

# LCLS Run 25 Users Town Hall

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February 6th 2025

# Agenda

Time (PST)	Topic	Presenter
<b>Plenary Session - <a href="#">Join via Zoom &gt;&gt;</a></b>		
9:00 am	Current LCLS Status & Plans	<b>Mike Dunne</b> Director, LCLS
9:15 am	Universal Proposal System	<b>Leilani Conradson / Paul Jones</b> LCLS User Office
9:23 am	User Executive Committee Update	<b>Silvia Pandolfi</b> LCLS UEC Vice Chair
9:26 am	Short Proposal Program Update	<b>Sandra Mous</b> LCLS Scientist
9:31 am	Accelerator Plans for Run 25	<b>Axel Brachmann / Tim Maxwell</b> Accelerator Dept. Head
9:40 am	Soft X-ray Instrument Capabilities (Introduce breakouts)	<b>James Cryan / Kristjan Kunnus /Georgi Dakovski</b> TMO/chemRIXS/qRIXS Instrument Leads
9:50 am	Hard X-ray Instrument Capabilities (Introduce Breakouts)	<b>Sebastien Boutet</b> Director of Operations
9:55 am	Data systems	<b>Jana Thayer</b> Data Systems Dept. Head
<b>Breakout Sessions/Office Hours by Instrument</b>		
10:10 am - 11:00am	<u>Session 1</u>	
	•TMO <a href="#">Join via Zoom &gt;&gt;</a>	James Cryan
	•MEC <a href="#">Join via Zoom &gt;&gt;</a>	Eric Galtier
	•MFX <a href="#">Join via Zoom &gt;&gt;</a>	Sebastian Dehe for Leland Gee
	•qRIXS <a href="#">Join via Zoom &gt;&gt;</a>	Georgi Dakovski
	•XCS/XPP <a href="#">Join via Zoom &gt;&gt;</a>	Matthieu Chollet & Takahiro Sato
	•chemRIXS <a href="#">Join via Zoom &gt;&gt;</a>	Kristjan Kunnus
	•CXI <a href="#">Join via Zoom &gt;&gt;</a>	Meng Liang

# Current LCLS Status & Plans

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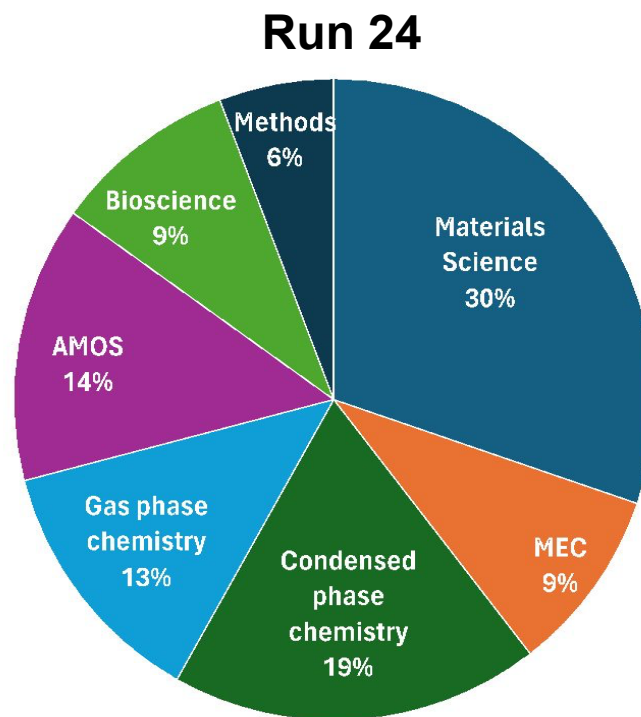
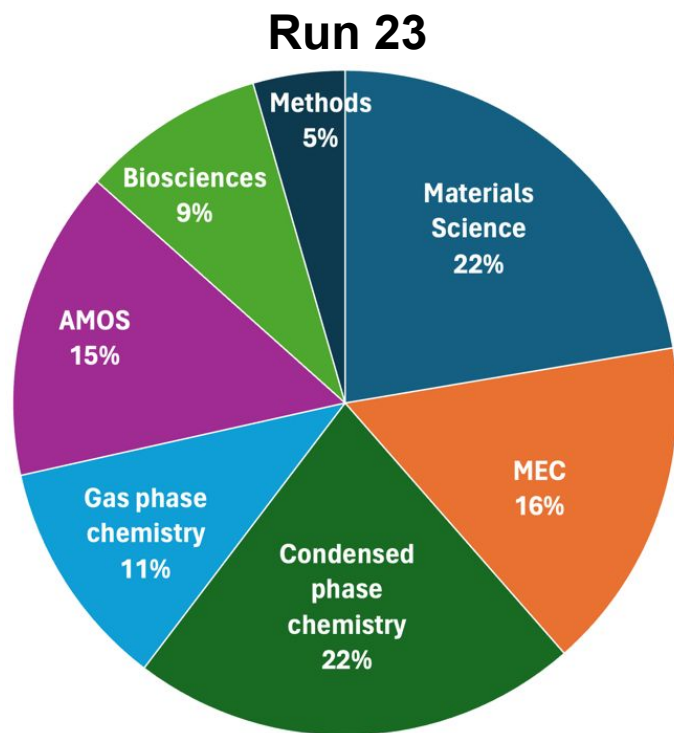
Mike Dunne

LCLS Director

February 6<sup>th</sup> 2025

# Recent proposal statistics

## Split by science area

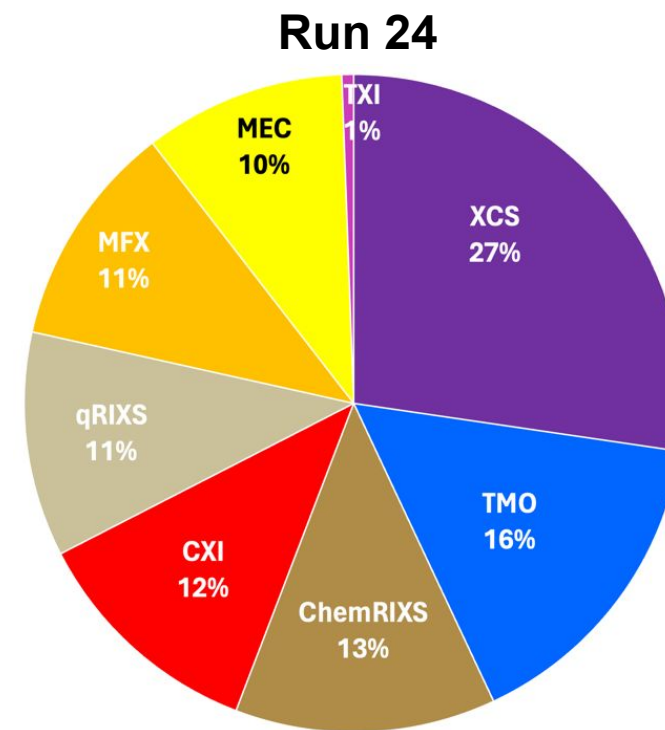


**158 proposals for Run 24 (March – July 2025)**

152 proposals for Run 23 (Aug 24 – Mar 25)

177 proposals for Run 22 (Jan – July 2024)

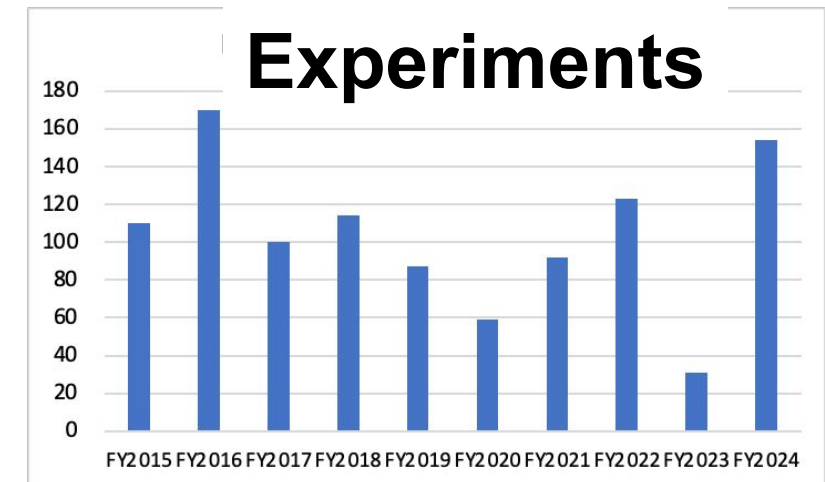
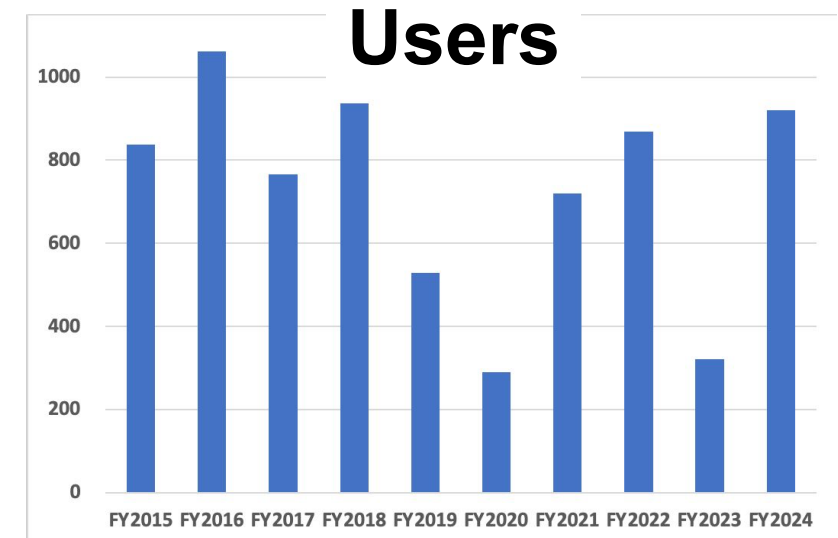
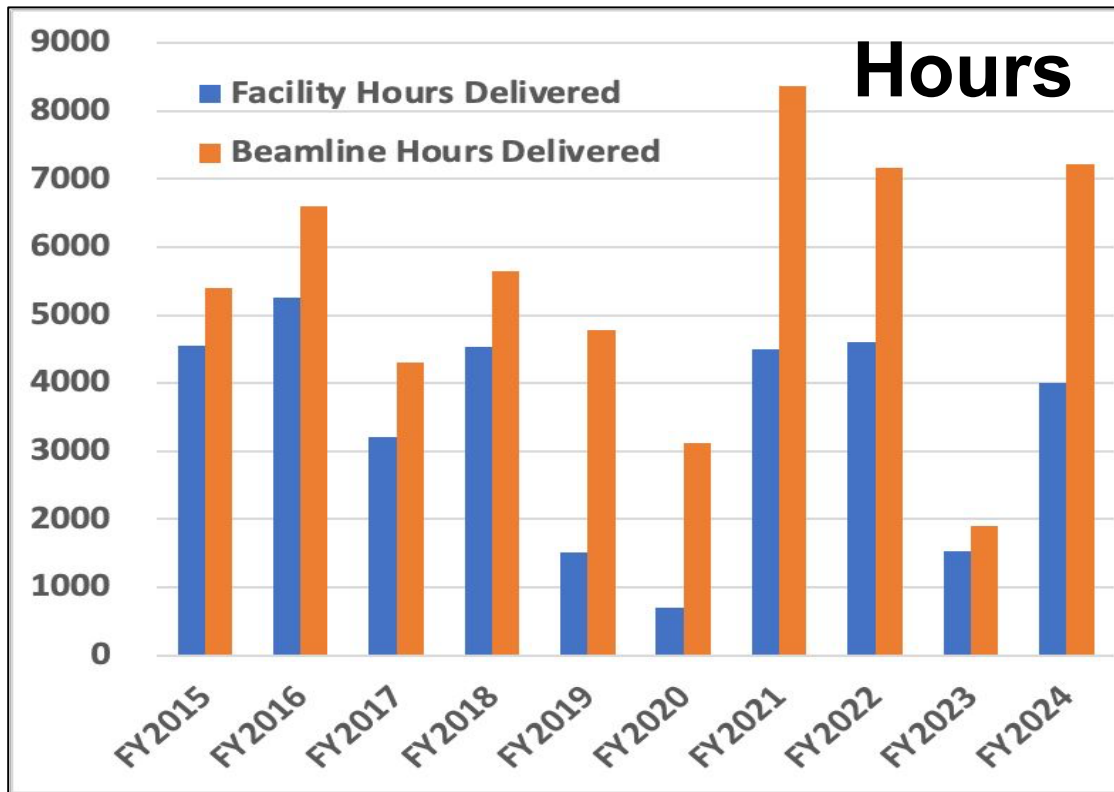
## Split by instrument



**Note:**

XPP upgrade for LCLS-II-HE started in December!

