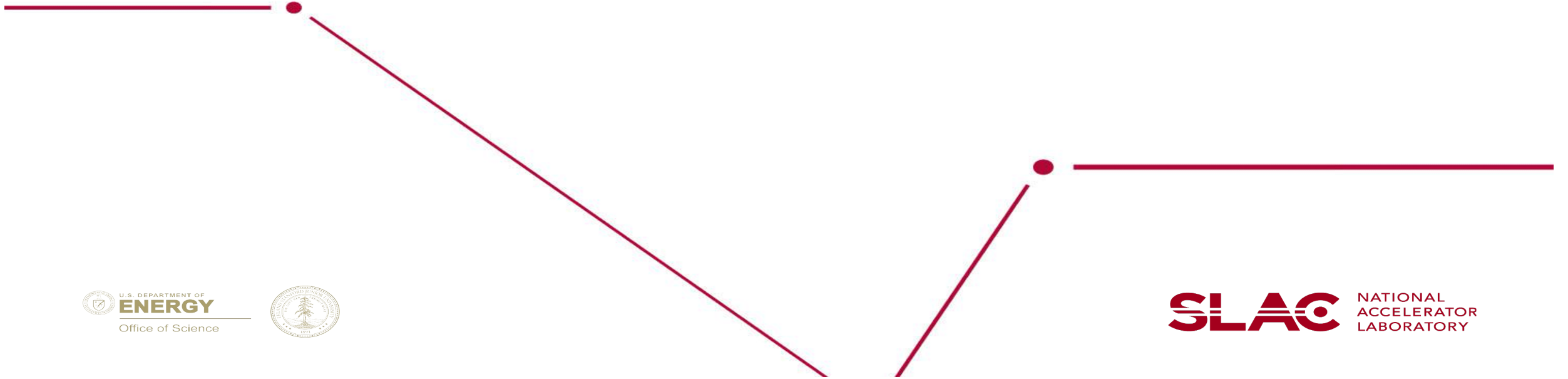


LCLS Material Sciences Town Hall Run 21

March 21st, 2022



Agenda



- LCLS II & How to get Involved in Early Science (A. Mehta) ~ 5 min
- qRIXS capabilities (G. Dakovski) ~ 5 min
- XCS capabilities (M. Chollet) ~ 5 min
- XPP capabilities (D. Zhu) ~ 5 min
-
- Q&A ~ 40 min

Overview: LCLS-II Upgrade for TMO and NEH2.2



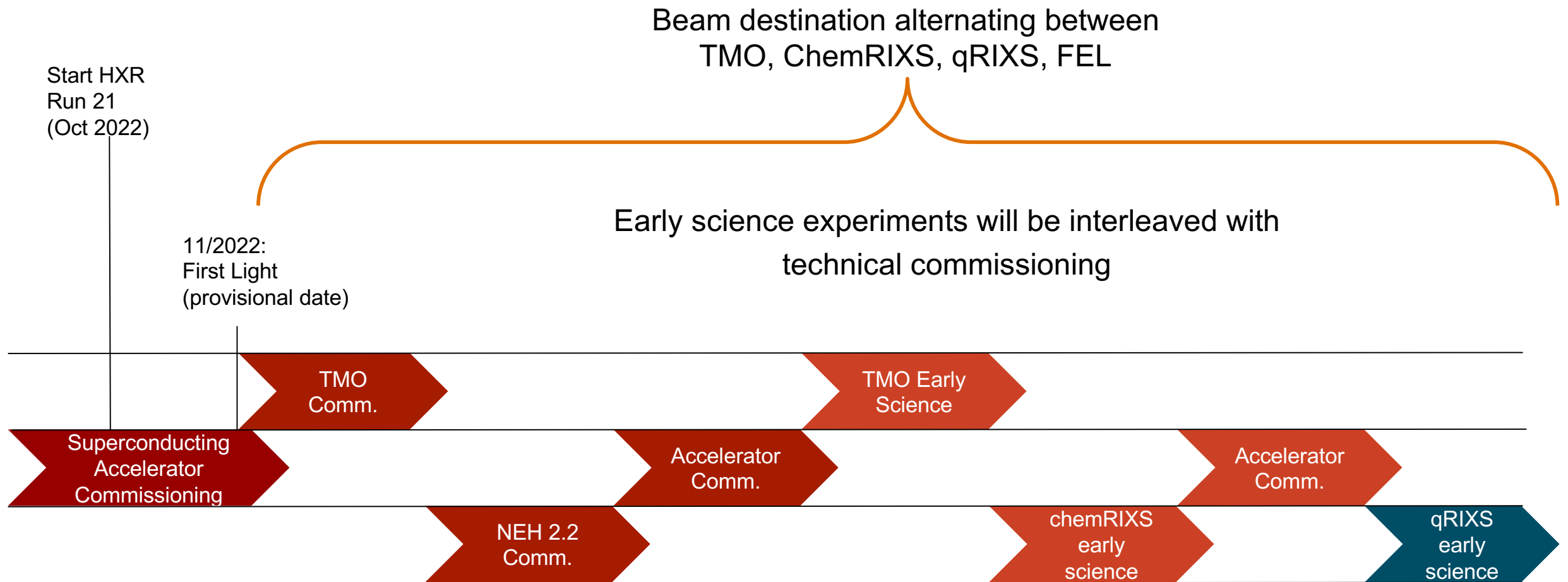
- LCLS-II superconducting accelerator will startup during 2022/23
- First Light planned for November 2022
- For Run 21, the soft X-ray instruments will focus on the high rep-rate beam (< 33KHz)
 - TMO, ChemRIXS, [qRIXS](#)
 - Technical commissioning followed by an LCLS-led, community-wide 'Early Science' period
 - No PRP proposals for Run 21 for these instruments
 - Users should submit ideas for the "Early Science" experiments (see next slides)
- For Run 21, the hard X-ray instruments will use the Cu – linac @120 hz

Timeline For Early Science Program



- **March 30, 2022:** Deadline for Letters of Interest to LCLS (same date as regular proposals)
 - One-page summary of science / instrument areas of interest, or
 - Bulleted list of experimental ideas
- **April - June 2022:** LCLS engages with User Community to develop the plan.
- **June 30, 2022:** LCLS announces Early Science experiments to User Community
- **September 1, 2022:** Deadline for interested users to submit a description of their proposed contribution to the specific Early Science experiments.
 - Experiments are open enrollment, subject to forming a balanced onsite team.
- **November 2022:** Provisional date for 'First Light' from SCRF beam, followed by:
 - FEL commissioning
 - Beamline/instrument commissioning
 - Early Science (likely in early 2023 onwards)

