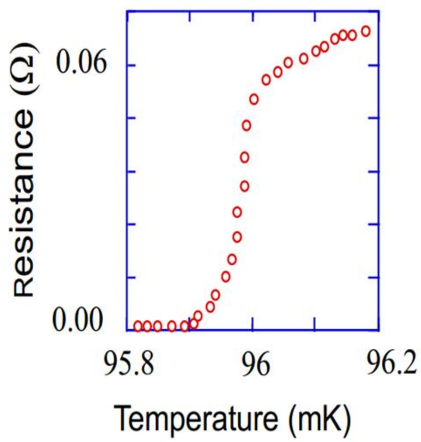
Objectives:

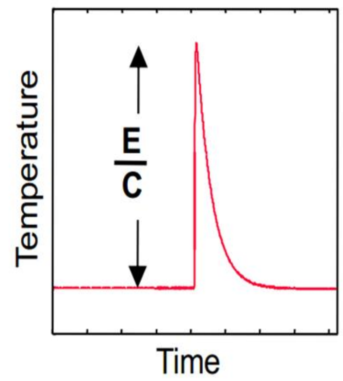


- Maximize throughput while
  - use 1 optical element
  - use CCD, commercially available
- Achieve RP 2,000 from 250 to 1,000 eV
- Accept "large" spot in dispersive direction
- Use 2 gratings, if needed
- Grating(s) need to be not state of-the-art
- Choose different photon energy with 1 motion of detector
- Alignment degrees of motion can be manual
- Needs to fit in the 90 deg geometry in chemRIXS
- Needs entrance apertures for the grating and
- Aluminum filter for the CCD

Transition Edge Sensor Spectrometer

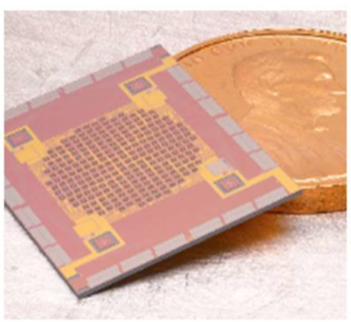


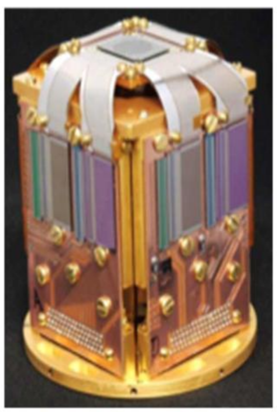




Capabilities:

- Large collection efficiency
- Fast readout
- 1 eV resolution (1 pixel) demonstrated
- 0.5 eV targeted (R%D effort)





TES spectrometers provide a unique combination of spectral resolution, efficiency, and broadband coverage

CDMS heritage

$$\Delta E \propto \sqrt{k_B T E_{max}}$$