# FY2024 was a productive year, with a return to the high levels of delivered hours and users seen in our peak historical years



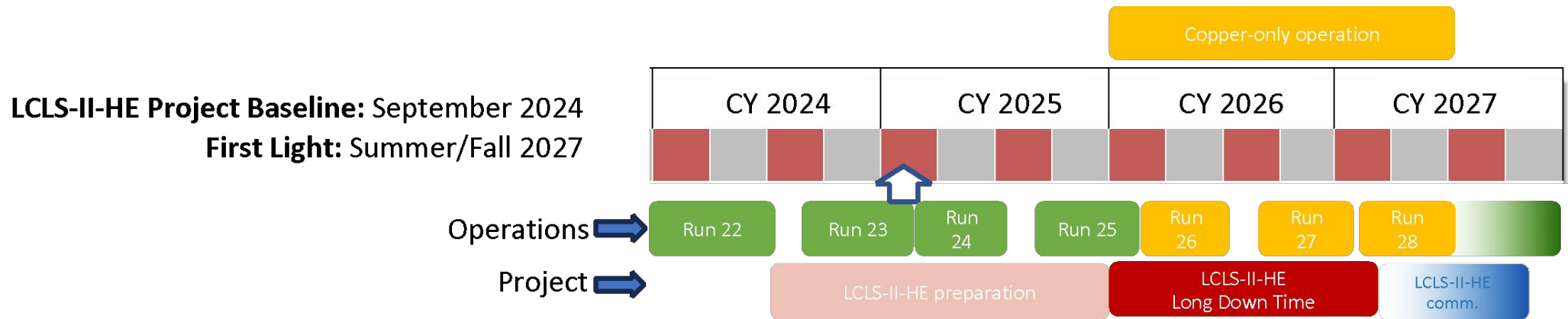
- FY24: **920** unique users (37% remote) for **154** experiments
- FY24 estimated annual publications at a high level (**203**)
- FY24 facility hours (**4005** = 3834 Cu + 171 SC)
- **FY25 planned** facility hours rises to **~7000** (4600 Cu + 2400 SC)

# Facility status – SC-based FEL

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- Highlights in Run 23 include sustained 8 kHz and sub-fs pulses (XLEAP)
- Increase of beam power limit **from 5 kW to 16 kW** for Run 24
  - Allows beam repetition-rate increase to 33 kHz and/or increased beam charge
  - Ongoing work to increase linac energy and improve beam emittance
- **Had to delay the restart of Run 23 in CY2025 due to vacuum leak in the SC linac gun**
  - Curtailed the final set of experiments in December
  - Invasive repair needed (multi-week) to replace a ceramic RF window
  - Restart is now underway
  - User science from 1 March to 17 March
- Recovered some beamtime by starting Run 24 early and finishing later
  - Run 24 (SC)      24 March to 20 July
  - Run 24 (NC)      27 March to 20 July

# Update on LCLS-II-HE downtimes, and impact on LCLS operations



An extended shutdown of the SC linac is needed (12 to 15 months)

- **Timing** of the Long Down Time (LDT) is driven by :
  1. LCLS-II-HE **Project readiness** for construction and installation work
  2. LCLS-SC **beam commissioning** to meet pre-determined performance goals (to reduce risk to HE)
  3. Delivery of LCLS-SC **user science program** (TMO, ChemRIXS, qRIXS)
- **Start of LDT deferred to January 2026** to allow additional time for beam ramping and user science
- **Run 25**
  - Cu linac (hard X-ray) users: 2 Sept 2025 to 31 Jan 2026
  - SC linac (soft X-ray) users: 15 Sept 2025 to 19 Dec 2025
  - With the limited beamtime to SC users, we will ask the PRP to provide particular attention to “*issues of programmatic and community diversity, access to new instruments*” to help ensure overall balance

# Summary of highlights for Run 25

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- Operation of **SC linac** at nominal 33 kHz (potential for higher rep-rate at constant power)
  - TMO-MRSCO/MBES and TMO-DREAM
  - ChemRIXS with new high throughput SVLS spectrometer and upgraded detectors
  - qRIXS
- Performance of **Cu linac** expected to enable 20-25 keV (previously 18keV limit)
  - XCS, MFX, CXI, MEC
  - XPP not available due to upgrade for LCLS-II-HE
    - Transition of user science to XCS: please consult with the instrument science team!
- New Dataset and Screening (DC&S) proposal mechanism (1-2 shifts) to be treated separately to full-scale proposals



# Universal Proposal System (UPS)

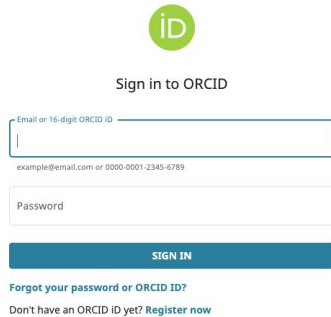
Paul Jones  <https://orcid.org/0000-0001-7538-4238>

Leilani Conradson  <https://orcid.org/0000-0002-4261-7135>

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February 6th 2025

# What To Expect



## Logging In

Authenticate into the system via your ORCID credentials

Do not request a new ORCID if you already have one - please use your existing ORCID

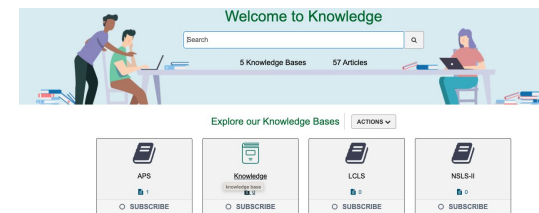


## Profile

Your UPS profile data is private and protected

Demographic data will only be used in aggregate

You decide how much info to share



## Knowledge Base

Under development - over time this will provide answers to FAQs

Fully searchable resources at your fingertips



## Dashboards

Configurability to put information from your most-used facilities front and center

# Important Notes

- **ALL members of the proposal team PIs, Co-PIs and Co-Proposers must register in UPS**
- Members of the proposal team can collaborate on draft proposals - once submitted, proposals cannot be edited
- Proposals not submitted by the submission deadline will be archived - they can be viewed, but not edited or re-used

## Useful Resources:

- Register / Login to UPS:  
<https://ups.servicenowservices.com/ups>
- Further information and tutorial video:  
<https://lcls.slac.stanford.edu/user-resources/proposals/universal-proposal-system-ups>
- Contact the User Office with questions:  
[lcls-user-office@slac.stanford.edu](mailto:lcls-user-office@slac.stanford.edu)

**Do not wait until the last minute to submit!**

**Welcome to the Universal Proposal System**  
A common platform for the management of user scientific proposals at APS, LCLS & NSLS-II

**Log in**  
LOG IN WITH ORCID

### World class

- State-of-the-art synchrotron radiation light sources at APS and NSLS-II offer continuous spectrum, high flux and brightness allowing scientists to probe the fundamental properties of matter.
- The free electron laser at LCLS generates ultra-bright, ultrafast, high coherence pulses, with the MeV-UED offering a powerful "electron camera" to study ultrafast atomic & molecular dynamics.

### Learn more

- User facilities provide open access to specialized instrumentation to scientists from universities, national laboratories, and industry.
- For approved, peer-reviewed projects, instrument time is available without charge to researchers who intend to publish their results in the open literature.
- Thousands of scientists conduct experiments at BES user facilities every year.

### Get started

- Create a free ORCID profile or use your existing ORCID ID to register to use the proposal system.
- Submit a proposal to request experimental time or submit a request against a proposal that has already been awarded time.
- Contact User Program staff with any questions – they are there to help!

U.S. DEPARTMENT OF ENERGY OFFICE OF SCIENCE X-RAY LIGHT SOURCES

### Participating Facilities

This tool is currently being used to support the proposal submission and review processes for the following facilities

#### Advanced Photon Source

**APS**

The APS, at Argonne National Laboratory, is one of only four third-generation, hard x-ray synchrotron radiation light sources in the world. The 1,104-meter circumference facility—large enough to house a baseball park in its center—includes 34 bending magnets and 34 insertion devices, which has a capacity of at least 68 beamlines for experimental research.

#### Linac Coherent Light Source

**LCLS**

The LCLS, at the SLAC National Accelerator Laboratory, is the world's first hard x-ray free electron laser facility and became operational in June 2010. This is a milestone for x-ray user facilities that advances the state-of-the-art from storage-ring-based third generation synchrotron light sources to a Linac-based light source.

#### National Synchrotron Light Source II

**NSLS-II**

NSLS-II is a state-of-the-art, medium-energy electron storage ring (3 GeV) that generates ultrabright, highly stable beams of synchrotron light, ranging from infrared to hard x-rays. It came online in 2014 and currently operates 29 beamlines with a capacity for about 60 beamlines when fully built out.

U.S. DEPARTMENT OF ENERGY Privacy and Security Notice

Facility websites: APS | LCLS | NSLS-II

# Need Help?

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## Universal Proposal System “Office Hours”

Date	Time
February 12, 2025	9:30 am Pacific Time
February 19, 2025	9:30 am Pacific Time
February 25, 2025	9:30 am Pacific Time
March 3, 2025	9:00 am Pacific Time
March 3, 2025	12:00 pm Pacific Time

Zoom links at: <https://lcls.slac.stanford.edu/news/lcls-run-25-call-proposals>

# LCLS UEC (User Executive Committee)

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Silvia Pandolfi, UEC Vice Chair

February 6<sup>th</sup>, 2025

# LCLS UEC (what is the role of UEC?)

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UEC is here to represent you!

UEC meets monthly with LCLS Management

UEC communicates the needs and desires of users regarding:

- LCLS operating policies and use of LCLS
- user support
- other issues of concern to users

UEC assigns LCLS awards during the User Meeting

Current Members of UEC & meeting Minutes: <https://lcls.slac.stanford.edu/lclsuo>

# Upcoming user meeting

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2025 LCLS/SSRL Users' Meeting: 22<sup>nd</sup>-26<sup>th</sup> September

Call for User Meeting Workshops is open (until March 28<sup>th</sup>)!

<https://forms.gle/qdUjAWTWynLLQ5sE6>

Please feel free to contact the LCLS UEC members with any suggestions or questions!

E-mail suggestions to

LCLS UEC [lcls-uec@slac.stanford.edu](mailto:lcls-uec@slac.stanford.edu)

or

User Office ([lcls-user-office@slac.stanford.edu](mailto:lcls-user-office@slac.stanford.edu))

# LCLS Run 25 Users Town Hall Dataset Collection & Screening

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Sandra Mous

February 6<sup>th</sup>, 2025



# LCLS Short Proposal Program

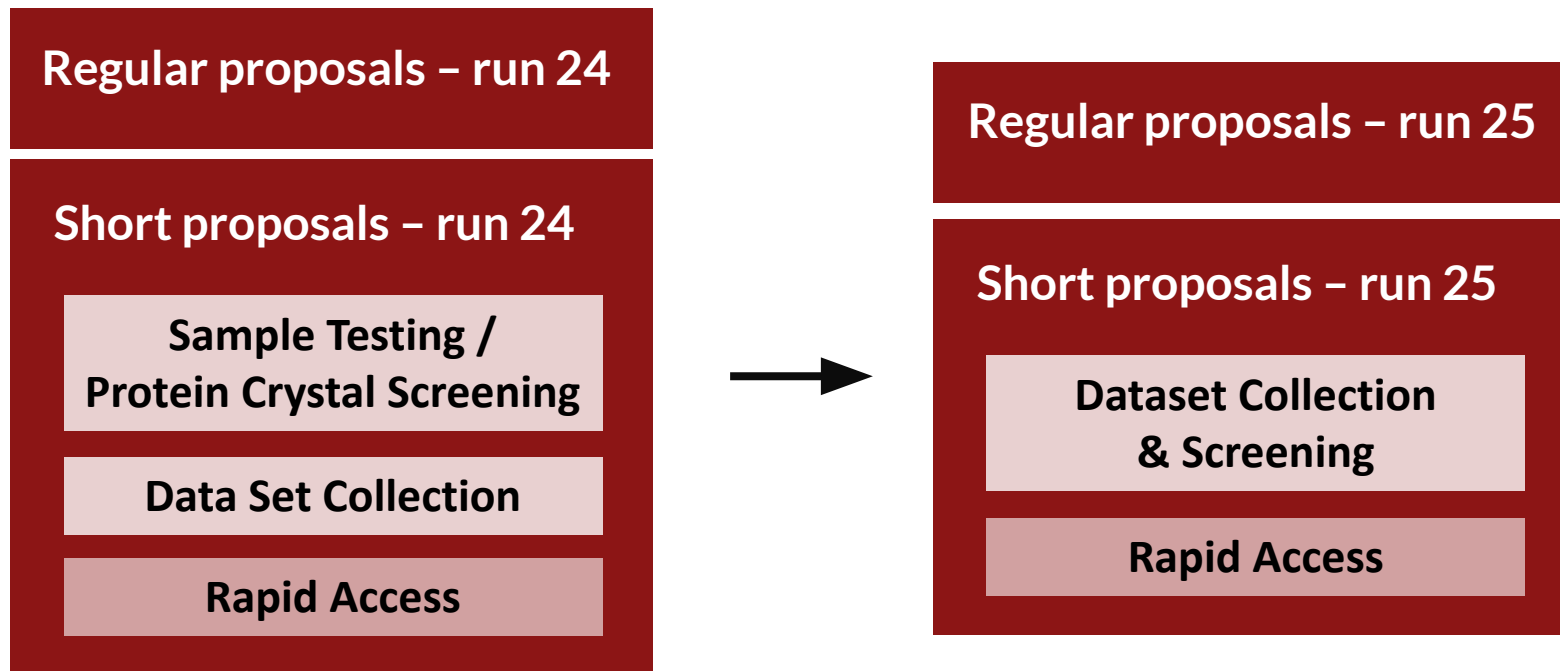
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- Offered alongside regular LCLS proposals
- Access mechanisms offered in the LCLS Run 24 Short Proposal Program:
  - **Sample Testing** (or Protein Crystal Screening - PCS): ideal for new user groups to gain first experience with XFEL beamtime and obtain preliminary results
  - **Data Set Collection**: enables user groups to complete data collection or test mature projects with a limited amount of beamtime (up to 24 hours)
  - **Rapid Access**: for time-sensitive experiments, provides short-term scheduling and rapid turnaround

# Unifying modes of access to LCLS

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- Merging some of the short proposal programs simplifies the modes of access to LCLS
  - **Dataset Collection & Screening:** short beamtime for testing or collecting a dataset using standard configuration
  - **Rapid Access:** rolling review and short-term scheduling