Early Science during Run 21 will follow a phased approach between the instruments, interleaved with FEL ramp-up



The Early Science process



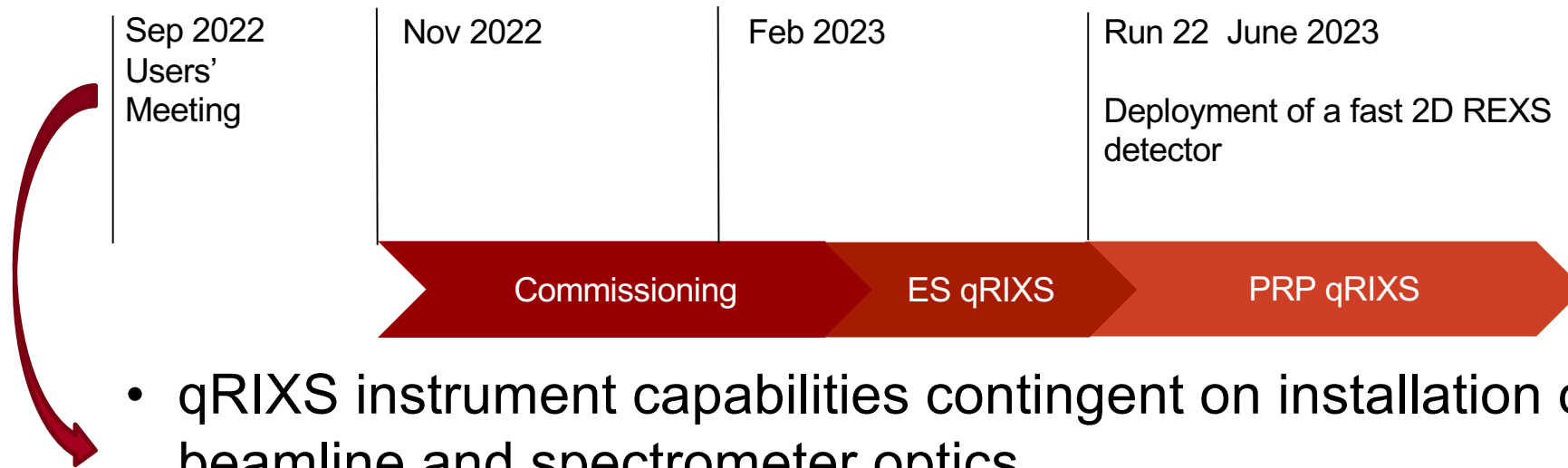
- Motivation:
 - The complexity brought by high repetition rate operation warrants the implementation of a 3-step approach:
 - i. Allocate sufficient time for technical commissioning of beamline and instruments at high repetition rate
 - ii. Early Science, bridging the gap from technical commissioning of new instrumentation to regular user access
 - iii. PRP proposals (planned for the next Run)
 - Enables a more flexible response to emerging LCLS-II performance, and beamline/instrument readiness
- Early Science
 - Based on ideas solicited from the community
 - Led by LCLS staff, with broad involvement from the community
 - Overseen by the LCLS Scientific Advisory Committee (SAC) and the Instrument Advisory Panels (IAPs)
- Interested groups should contact the relevant department heads - deadline 30 March
 - **TMO**: James Cryan (AMOS, jcryan@slac.stanford.edu)
 - **ChemRIXS**: Thomas Wolf (Chemical Sciences, thomas.wolf@slac.stanford.edu)
 - **qRIXS**: Apurva Mehta (Materials Sciences, mehta@slac.stanford.edu)
- Experiment ideas will then be prioritized by LCLS staff and the instrument advisory panels.
- The resultant early science plans will be advertised to the user community to solicit participation.

2-page summary:

- What is the science case?
- Why is LCLS needed?
- Crucial performance parameters:
 - X-ray energy, scanning
 - Optical wavelength, timing
 - Detectors, diagnostics, sample, etc.
- How many shifts are needed? Signal levels?
- Who needs to participate and what can they contribute?
- Is there theoretical support, what would make the experiment a “success”?

qRIXS Instrument Capabilities

qRIXS Instrument: Notional timeline



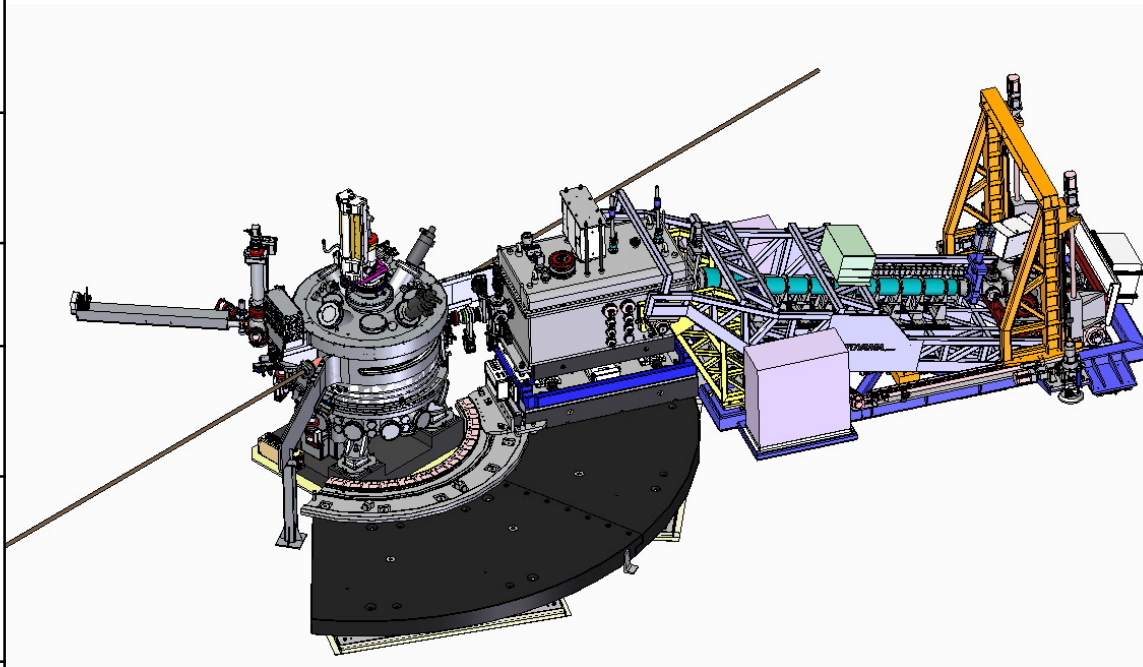
- qRIXS instrument capabilities contingent on installation of critical beamline and spectrometer optics
- Update the science community at the SSRL/LCLS Users' Meeting
- If optics are significantly delayed, we will prioritize low energy resolution experiments in the qRIXS Sample Chamber.