# Overview of changes to the program

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- **Experimental requirements:** DC&S proposals will need to make use of a standard configuration already in place for a regular LCLS experiment to maximize the throughput of an existing set-up
  - A list of select hard X-ray configurations has been made available in the call for proposals
  - DC&S proposals will not be carried over if a suitable configuration is not available
  - To apply for a short amount of beamtime using a non-standard configuration (or configurations not listed in the call for DC&S proposals), users will be asked to submit a regular proposal
- **Proposal templates:** user groups are asked to make use of the templates provided in the proposal call
  - The template addresses key review criteria
- **Alignment of submission deadline:** DC&S proposals are due at the same time as regular proposals
- **Concurrent review:** DC&S proposals are reviewed by the PRP at the same time as regular proposals
  - This helps ensure proposals are reviewed on time for scheduling considerations
- **Ranking:** DC&S proposals will be ranked separately from regular proposals
  - Acceptance is dependent on the available shifts and set-ups and may not strictly reflect the PRP ranking

# Availability

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- Scientific areas
  - Biology
  - Materials Science
  - Solution Phase Chemistry and Biochemistry
  - Gas Phase Photochemistry
  - Matter in Extreme Conditions
- Frequently deployed configurations only
  - XCS: horizontal liquid jet for solution scattering and hard X-ray spectroscopy
  - MFX: horizontal liquid jet for solution scattering or crystallography
  - MFX: droplet-on-tape for crystallography
  - MFX: fixed targets in air
  - CXI: liquid jet in the micron-focus chamber (no pump laser)
  - CXI: gas phase scattering in the micron-focus chamber with 200 nm or 266 nm pump laser
  - MEC: X-ray diffraction with uniaxial compression
  - MEC: X-ray imaging with long pulse laser side irradiation

# Contact information

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- Questions or feedback?
  - Please reach out to Sandra Mous ([smous@slac.stanford.edu](mailto:smous@slac.stanford.edu)) or respective instrument lead

# LCLS Run 25 Users Town Hall Accelerator Update

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Axel Brachmann, Tim Maxwell, Yuantao Ding

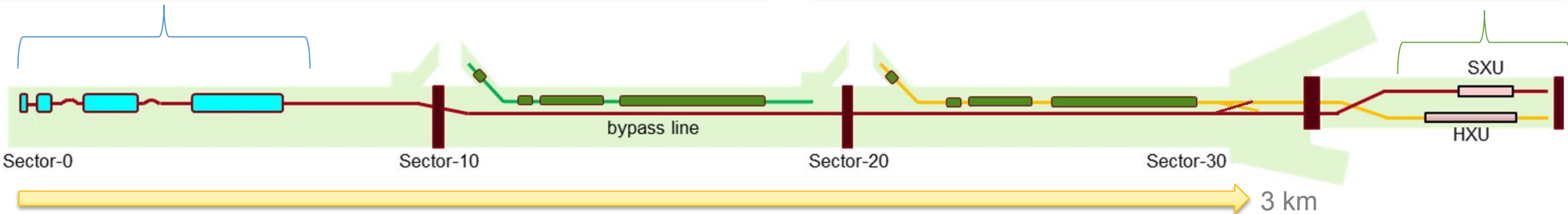
February 6<sup>th</sup>, 2025

# LCLS NC/SC Linac FEL Complex

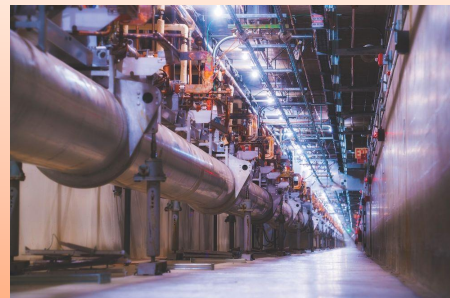
**Superconducting Linac**  
4 GeV,  
High rep rate, CW RF



**Soft and Hard X-ray  
Variable Gap  
Undulators (VGUs)**



*Linac gallery and new cryoplant viewed  
from Sector 0*



**Normal Conducting Linac**  
3.5-17 GeV,  
120 Hz Pulsed RF



# Hard X-ray, Normal Conducting Linac Capabilities



# HXR single-pulse SASE w/ NC Linac

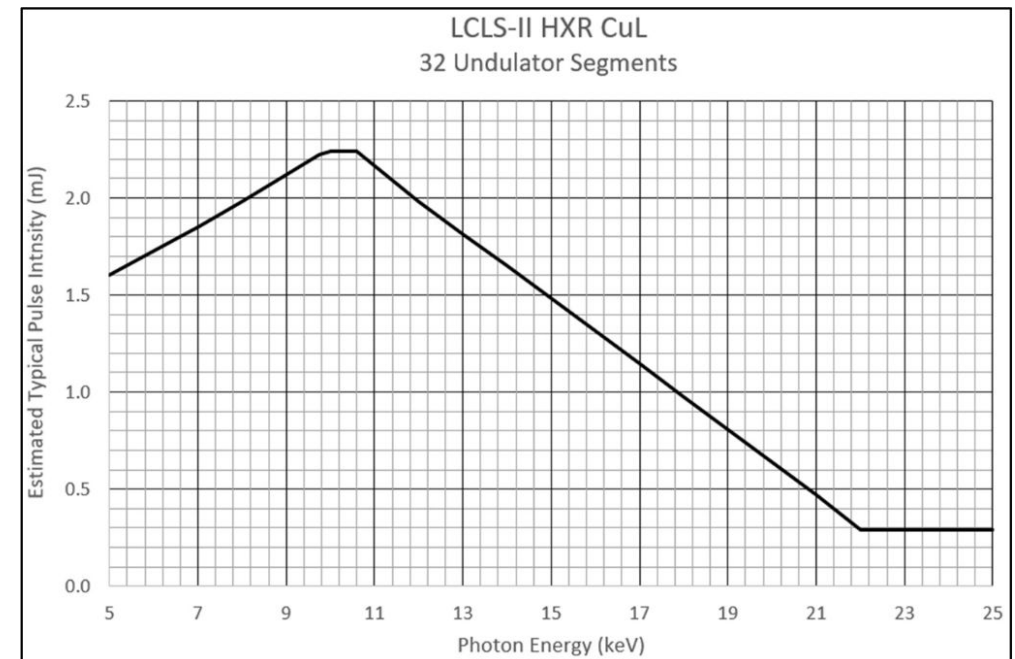
High photon energy (to 25 keV) and pulse energy (0.5-2mJ)

Varies w/ duration, energy, beamline transmission, etc.

Beam Parameters	Symbol	Cu-HXU x-rays		Unit
		$\omega_{\max}$	$\omega_{\min}$	
<b>Photon Energy</b>	<b><math>h\omega</math></b>	<b>25000</b>	<b>1000</b>	<b>eV</b>
Fundamental wavelength	$\lambda_r$	0.5	12.4	Å
Final linac e- energy	$\gamma mc^2$	16.5	3.5	GeV
FEL 3-D gain length	$L_G$	4	1	m
Peak power	$P$	20	80	GW
Pulse duration range (FWHM)		10 – 50		fs
<b>Nominal pulse duration (FWHM)</b>	<b><math>\Delta\tau_f</math></b>	<b>~30</b>		<b>fs</b>
<b>Max Pulse Energy*</b>	<b><math>U</math></b>	<b>0.6</b>	<b>2</b>	<b>mJ</b>
Photons per pulse*	$N_\gamma$	0.15	14	$10^{12}$
Peak brightness*	$B_{pk, SASE}$	7800	425	$10^{30} \S$
Average brightness (120Hz)*	$\langle B \rangle$	280	16	$10^{20} \S$
SASE bandwidth (FWHM)	$\Delta\omega/\omega$	30	2	eV
Photon source size (rms)	$\sigma_s$	8	20	$\mu\text{m}$
Photon far field divergence (FWHM)	$\Theta_{FWHM, x, \infty}$	1	12	$\mu\text{rad}$
<b>Max. Beam Rate</b>	<b><math>\phi_{FEL}</math></b>	<b>120</b>		<b>Hz</b>
Avg. x-ray beam power	$P_x$	0.07	0.24	W
Linear Polarization (100%)	$\langle P \rangle$	Vertical		

\*Assuming nominal duration and undulator strength

$\S$ Brightness units are photons/sec/mm<sup>2</sup>/mrad<sup>2</sup>/0.1%-BW

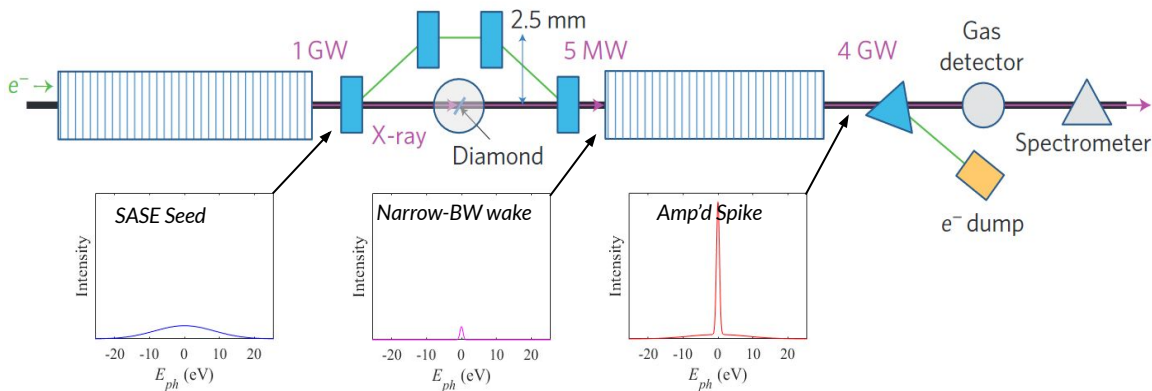


# Hard X-ray Self-Seeding (HXRSS)

## Spectral brightness enhancement for narrow bandwidth experiments

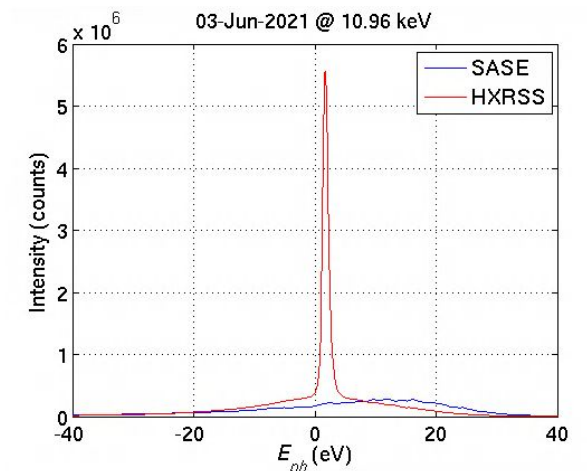
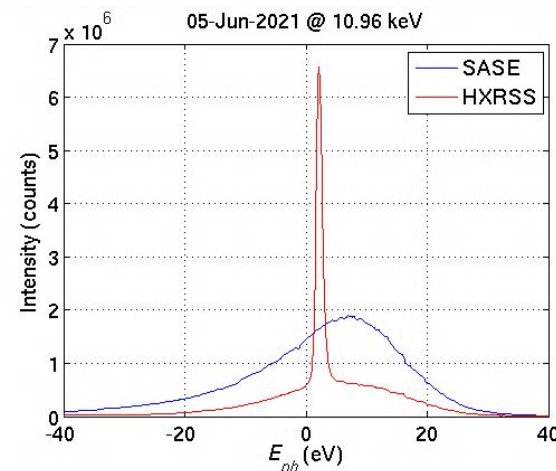
- Updated for LCLS-II vertically polarized HXU (90° rotation of crystal optics)
- 3-6x spectral brightness at sample vs. SASE

Photon energy	4.5 – 11 keV
Bandwidth (FWHM)	0.35 – 1.5 eV
Max pulse energy	0.2 – 0.5 mJ
Duration	30 fs



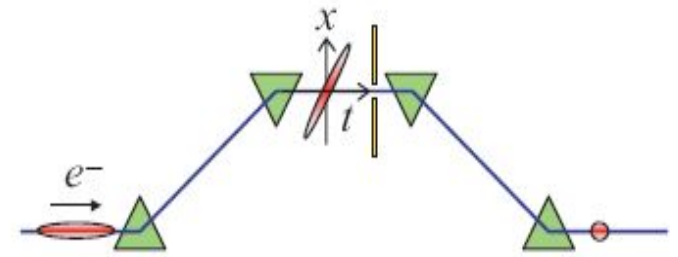
*Initial SASE passes diamond wake monochromator, narrow BW amplified in 2<sup>nd</sup> half of undulator*

**Full SASE vs. HXRSS average spectra at 11 keV**



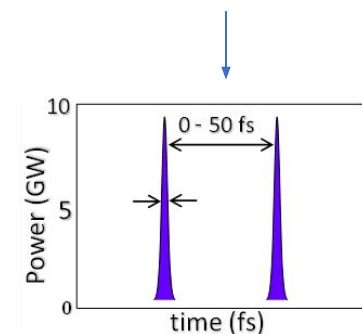
# Short Pulses

- **~5-10 fs HXR pulses readily achievable** with corresponding reduction in pulse energy (change of charge, use of “slotted foil”)
- Methods are available for **< 1 fs HXR pulses**, approaching single SASE spike limit



**Slotted foil** inserted in beam to spoil lasing in time

Make short single or double pulses



Technique	Min Pulse Duration	Energy/Pulse	single-spike rate
Slotted foil / optics / taper	400 as	5 uJ (76% fluct.)	65%
Non-linear bunch compression	200 as	10 uJ	45%
HXR XLEAP (experimental)			