qRIXS Instrument: Sample Chamber + Spectrometer Arm

X-ray Parameters		Laser Parameters	
Repetition rate (kHz)	33	Repetition rate (kHz)	33
Energy Range (eV)	250 - 1100	Wavelength (nm)	800
Spot Size (um), H x V	10 x 10, min 1000 max	Pulse Duration (fs)	<40 @ 800 nm
Energy per pulse (nJ)	>10	Energy per pulse (μJ)	300
Pulse Duration (fs)	<200	Spot size (μm)	50 min
Beamline Resolving Power	>20,000	Polarization control	Horizontal and vertical, circular
Combined Spectrometer resolving power	10,000 @ 931 eV	Arrival time monitor precision (fs)	<20
Polarization	Linear horiz.		

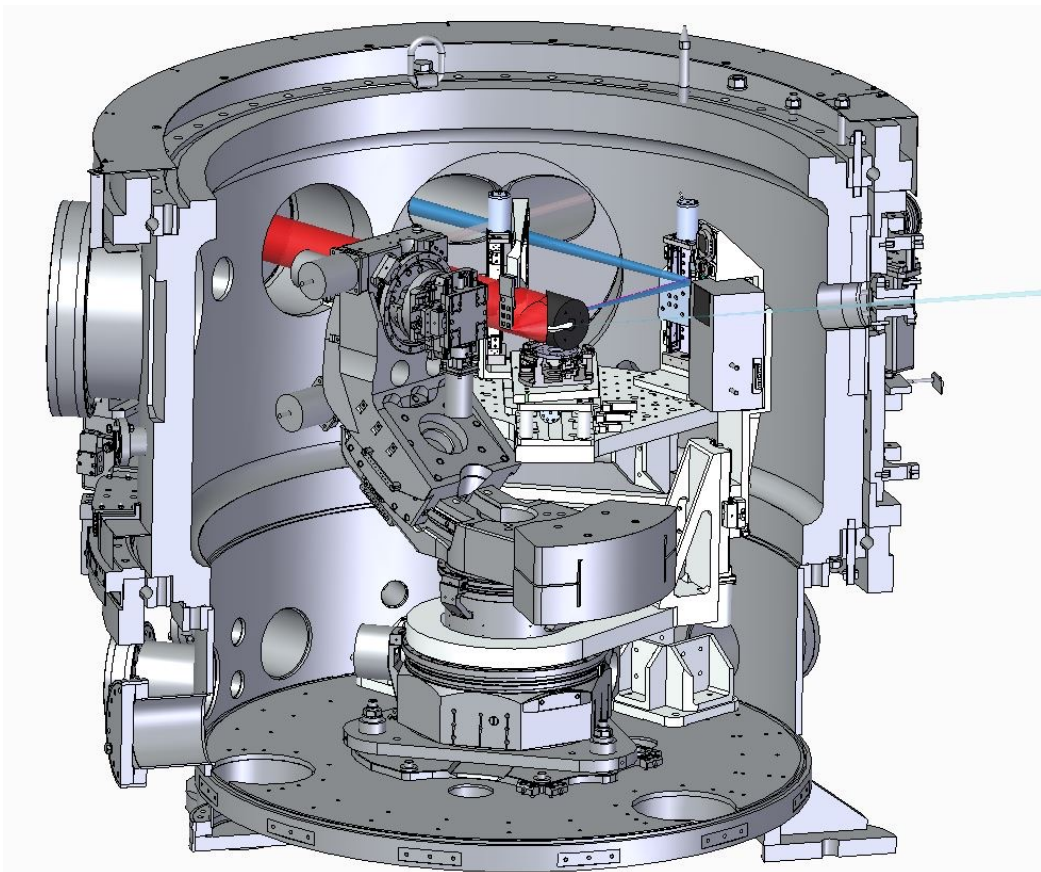
For more details:

<https://lcls.slac.stanford.edu/instruments/neh-2-2/neh-2-2-Capabilities>



qRIXS Instrument: Sample Chamber capabilities

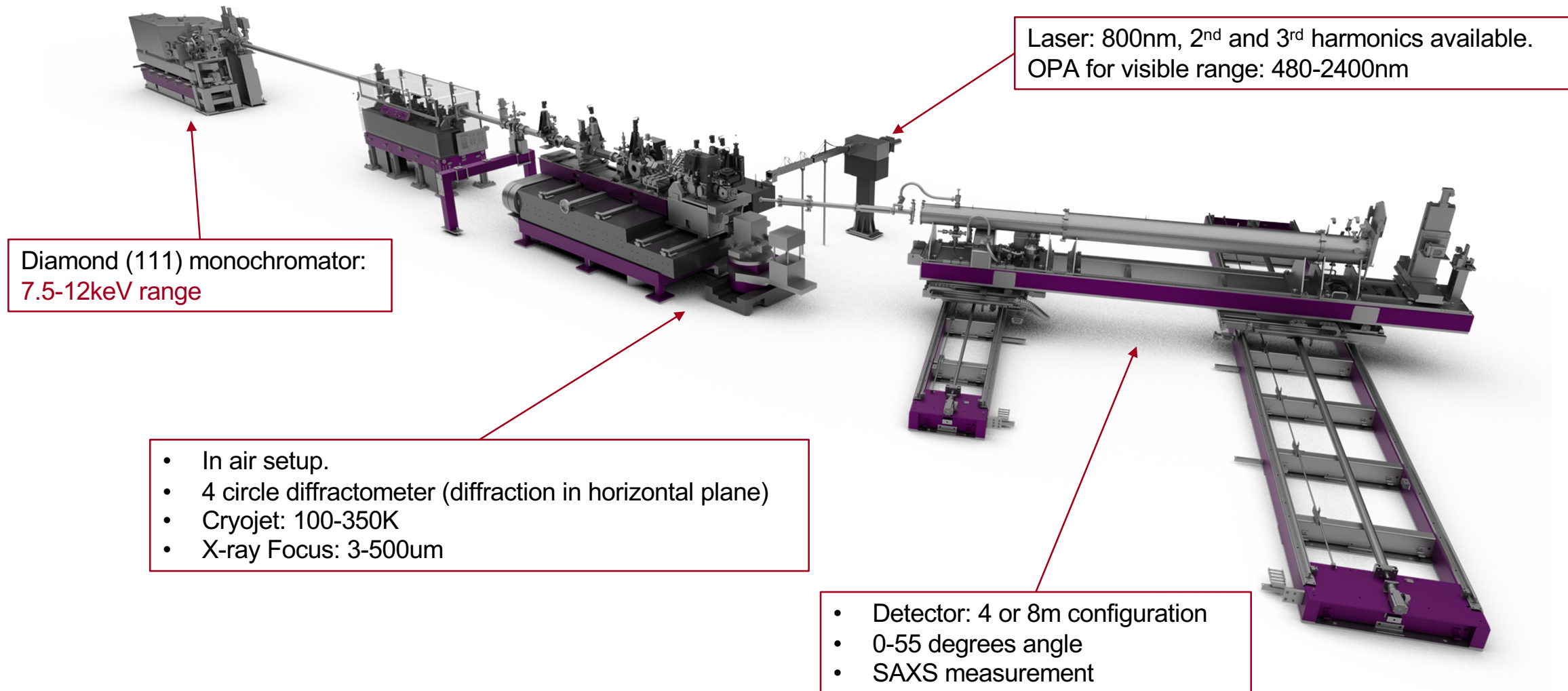
Techniques: XRD, REXS, XRR, XAS



- In-vacuum diffractometer, 6 degrees of freedom
- Bulk samples and thin films on substrates
- Load-lock chamber
- Sample cooling, ~ 25 K
- Diagnostic paddle for calibration targets, spatio-temporal overlap, etc.
- Laser in- and out- coupling
- Avalanche photodiode detectors for x-ray absorption and diffraction
- Arrival time monitor
- Lasers: 800 nm
- Overall temporal resolution: ~ 60 fs

XCS Instrument Capabilities

Time-resolved hard X-ray coherent scattering and small angle scattering on condensed matter systems in air.

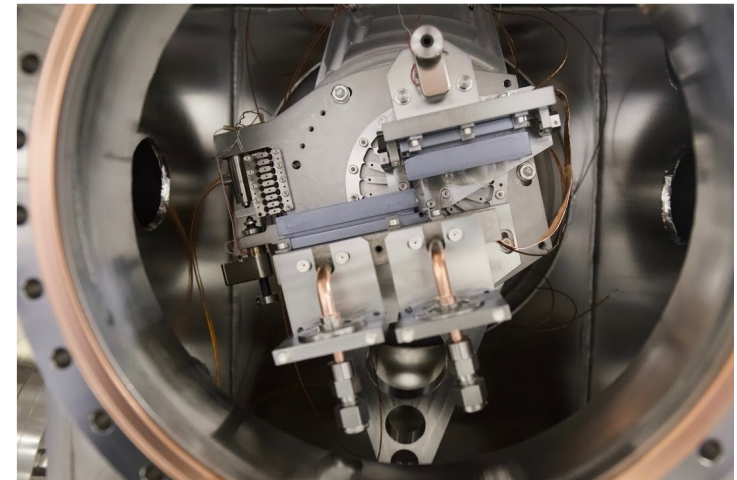
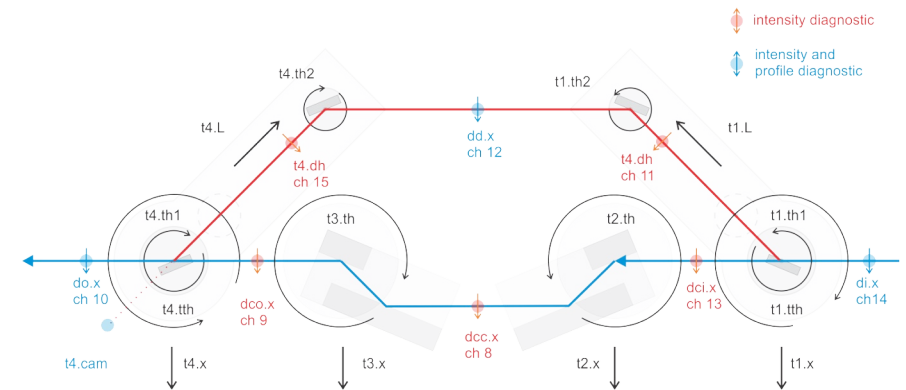


Other capabilities @ XPP:

- Split & Delay for XPCS: Wavefront splitting design. Energy range 6.5 to 13keV with a delay range from -50ps to 550ps.
- Up to 25keV X-ray
- Scannable Channel Cut Monochromator (CCM): Si(111) crystals. Energy range 7-25keV for XAS
- X-ray Pulse picker for single shot or non 120Hz operations.

Detectors:

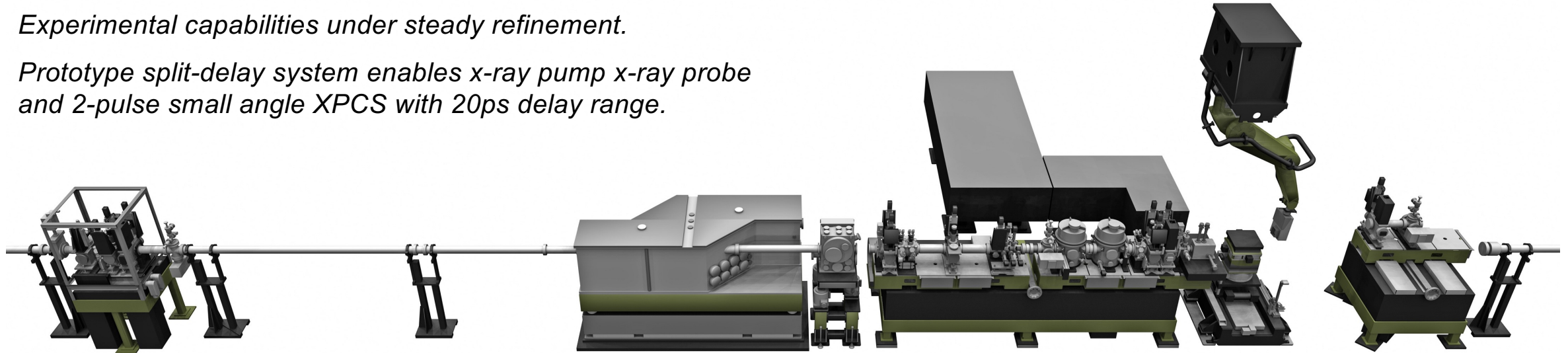
- Epix10k and epix10k-2m: 135k pixels and 2M pixels with 100um pixel size
- Epix100: 50um pixel size
- Jungfrau 0.5M and 1M: 75um pixel size