Discuss special requirements with your LCLS POC

# Advanced Multi-Pulse/Color Modes

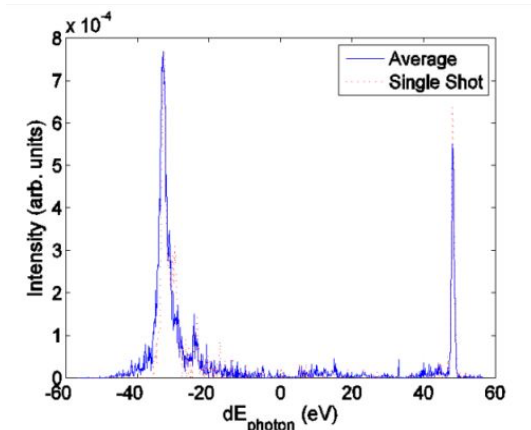
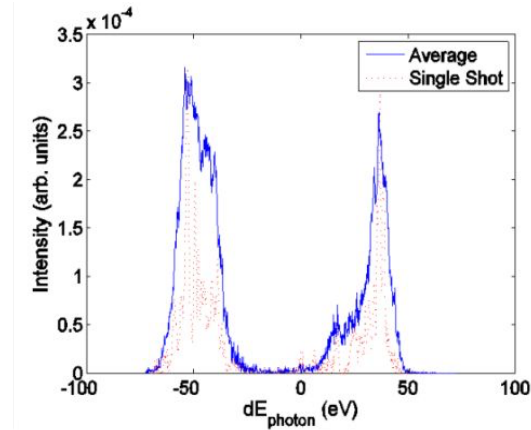
Multiple accelerator-based means for x-ray pump, x-ray probe on variety of time scales

## One electron bunch:

- Double slotted foil

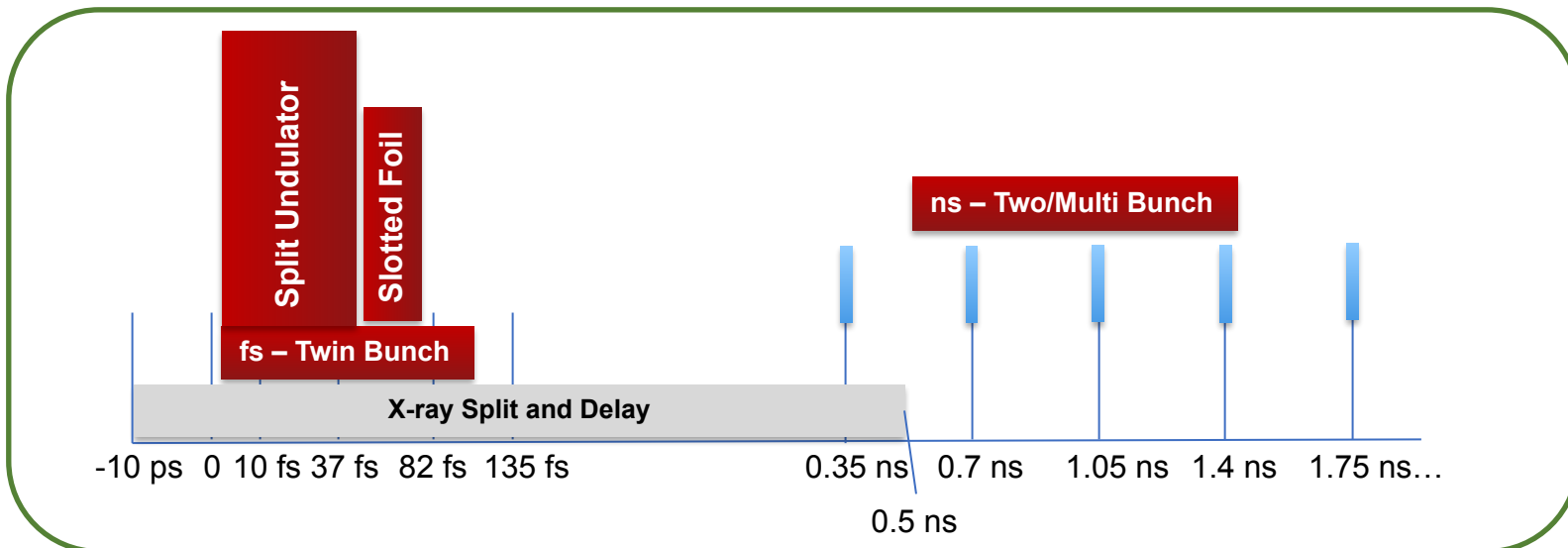
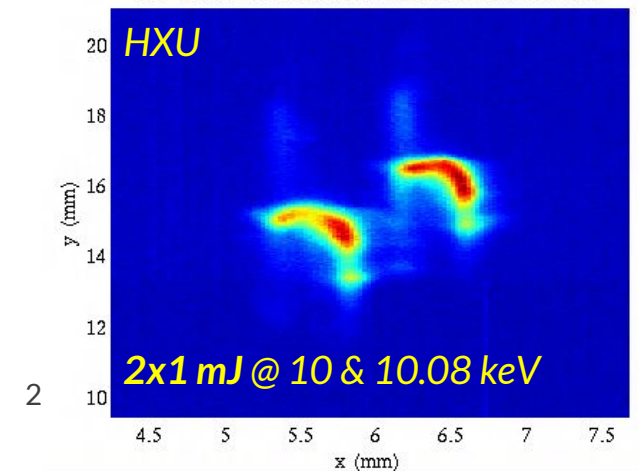
## Two electron bunches:

- fs spacing: Injector laser pulse splitting (“twin bunches”)
- ns spacing: Multiple laser pulses at cathode (“two/multi bunches”)



## Two-bunch XTCMV Images (ns spacing)

Profile Monitor OTRS:DMPH:695 27-Jun-2021 10:49:58



# Advanced Multi-Pulse/Color Modes

Multiple accelerator-based means for x-ray pump, x-ray probe on variety of time scales

Technique	Pulse Separation	Pulse Duration	Energy Separation	Max Energy/Pulse
Split Undulator SASE	0 - 30 fs	15 fs	Up to factor 1.2 ratio in photon energies	40 uJ (25 fs pulse duration)
Double Slotted Foil	7-20 fs	~ 10 fs	+/-1.5%	100-200 uJ
Twin Bunches				
Two SASE Pulses	20 - 125 fs	~ 10 fs	0.2-2%	0.3 mJ (20 fs duration)
With slotted foil (shorter pulses)	+/- 50 fs	~5-10 fs	~2%	40 uJ
Two-(multiple) bunch				
Two bucket	350 ps increments, up to 120 ns	20 fs	~ 1%	0.5-1 mJ (30 fs duration SASE)
Multi bucket (4 or 8 bunches)	Two trains of 4 pulses. 700 ps between each pulse in the same train.	20 fs	~ 1%	To be tested



Soft X-ray, Superconducting Linac Capabilities

# SXR single-pulse SASE w/ SC Linac

Beam Parameters	Symbol	SC-SXU x-rays			Unit
		$h\omega_{\max}$	$h\omega_{\text{nominal}}$	$h\omega_{\min}$	
<b>Photon Energy</b>	$h\omega$	1300	800	200	eV
Fundamental wavelength	$\lambda_r$	9.5	15.5	62.0	Å
Final linac e- energy	$\gamma mc^2$	3.5-4.0			GeV
FEL 3-D gain length	$L_G$	TBD			m
Peak power	$P$	3	2.5 - 7	8	GW
Pulse duration range (FWHM)		20 – 40			fs
<b>Nominal pulse duration (FWHM)</b>	$\Delta\tau_f$	20			fs
<b>Max Pulse Energy*</b>	$U$	0.06	0.05 - 0.14	0.16	mJ
Photons per pulse*	$N_\gamma$	0.28	0.4 - 1.1	5.0	$10^{12}$
Peak brightness*	$B_{pk, SASE}$	20	8.6 - 24	1.7	$10^{30} \S$
Average brightness* (@33 kHz)	$\langle B \rangle$	137	57 – 161	12	$10^{20} \S$
SASE bandwidth (FWHM)	$\Delta\omega/\omega$	4	3	3	eV
Photon source size (rms)	$\sigma_s$	TBD			μm
Far field divergence (FWHM)	$\Theta_{FWHM, x, \infty}$	TBD			μrad
<b>Max. Beam Rate</b>	$\varphi_{FEL}$	1,000 – 40,000 **			Hz
Avg. x-ray beam power (@33kHz)	$P_x$	2.0	1.7-4.6	5.3	W
<b>Linear Polarization (100%)</b>	$\langle P \rangle$	Horizontal			

**Pulse energies of >100 μJ in <40 fs**

<https://lcls.slac.stanford.edu/machine/parameters>

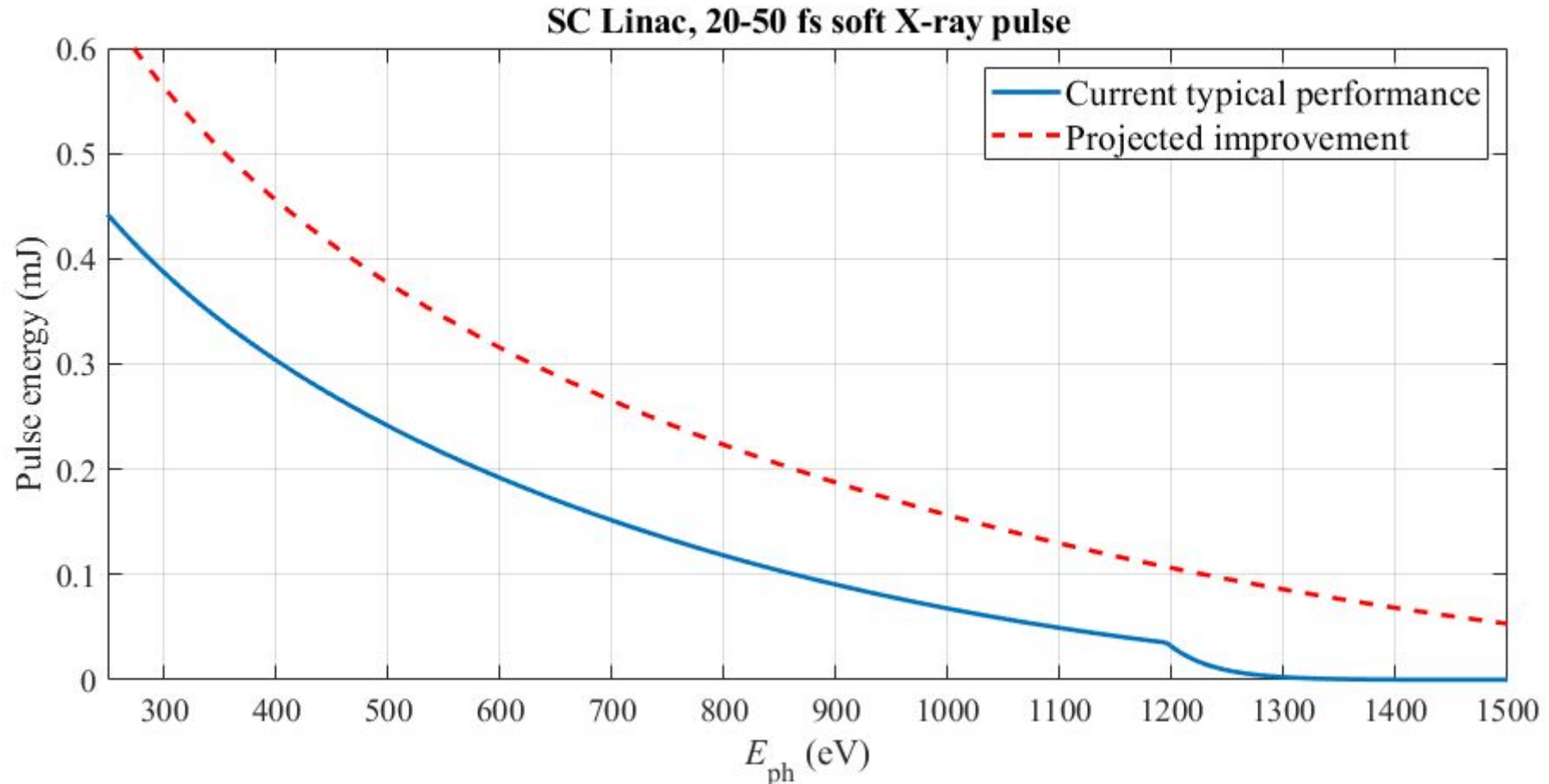
\* Assuming nominal duration and undulator strength

§ Brightness units are photons/sec/mm<sup>2</sup>/mrad<sup>2</sup>/0.1%-BW

\*\* Highest rate will depend on accelerator protection and beamline acceptance

# SC Linac Beam Quality Ramp Up

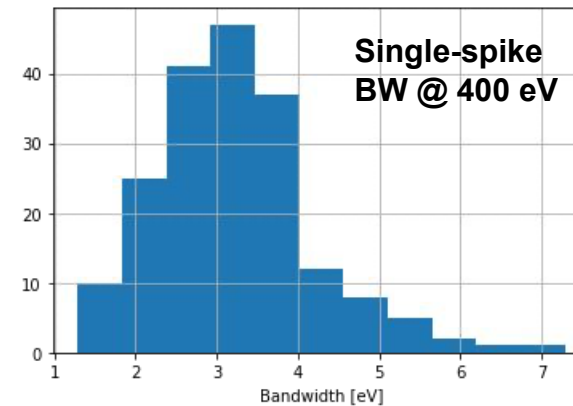
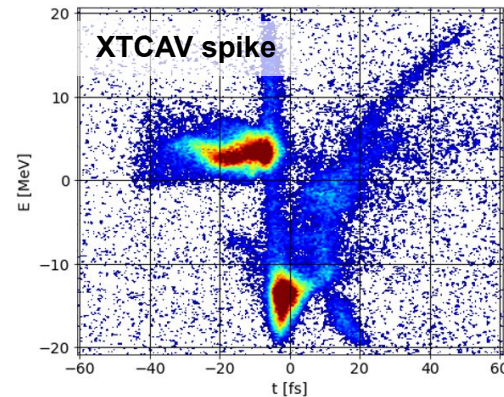
- Projected intensity has been achieved at 70 pC in Run 23





# Shorter Pulses

- Laser heater shaping (few fs pulses) and XLEAP (sub-fs pulses) demonstrated with NC Linac
- XLEAP capability *demonstrated* to 1 fs and better w/ SC linac