XPP Instrument Capabilities

XPP status and standard configuration

- *Experimental capabilities under steady refinement.*
- *Prototype split-delay system enables x-ray pump x-ray probe and 2-pulse small angle XPCS with 20ps delay range.*



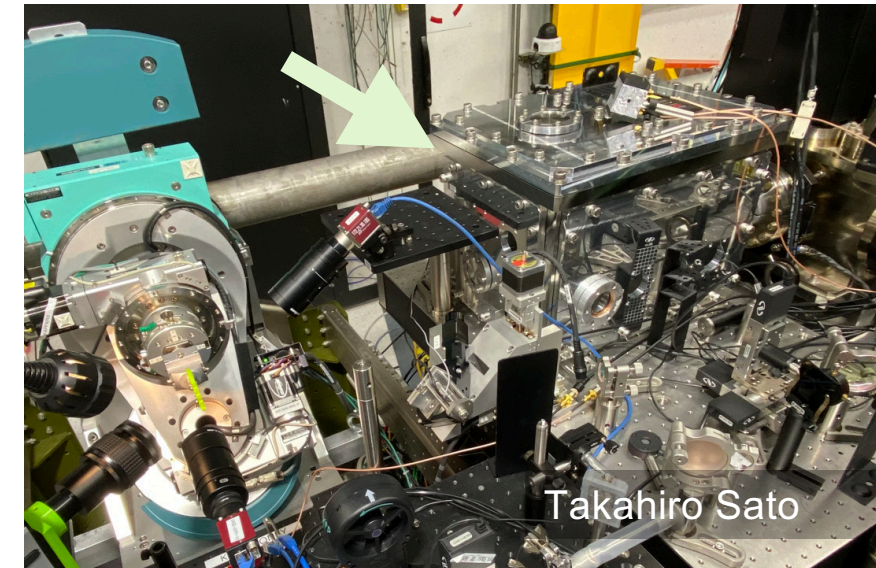
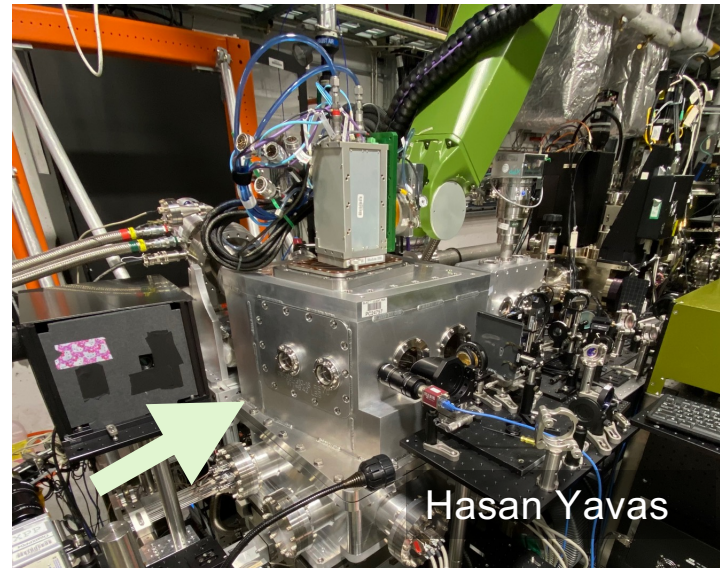
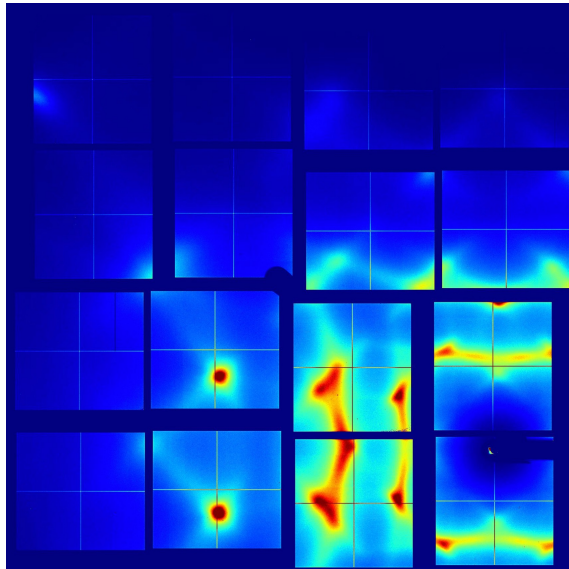
Time-resolved diffraction and scattering

- Flexible in-air diffractometer for solid samples
- Nitrogen cryojet cooling down to 100K
- Flexible optical excitation capability from UV to **THz**.
- ePix10k, ePix100, and Jungfrau detectors available for diffraction and scattering measurement
- 50-100 fs time resolution

Time-resolved Absorption Spectroscopy

- Liquid jet sample delivery.
- Energy scan with the Si(111) mono to cover both XANES and EXAFS regime.
- Flexible optical excitation capability from UV to near IR.
- ePix100 for XES, RXES, ePix10k for forward WAX.
- 50-100 fs time resolution

New capabilities introduced as 'Standard' in run 21



- **trWAX** for material science at 20keV+, vacuum environment supporting fixed target rapid replacement.
- New experimental endstation for **trXRD at low temperature** (20-30K) will be offered with THz excitation capability.
- **Hard x-ray polarization control** established to switch on a near pulse-to-pulse bases between circular and linear inside the new laser in coupling chamber.
- **High resolution mono** (<100meV) and **nanofocusing**.