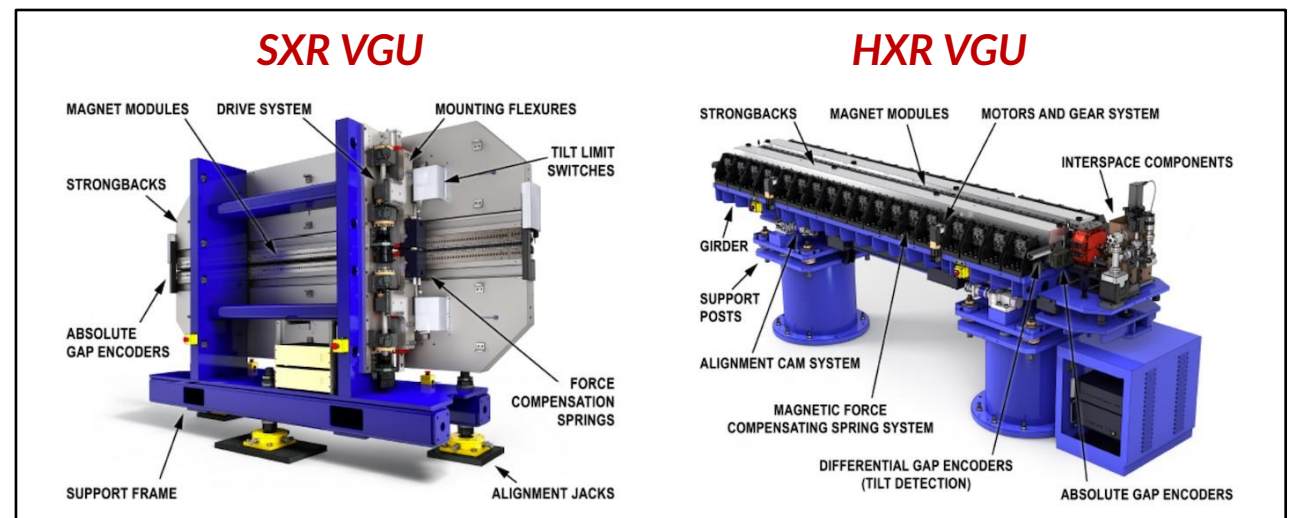
Technique	Min Pulse Duration	Linac (Max Rate)	Energy range	Energy/Pulse	Single Spike rate
Laser Heater Shaping	< 8 fs	SC (1 kHz+)	SXR	10-20 $\mu$ J	TBD
XLEAP	< 1 fs (TBD)	SC (1 kHz+)	SXR	TBD	TBD

**fs and sub-fs pulses demonstrated  
w/ SC linac in Run 23**

# Photon Energy Scanning

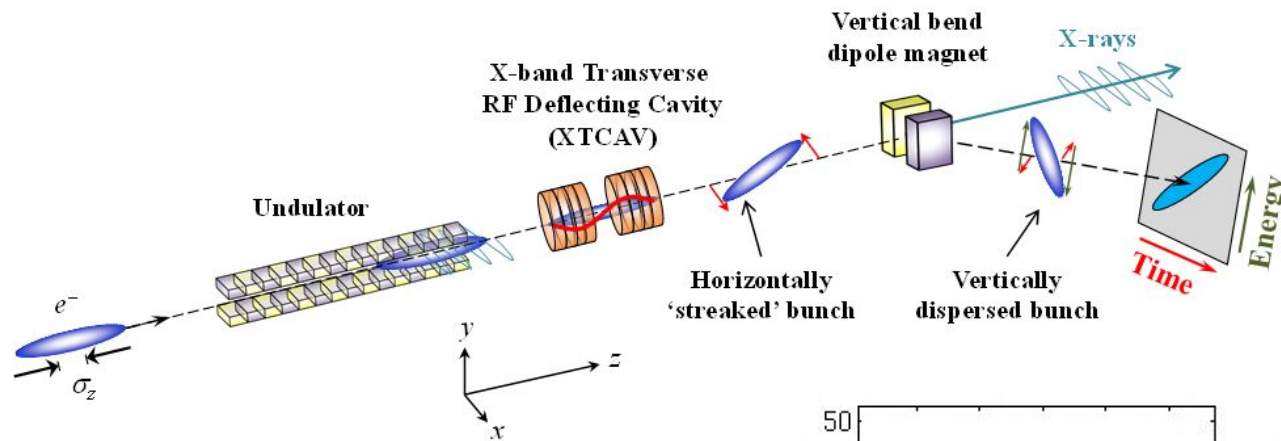
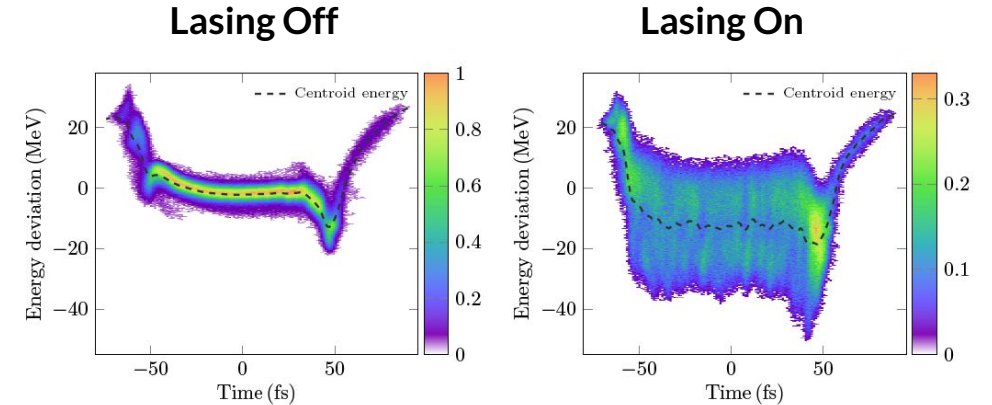
Linac+Und	Mode	Energy delta	Speed/step	Notes
NC + HXR	Und Gap (coarse)	20%	seconds	Range is performance limited
	Vernier (fine)	1-2%	milliseconds	
SC + SXR	Und Gap (coarse)	50-100%	seconds	Range is performance limited
	Vernier (fine)	1-2%	milliseconds	(Tested, affects performance)

User control of photon energy scans ready and available via new variable gap undulators

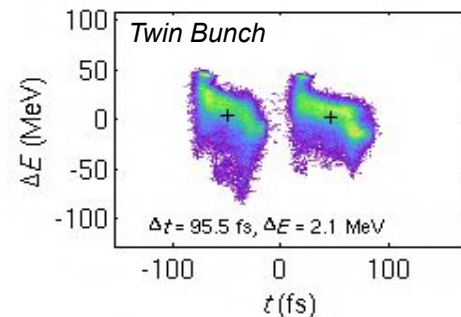
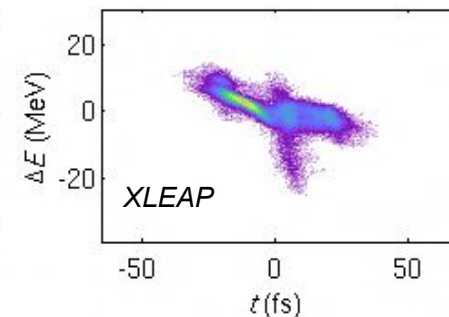
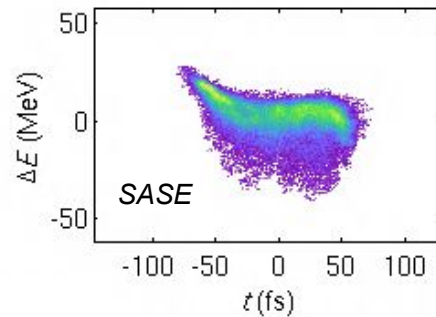


# XTCAV: Femtosecond “streak camera” for e<sup>-</sup> beam

- 120 Hz images of e<sup>-</sup> beam time-energy distribution
- Observe energy loss due to FEL, calculate x-ray temporal profile shot-by-shot w/ fs resolution
- Available for recording/analysis at beamlines in coordination with ACR



**XTCAV available for both undulators and linacs in Run 25 (120 Hz max)**



# SC Linac Summary

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- **Rate:** Up to 33 kHz delivery over Run 25
- **Intensity/quality:** Continued improvement for lower charge/duration
- Special capabilities for Run 25:
  - **Photon energy scans**
  - **Short pulses (fs to sub-fs)**

# Communication with the Accelerator Team

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- Weekly 'User Meeting' with the ACR team:  
*Wednesday before your experiment starts, share experiment background and summarize key x-ray parameters: photon energy, pulse energy, pulse length, other special conditions/requests important for FEL source requirements. (~10 min presentation each)*
- LCLS POC is the conduit for communication with the Accelerator teams

**Thank you and Good Luck**

# TMO in Run 25

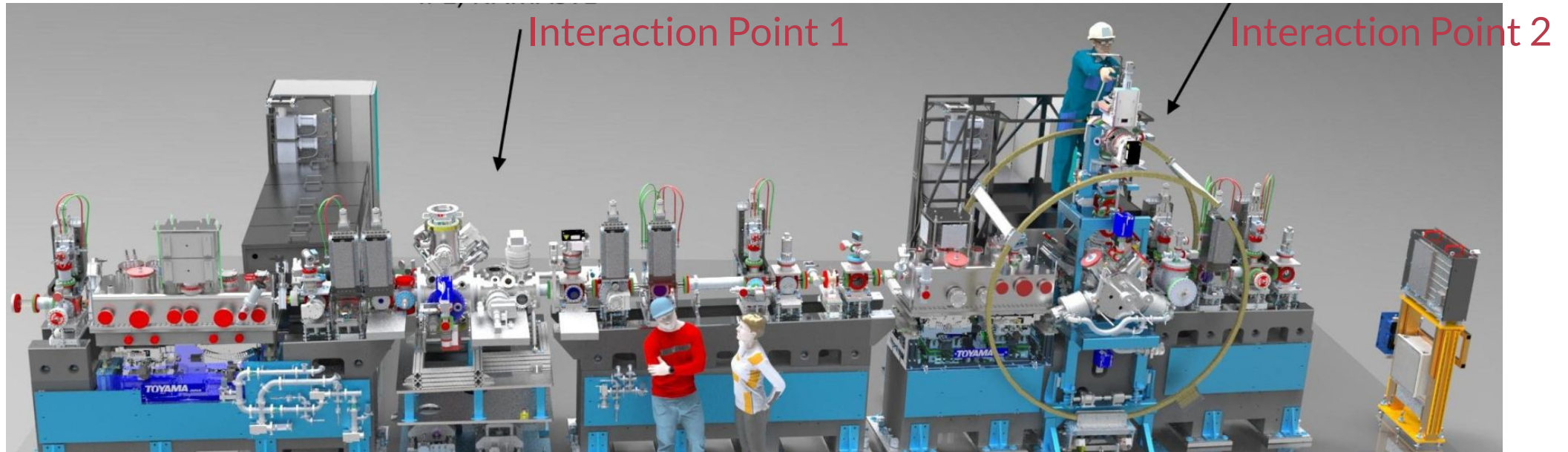
## LCLS Run 25 Users Town Hall

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February 6th 2025

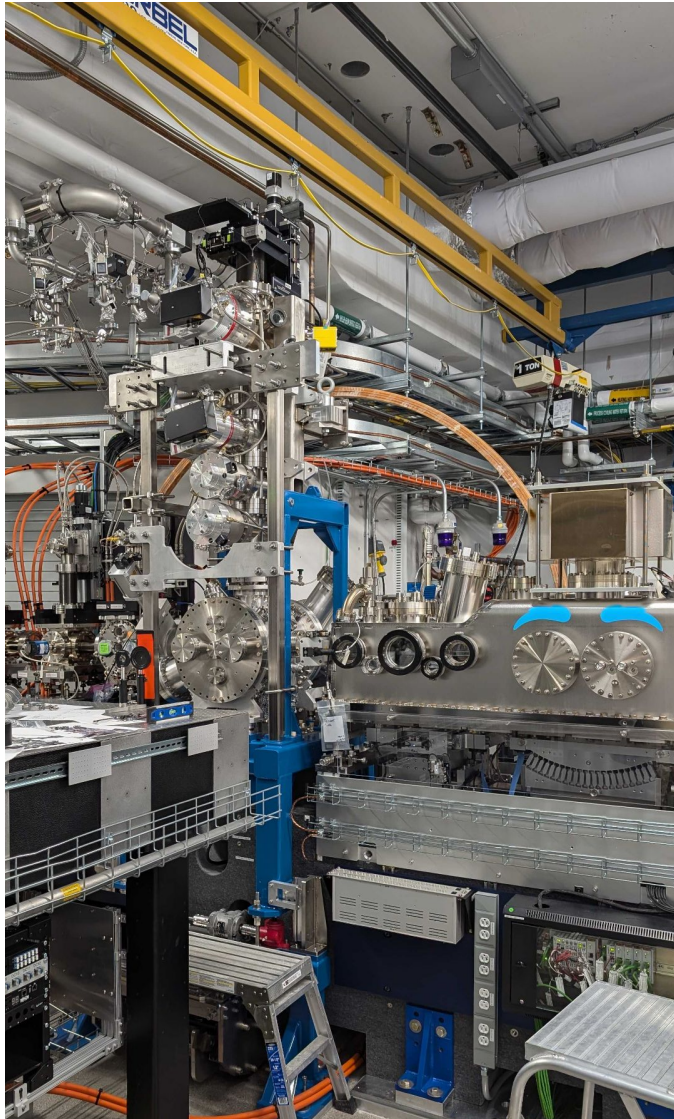
James Cryan and the TMO Team

# TMO in Run 25



- We will offer a standard configuration for both IP1 (MRCO/MBES) and IP2 (DREAM)
  - Interaction points can not be operated simultaneously at this point.
  - We hope to develop this capability.
- Expect X-ray repetition rates up to 33 kHz (possibility to exceed)
- Atto/atto capabilities

# Dynamic REAction Microscope (DREAM)



Commissioning





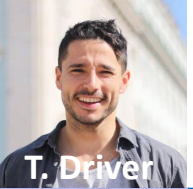



ES  
DREAM

PRP DREAM

- Assembly almost complete
- Plan for laser-only commissioning during remainder of Run 23.
- Bulk of X-ray commissioning during Run 24
- Early Science experiments at end of Run 24:
- Following Early Science, we will move into PRP experiments



# TMO Instrument Team @ LCLS

	TMO Instrument Lead	
		TMO Instrument Scientists
		
		
	TMO Research Associates	

		TMO Engineering Team	
		TMO Area Manager and Support Team	
		TMO Controls Team	
			Graduate Students

# ChemRIXS in Run 25

## LCLS Run 25 Users Town Hall

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February 6th 2025

Kristjan Kunnus and the ChemRIXS Team

# ChemRIXS Run 25 call

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## Liquid standard configuration

Liquid samples, sheet or round jets.