Backup



Points of contact - by science area and by instrument



LCLS Instrument Contacts:

- **Time-resolved AMO (TMO)** - James Cryan (jcryan@slac.stanford.edu)
- **ChemRIXS** - Georgi Dakovski (dakovski@slac.stanford.edu) or Kristjan Kunnus, (kristjan@slac.stanford.edu)
- **qRIXS** - Georgi Dakovski (dakovski@slac.stanford.edu)
- **X-ray Pump Probe (XPP)** - Diling Zhu (dlzhu@slac.stanford.edu)
- **X-ray Correlation Spectroscopy (XCS)** - Matthieu Chollet (mchollet@slac.stanford.edu)
- **Macromolecular Femtosecond Crystallography (MFX)** - Alex Batyuk (batyuk@slac.stanford.edu)
- **Coherent X-ray Imaging (CXI)** - Meng Liang (mliang@slac.stanford.edu)
- **Matter in Extreme Conditions (MEC)** - Gilliss Dyer (gilliss@slac.stanford.edu)

LCLS Scientific Department Head Contacts:

- Atomic, Molecular and Optical Sciences - James Cryan (jcryan@slac.stanford.edu)
- Biological Sciences - Mark Hunter (mhunter2@slac.stanford.edu)
- Chemical Sciences - Thomas Wolf (thomas.wolf@slac.stanford.edu)
- Laser Science - Joe Robinson (jsrob@slac.stanford.edu)
- Materials Science - Apurva Mehta (mehta@slac.stanford.edu)
- Matter in Extreme Conditions - Gilliss Dyer (gilliss@slac.stanford.edu)

HXR single-pulse SASE w/ NC Linac

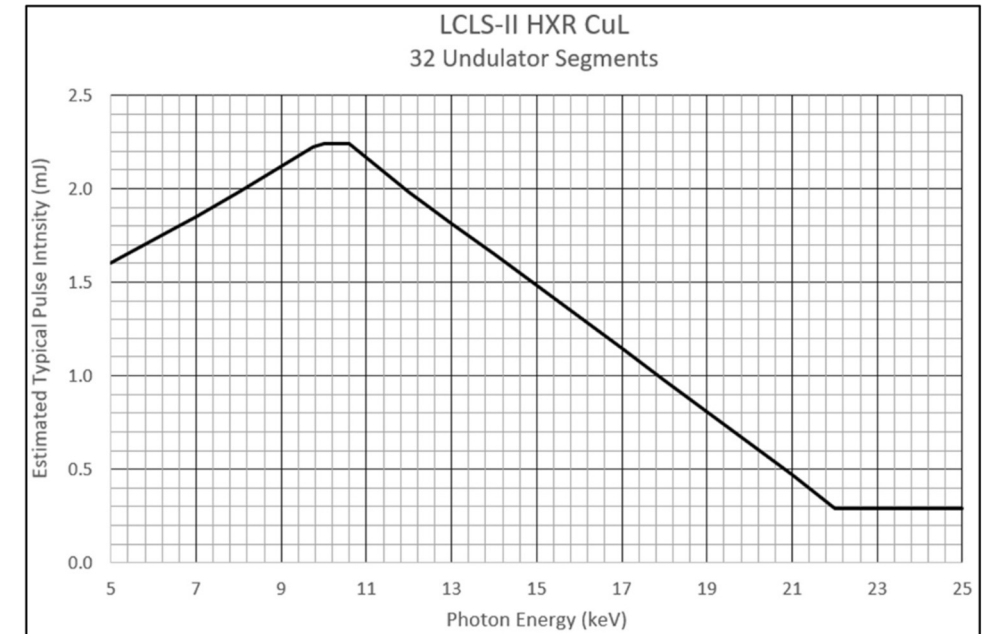
Beam Parameters	Symbol	Cu-HXU x-rays		Unit
		ω_{\max}	ω_{\min}	
Photon Energy	$h\omega$	25000	1000	eV
Fundamental wavelength	λ_r	0.5	12.4	Å
Final linac e- energy	γmc^2	16.5	3.5	GeV
FEL 3-D gain length	L_G	4	1	m
Peak power	P	20	80	GW
Pulse duration range (FWHM)		10 – 50		fs
Nominal pulse duration (FWHM)	$\Delta\tau_f$	~30		fs
Max Pulse Energy*	U	0.6	2	mJ
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)	σ_s	8	20	μm
Photon far field divergence (FWHM)	$\theta_{FWHM, x, \infty}$	1	12	μrad
Max. Beam Rate	φ_{FEL}	120		Hz
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/mm²/mrad²/0.1%-BW

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

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



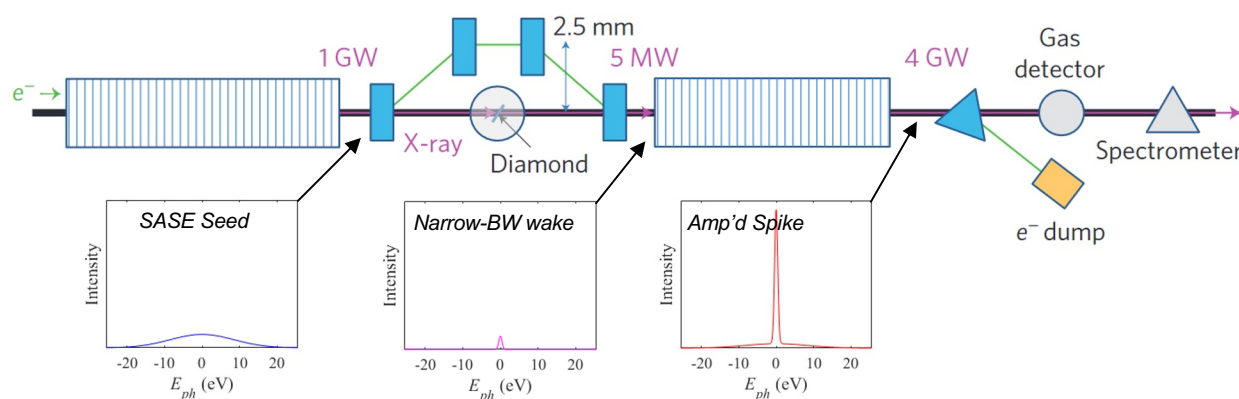
<https://lcls.slac.stanford.edu/parameters>

Hard X-ray Self-Seeding (HXRSS)

Spectral brightness enhancement for narrow bandwidth experiments

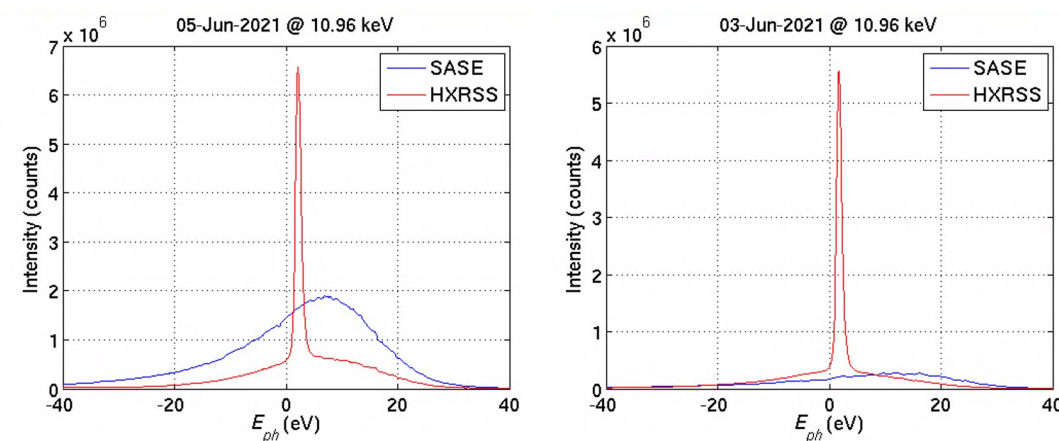
- Updated for LCLS-II *vertically* polarized HXU (90° rotation of crystal optics)
- Now used for 3 experiments, 3-6x spectral brightness at sample vs. SASE

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 2nd half of undulator

Full SASE vs. HXRSS average spectra at 11 keV



Advanced Multi-Pulse/Color Modes

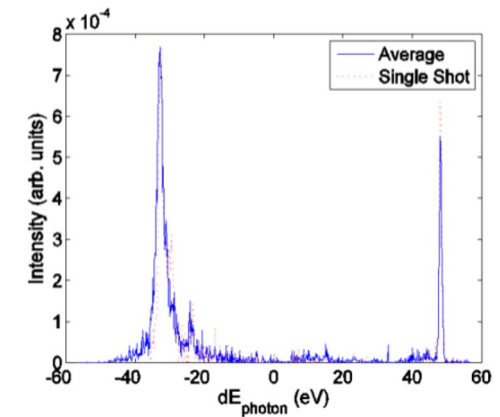
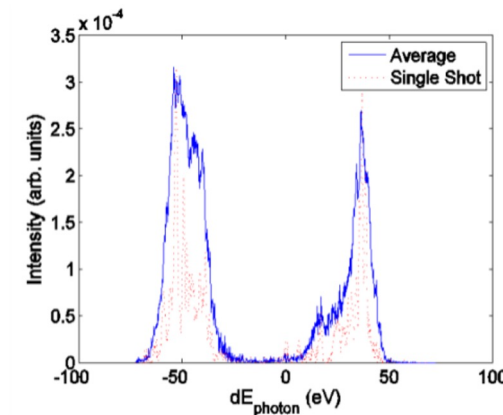
Multiple accelerator-based means for x-ray pump, x-ray probe on variety of time scales

One electron bunch:

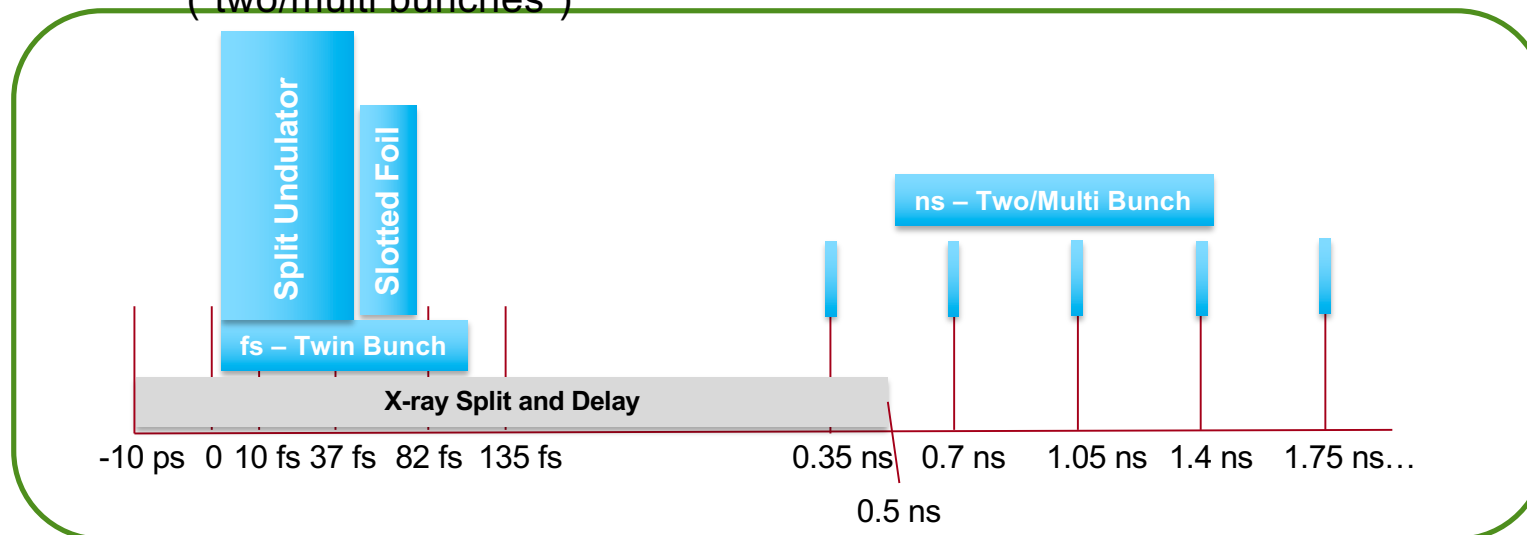
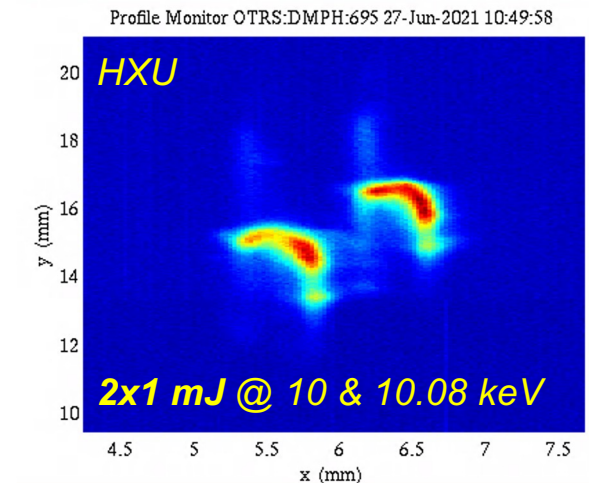
- Double slotted foil

Two electron bunches:

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



Two-bunch XTCAV Images (ns spacing)



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	0 - 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