- Time-resolved XAS with monochromatic beam (scanning)
  - Transmission experiments (sheet jets)
  - Total Fluorescence Yield (TFY) mode
  - Partial Fluorescence Yield (PFY) mode
- Time-resolved RIXS/XES

## Upgrades

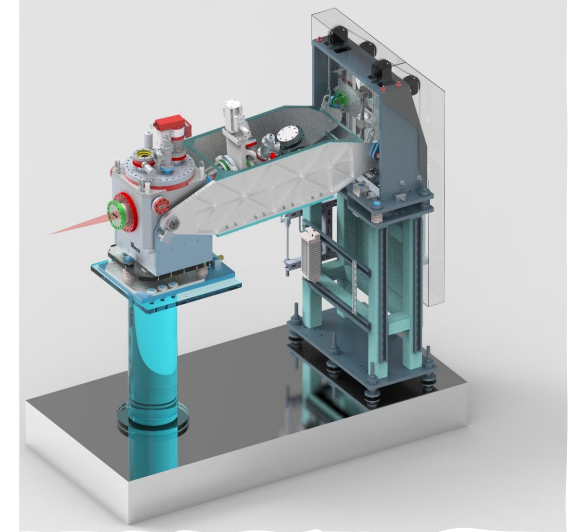
We are planning to commission during Run 24:

- High throughput RIXS spectrometer.
- Improved transmission XAS capabilities (new detectors, dual-beam).

## Non-standard configurations

- Please contact beamline scientist for:
  - Zero-order operation at high rep-rate (e.g. attosecond XLEAP experiments).
  - Solid samples or special sample delivery requirements.

## Spectrometer upgrade:



# ChemRIXS Run 25 key parameters

## X-ray

Repetition rate (Hz)	Up to 33 kHz
Energy Range (eV)	250 - 1600 eV
Pulse Duration (fs)	20 fs (nominal, SASE)
Energy per pulse at the IP (monochromatic)	>100 nJ (250 - 1000 eV) >10 nJ (1000 - 1300 eV) >1 nJ (1300 - 1600 eV)
Beamline Resolving Power	>2000
Spot Size, FWHM (range)	10 - 1000 ( $\mu\text{m}$ ) diameter
Polarization	Linear, Horizontal

## Laser

Repetition rate (Hz)	Synchronized up to 33 kHz				
Wavelength (fs)	800	400	266	480 - 600	600 - 900
Pulse Duration (fs)	20	30	35	<50	<50
Energy per pulse ( $\mu\text{J}$ ) (on target)	500	50	5	>15	>5
Spot Size, FWHM (800 nm)	50 to 100 $\mu\text{m}$				
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 should be available. Overall temporal resolution will be dependent on machine and instrument configuration.				

Please contact us for any questions  
**K. Kunnus**  
[kristjan@slac.stanford.edu](mailto:kristjan@slac.stanford.edu)

# qRIXS in Run 25

## LCLS Run 25 Users Town Hall

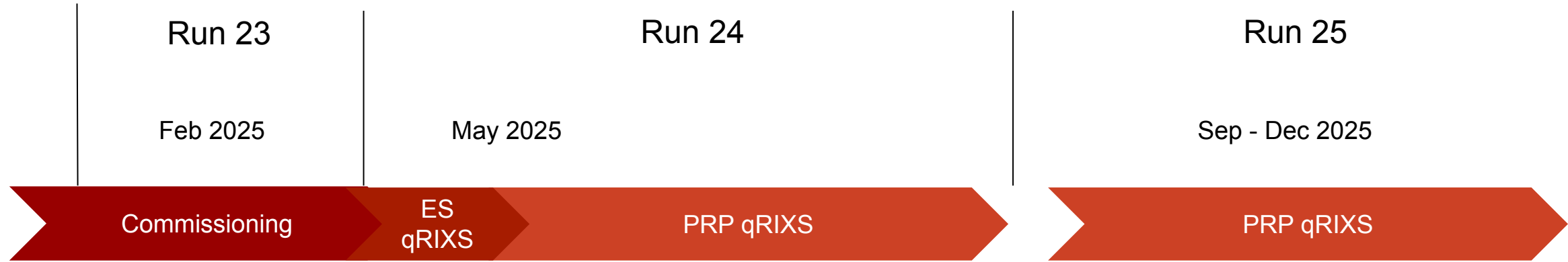
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February 6 2025

Georgi Dakovski and the qRIXS Team

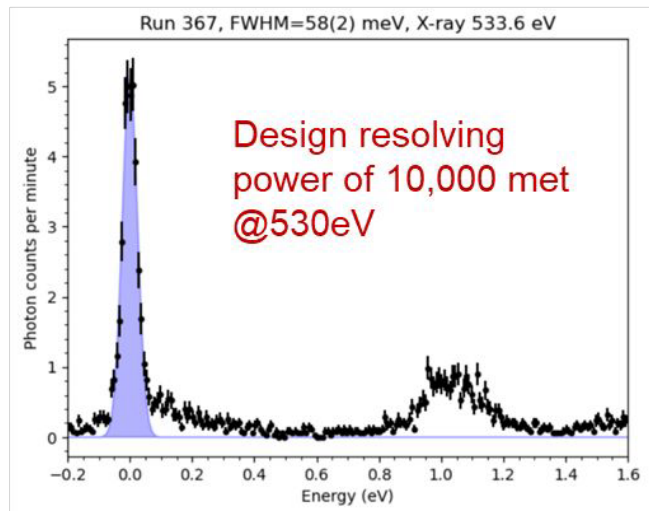
# qRIXS Instrument: Notional timeline

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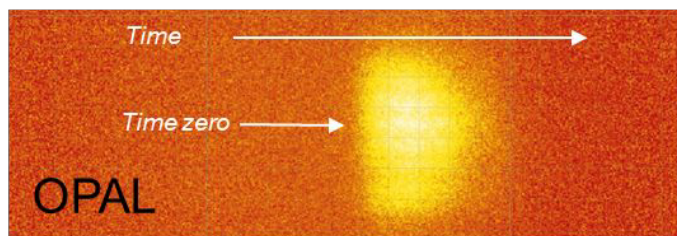


- qRIXS is installed; vacuum, motion and detectors are functioning
- Commissioning in Run 23 is underway
- Early Science phase will be scheduled for the beginning of Run 24, based on commissioning progress
  - For Users community engagement, please contact Apurva Mehta, [mehta@slac.stanford.edu](mailto:mehta@slac.stanford.edu) (Materials Science Department Head)
- The remainder of Run 24 and Run 25 will be for PRP experiments

# qRIXS commissioning is underway

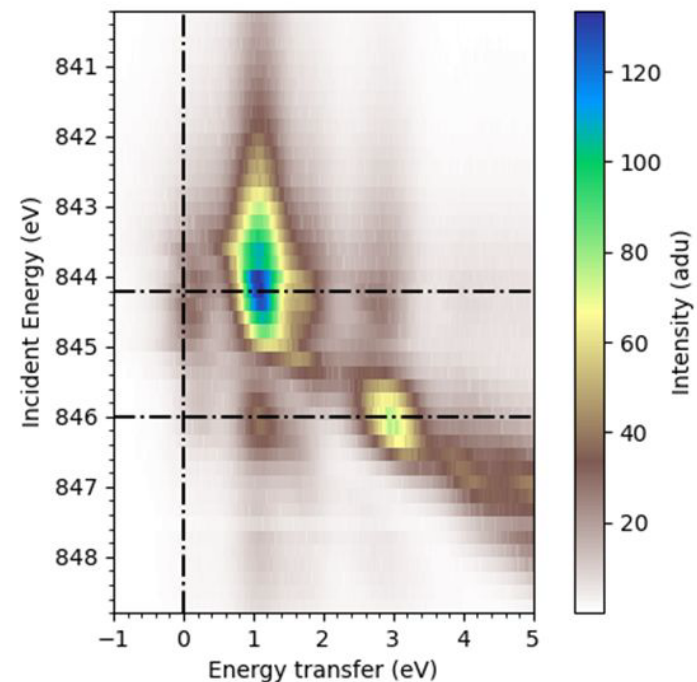


First Arrival Time Monitor results using SC & 1030nm beams



qRIXS began commissioning @8.3kHz, 400 – 930eV

Fast RIXS map of NiO at the Ni  $L_3$  edge



# Hard X-ray Instruments in Run 25

## LCLS Run 25 Town Hall

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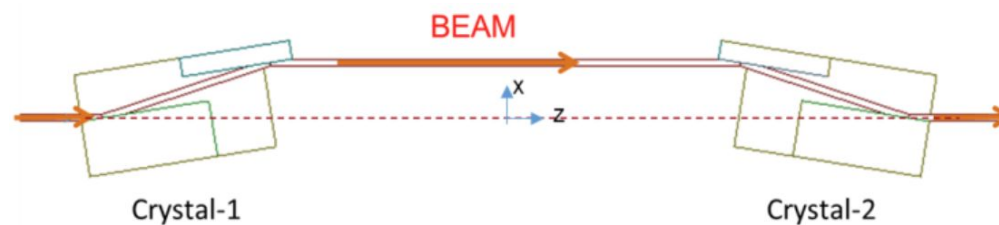
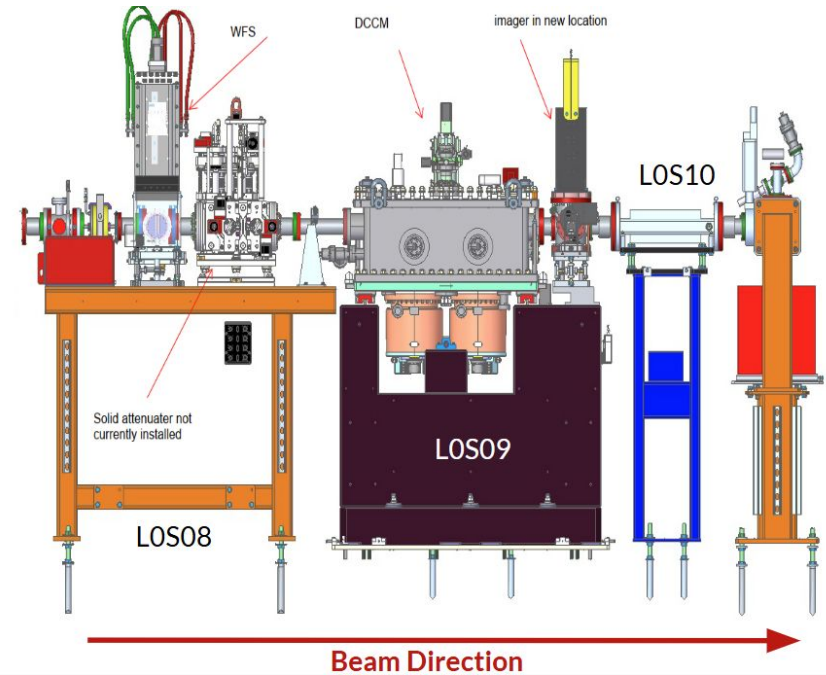
February 6 2025

Sebastien Boutet for all LCLS Hard X-ray  
Instrument Team Members



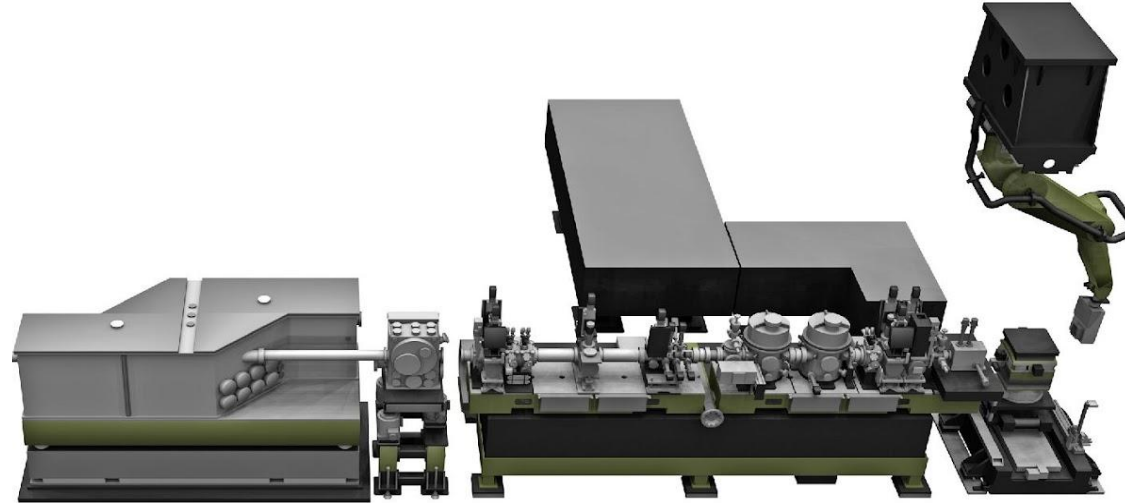
# New Capability: DCCM in The FEE Will Be Available

- The Double channel-cut crystal monochromator (DCCM) is currently installed in the Front End Enclosure (FEE).
- Will be commissioned in Run 23 & 24
- Will be available to users for run 25.
- Can send monochromatic beam to the far hall.
  - $\Delta E/E$  of  $1E-4$
- Can be used to calibrate XRT spectrometer.
- **Can be used for XAS experiments.**



# XPP (Not Available in Run 25)

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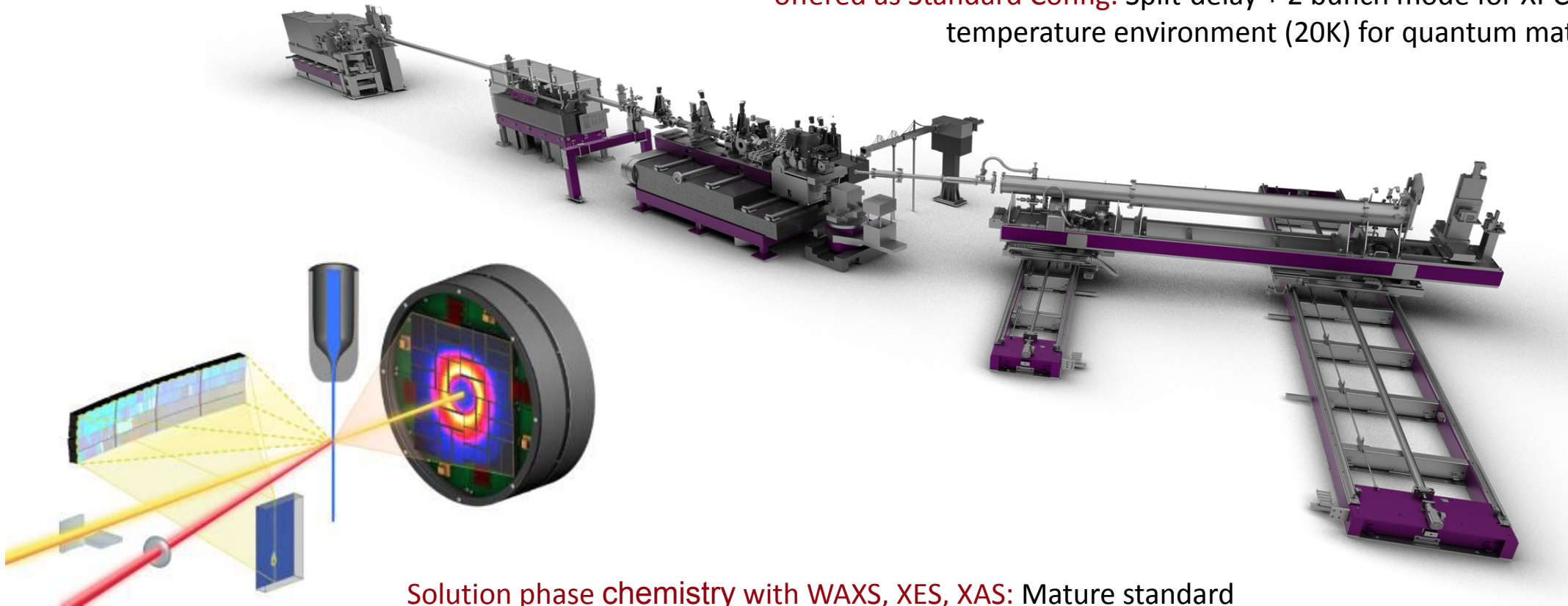


## LCLS-II-HE Upgrade

- The XPP Instrument is not available for beamtime in Run 25
- It will be undergoing a rebuild for LCLS-II-HE
- Much of the capabilities of XPP are available at other Hard X-ray Instruments
- Please contact LCLS scientists to discuss how to best support your needs at other instruments

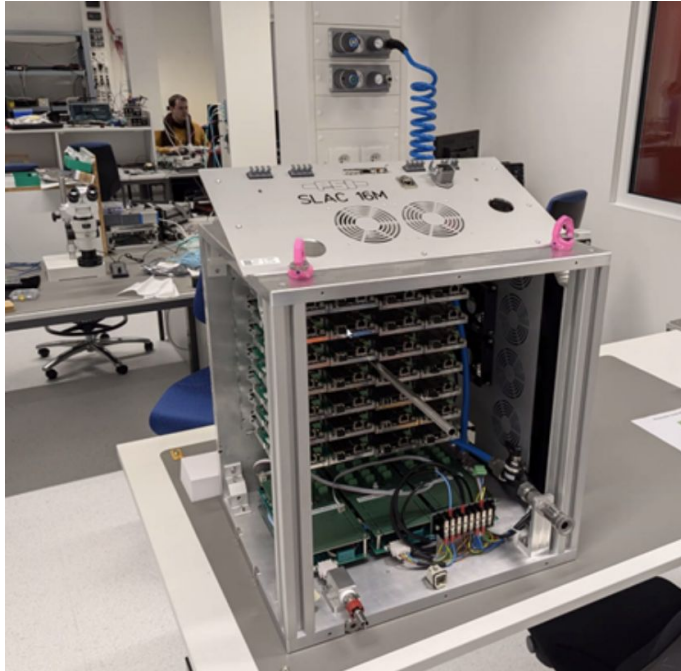
# XCS

Time-resolved coherent diffraction and small angle coherent scattering offered as Standard Config. Split-delay + 2 bunch mode for XPCS. Low temperature environment (20K) for quantum materials.



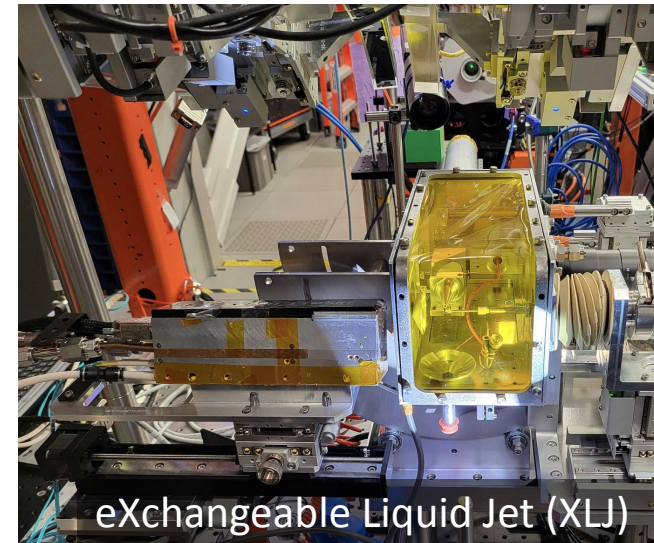
Solution phase chemistry with WAXS, XES, XAS: Mature standard configuration, broad UV-Vis-near-IR pump wavelength coverage. Enhanced suite of multi-crystal spectrometers.

# MFX

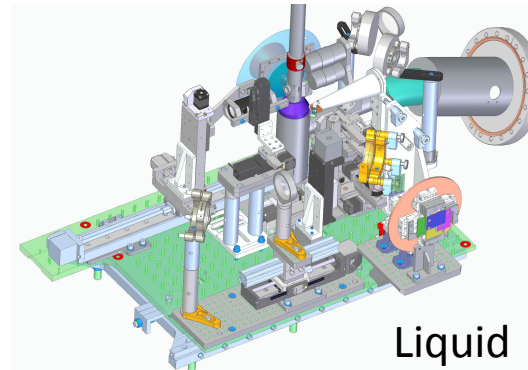
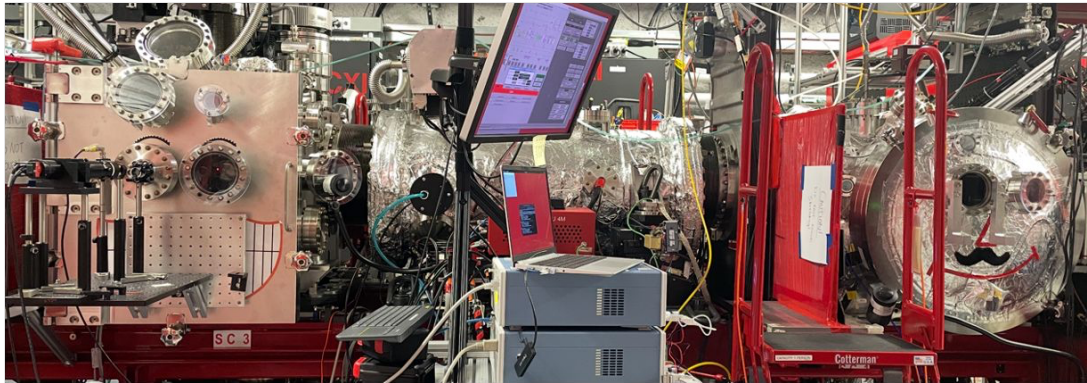


Jungfrau 15M

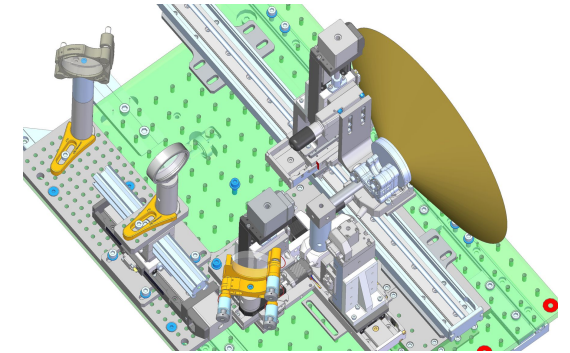
- **Key Capabilities:** Femtosecond Crystallography and time-resolved forward scattering (WAXS/SAXS).
- **Femtosecond Pump Laser:** Collinear incoupling geometry with wavelength coverage from UV to near IR.
- **Jungfrau 15M:** Fast large area detector to be commissioned in Run 24
- **eXchangeable Liquid Jet Endstation:** Helium environment horizontal and vertical jet sample delivery compatible with emission spectroscopy and forward scattering. Dedicated mutli crystal spectrometer. Compatible with collinear optical pump.
- **Droplet on Demand:** Semi-automated droplet delivery system with low sample consumption



eXchangeable Liquid Jet (XLJ)



Liquid  
jet



Gas cell

**Serial Femtosecond Crystallography:** variety of sample injection options from jets (GDVN, high-viscosity, MESH, mixing) to fixed target. High photon energy (18 keV) available for 0.8 Å resolution.

**Gas Phase Photochemistry:** In vacuum gas cell, short-pulse UV pump (<50fs), multisample gas exchange manifold.

**Nanofocus for high field physics and nonlinear x-ray science:** 100nm KB system allows reaching power density of  $10^{20}$  W/cm<sup>2</sup>. Improved nanofocus monitoring with wavefront sensor.

# MEC

Discuss with the staff to evaluate the use of these capabilities for your experiment!

## Long Pulse Laser

- Delivery of up to 100J in 10 ns on target
- Peak power of 10 GW for any temporal configuration
- Pulse shaping (e.g. flat top, ramp)
- CPP: 150, 300 and 600  $\mu\text{m}$

## Short Pulse Laser

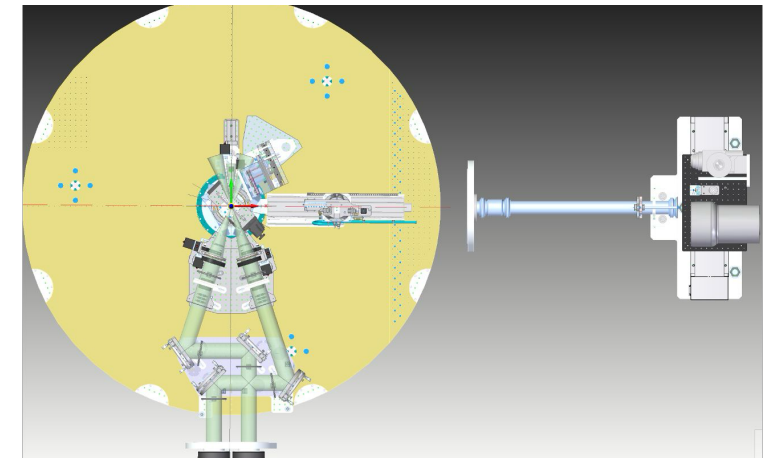
- Delivery of up to 1J in 45 fs at 800 nm, or 0.54J at 400 nm
- high intensity platform: peak intensity  $> 10^{19} \text{ W/cm}^2$
- at 800 nm, 45° angle of incidence allowed between high intensity mode and FEL
- low intensity platform: peak intensity  $\ll 10^{16} \text{ W/cm}^2$

## Multiple submission avenues

- Regular PRP proposal
  - up to 50% towards Inertial Fusion Energy
  - about 50% standard configuration
- Data Set Collection
  - 1-2 shifts
  - no requirement for previous X-rays beamtimes
  - reviewed by PRP
- Rapid Access
  - VISAR only shots
  - can be submitted at any time during the year
  - reviewed by the MEC team

## Std configurations

1. X-Ray Diffraction configuration with long pulse laser in collinear geometry (vs the FEL)
2. X-Ray Imaging geometry with Long Pulse Laser perpendicular to the FEL, X-Ray Diffraction with 1x ePix10k



Run 25

Run 26

~Nov 2025

~Feb 2026

~Mar 2026

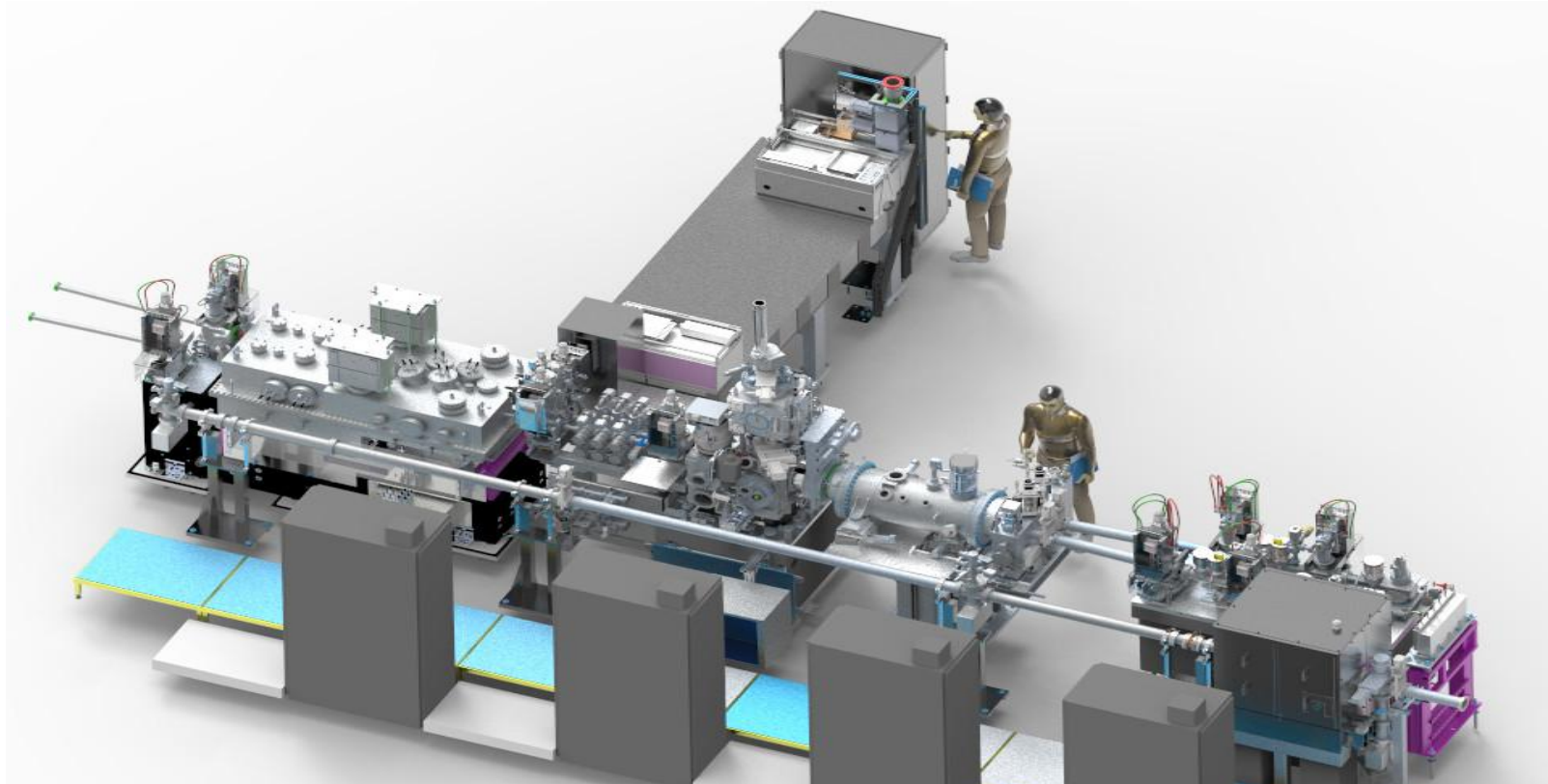
Commissioning

ES TES

PRP TES

**TXI commissioning:** We will commission the Tender Spectroscopy Endstation as the first TXI capability, with Early Science planned for run 26.

Visit the breakout sessions/office hours for more details.



Instrument Lead: Andy Aquila

# Data Systems

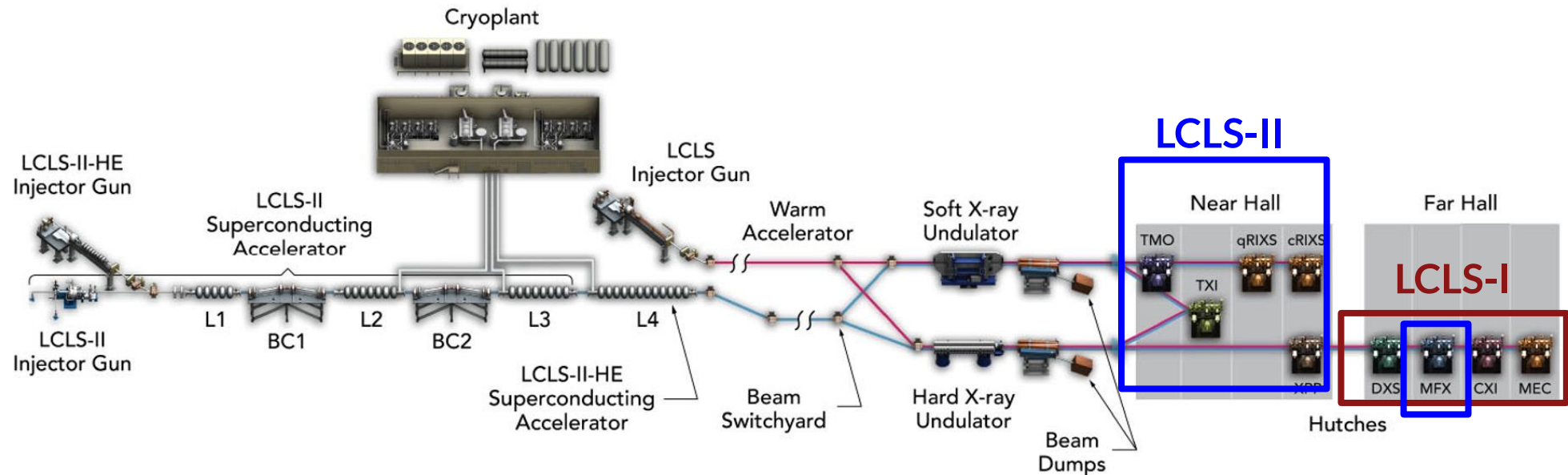
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February 6th 2025



# Reminder: LCLS-I and LCLS-II Use Different Data Systems

LCLS-I and LCLS-II have different DAQ, psana analysis framework, and AMI



**LCLS-I** is used for hard x-ray instruments **XCS, CXI, and MEC** - limited to 120 Hz and ~10 GB/s

**LCLS-I** psana analysis framework (psana) documentation: <https://confluence.slac.stanford.edu/display/PSDM/LCLS+Data+Analysis>

**LCLS-II** is used for the new instruments in **TMO, RIX, XPP, MFX** - up to 1 MHz and ~TB/s

**LCLS-II** psana analysis framework (psana2), documentation:

<https://confluence.slac.stanford.edu/display/LCLSIIData/LCLS-II+Data+Acquisition+and+Analysis>.

**AMI2** available in TMO, RIX, XPP, and MFX: <https://confluence.slac.stanford.edu/display/LCLSIIData/ami>

# What's new?

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- MFX is moving to LCLS-II DAQ/analysis
- LCLS-I will begin supporting AMI2 to allow users to acclimate to the new online monitoring system, designed to handle the high rate demands of LCLS-II. Users can start to use AMI2 in MFX.
- TMO and RIX data reduction: High Speed Digitizers are emitting both reduced (Feature Extracted, or FEX, data) and non-reduced (non-FEX) data.
  - Data Reduction in TMO/RIX digitizers is zero suppression; it is recommended that users analyze both FEX and non-FEX data in parallel to verify that they agree to within statistical errors
  - Please contact [pcds-ana-1@slac.stanford.edu](mailto:pcds-ana-1@slac.stanford.edu) or your POC with questions.
- Data center (S3DF) outages announcements: <https://confluence.slac.stanford.edu/display/PCDS/Outages>

# How is S3DF Different From psana?

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## Changes to expect when migrating from psana to S3DF

- **All** users/experiments, including old experiments, will use S3DF as a replacement for psana
- By October 2024, legacy systems will be retired.
- Changes from psana to S3DF:
  - Home directory (backed up) is now be in weka (/sdf/home/<first letter of username>/<username>)
  - Shared software packages and tools are in /sdf/group/lcls/ds
    - /sdf/group/lcls/ds/anapsana1/psana2 releases, detector calibration, etc.
    - /sdf/group/lcls/ds/tools smalldata-tools, cctbx, crystfel, om, ...
    - /sdf/group/lcls/ds/dm data-management releases and tools
  - LCLS experimental data is accessible on the interactive and batch nodes (but not the login nodes)
    - Offline storage: /sdf/data/lcls/ds/<instr>/<expt>/<expt-folders>
    - FFB storage /sdf/data/lcls/drpsrcf/ffb/<instr>/<expt>/<expt-folders>
  - S3DF batch compute uses Slurm batch processing and requires a Slurm account to submit a job in order to track resource usage per experiment. The slurm account is lcls:<experiment-name>
    - Contact your POC if you require a reservation with a certain number of nodes.
    - We are investigating on-shift/off-shift priority mechanisms; keep an eye on confluence as our policies and recommendations may be in flux as we learn which techniques provide users with the best performance.

# Try out Automated Run Processing (ARP)

Automated Run Processing (ARP) capabilities are available via eLog → Workflow → Definitions

- The Automatic Run Processor (ARP) is a web service that allows for automatic workflows and for the easier submission of batch jobs via a web interface: see eLog → Workflow → Definitions
- A script that submits the batch job is all that is needed for this system to work.
- ARP will automatically launch the configured workflow and return status and results to eLog.
- Examples and documentation: <https://confluence.slac.stanford.edu/pages/viewpage.action?pageId=219269619>
- Working on some standardized workflows for complex analysis tasks.
- For more information on using this resource, reach out to Silke Nelson ([snelson@slac.stanford.edu](mailto:snelson@slac.stanford.edu))

Name	Executable	Control	Parameters	Location	Trigger	As user	
DataQualityPlots	/cds/data/drpsrcf/xcs/xcslx2619/scratch/smalldata_tools/arp_scripts/submit_plots.sh		--postStats --queue ffb12q --directory /cds/data/drpsrcf/xcs/xcslx2619/scratch/hdf5/smalldata	SRCF_FFB	RUN_PARAM_IS_VALUE SmallData_ffb == done	snelson	 
PedestalPlots	/reg/g/psdm/sw/tools/smalldata_tools/pedplot/arp_scripts/submit_plots.sh		--queue psfehprioq --pedestals	SLAC	RUN_PARAM_IS_VALUE pedestal == done	snelson	 
cube	/cds/data/drpsrcf/xcs/xcslx2619/scratch/smalldata_tools/arp_scripts/cubeRun.sh		--cores 60 --postRuntable --queue ffbh2q	SRCF_FFB	MANUAL	yanwen	 
smd	/cds/data/drpsrcf/xcs/xcslx2619/scratch/smalldata_tools/arp_scripts/submit_smd.sh		--queue ffbh2q --norecorder --postRuntable --cores 60 --wait --epicsAll	SRCF_FFB	START_OF_RUN	yanwen	 

# S3DF Quick Reference

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S3DF Quick Reference: <https://s3df.slac.stanford.edu/public/doc/#/>

SSH	s3dflogin.slac.stanford.edu
NoMachine	s3dfnx.slac.stanford.edu
OnDemand	<a href="https://s3df.slac.stanford.edu/ondemand">https://s3df.slac.stanford.edu/ondemand</a>
Globus Endpoint	slac#s3df
Help (slack channel)	slac.slack.com#comp-sdf
Help (email)	s3df-help@slac.stanford.edu
Banking & Accounting	<a href="https://s3df.slac.stanford.edu/coact">https://s3df.slac.stanford.edu/coact</a>
S3DF Dashboard & Monitoring	<a href="https://s3df.slac.stanford.edu/monitoring">https://s3df.slac.stanford.edu/monitoring</a>

# Questions?

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# Agenda

Time (PST)	Topic	Presenter
<b>Plenary Session - <a href="#">Join via Zoom &gt;&gt;</a></b>		
9:00 am	Current LCLS Status & Plans	<b>Mike Dunne</b> Director, LCLS
9:15 am	Universal Proposal System	<b>Leilani Conradson / Paul Jones</b> LCLS User Office
9:23 am	User Executive Committee Update	<b>Silvia Pandolfi</b> LCLS UEC Vice Chair
9:26 am	Short Proposal Program Update	<b>Sandra Mous</b> LCLS Scientist
9:31 am	Accelerator Plans for Run 25	<b>Axel Brachmann / Tim Maxwell</b> Accelerator Dept. Head
9:40 am	Soft X-ray Instrument Capabilities (Introduce breakouts)	<b>James Cryan / Kristjan Kunnus /Georgi Dakovski</b> TMO/chemRIXS/qRIXS Instrument Leads
9:50 am	Hard X-ray Instrument Capabilities (Introduce Breakouts)	<b>Sebastien Boutet</b> Director of Operations
9:55 am	Data systems	<b>Jana Thayer</b> Data Systems Dept. Head
<b>Breakout Sessions/Office Hours by Instrument</b>		
10:10 am - 11:00am	<u>Session 1</u>	
	•TMO <a href="#">Join via Zoom &gt;&gt;</a>	James Cryan
	•MEC <a href="#">Join via Zoom &gt;&gt;</a>	Eric Galtier
	•MFX <a href="#">Join via Zoom &gt;&gt;</a>	Sebastian Dehe for Leland Gee
	•qRIXS <a href="#">Join via Zoom &gt;&gt;</a>	Georgi Dakovski
	•XCS/XPP <a href="#">Join via Zoom &gt;&gt;</a>	Matthieu Chollet & Takahiro Sato
	•chemRIXS <a href="#">Join via Zoom &gt;&gt;</a>	Kristjan Kunnus
	•CXI <a href="#">Join via Zoom &gt;&gt;</a>	Meng Liang