Discuss special requirements with your LCLS POC

SXR single-pulse SASE w/ NC Linac

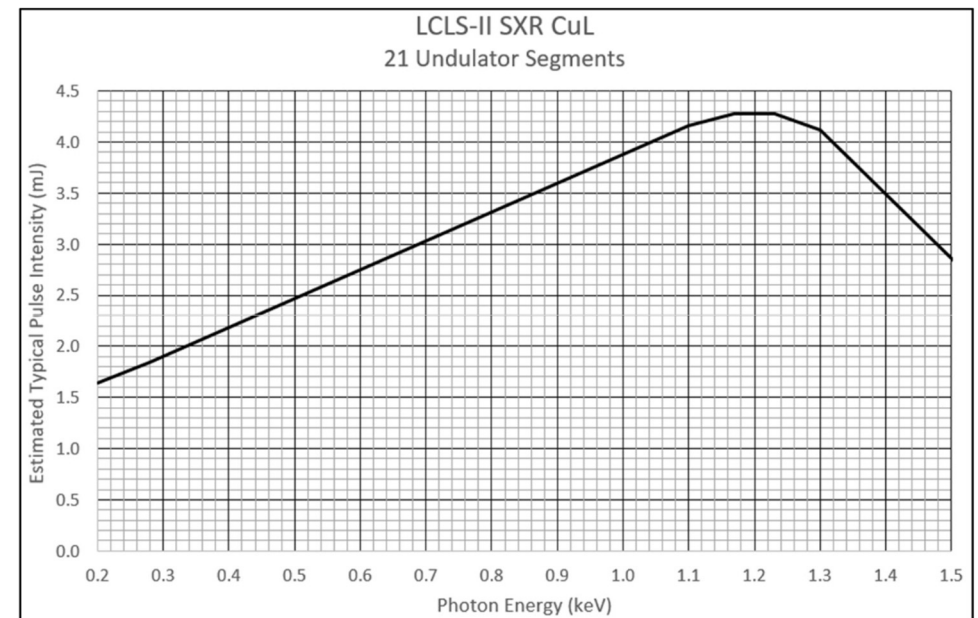
Beam Parameters	Symbol	Cu-SXU x-rays		Unit
		ω_{\max}	ω_{\min}	
Photon Energy	$h\omega$	5000	200	eV
Fundamental wavelength	λ_r	2.5	62	Å
Final linac e- energy	γmc^2	10	3.5	GeV
FEL 3-D gain length	L_G	2.5	1	m
Peak power	P	50	30	GW
Pulse duration range (FWHM)		10 – 250		fs
Nominal pulse duration (FWHM)	$\Delta\tau_f$	50		fs
Max Pulse Energy*	U	2.5	1.5	mJ
Photons per pulse*	$N\gamma$	3.1	47	10^{12}
Peak brightness*	$B_{pk, SASE}$	2250	19	$10^{30} \S$
Average brightness (120Hz)*	$\langle B \rangle$	138	1.5	$10^{20} \S$
SASE bandwidth (FWHM)	$\Delta\omega/\omega$	10	2	eV
Photon source size (rms)	σ_s	16	46	μm
Photon far field divergence (FWHM)	$\Theta_{FWHM, x, \infty}$	3	25	μrad
Max. Beam Rate	φ_{FEL}	120		Hz
Avg. x-ray beam power	P_x	0.3	0.18	W
Linear Polarization (100%)	$\langle P \rangle$	Horizontal		

*Assuming nominal duration and undulator strength

\S Brightness units are photons/sec/mm²/mrad²/0.1%-BW

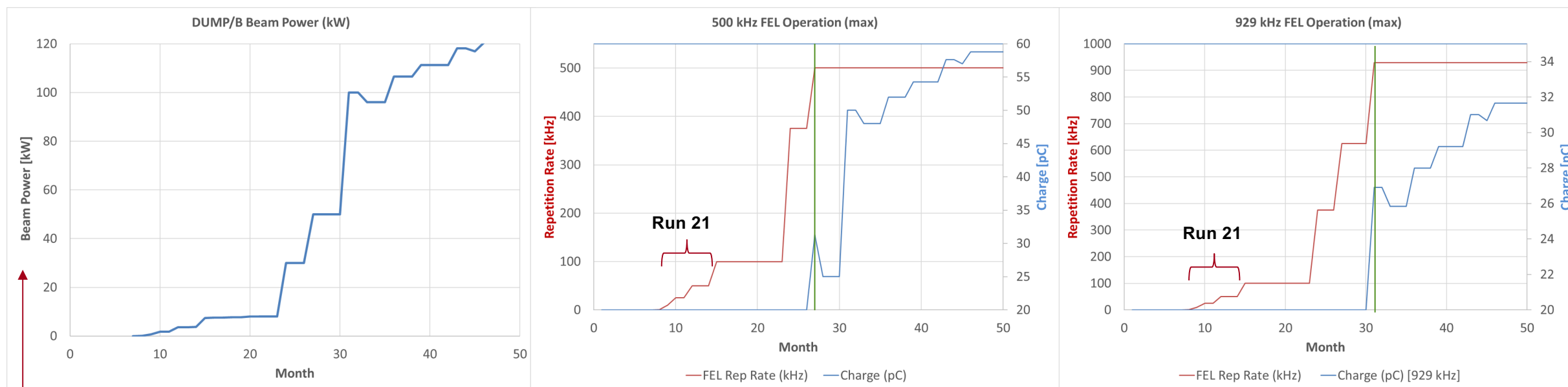
Ready and able, but not planned
for operation in Run 21

SXR line devoted to ramp of new SC
linac and Early Access science...



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

SC Linac Rate Ramp-Up



- Beam Power related to $[\text{Repetition Rate} * \text{Charge}]$, limited to 120 kW max at final beam dumps
- Beam losses & undulator irradiation are major potential issues/hazards
- Facility has 2 year plan for beam/radiation monitoring with a gradual increase of power
- First light mid November 2022 (20 pC, 1 kHz) then gradual ramp to 10's kHz thru Run 21

20 pC with ramp of beam rate from 1 to 33 kHz, dedicated delivery to the SXU

SXR single-pulse SASE w/ SC Linac



Beam Parameters	Symbol	Cu-HXU x-rays			Unit
		$h\omega_{\max}$	$h\omega_{\text{nominal}}$	$h\omega_{\min}$	
Photon Energy	$h\omega$	1300	800	200	eV
Fundamental wavelength	λ_r	9.5	15.5	62.0	Å
Final linac e- energy	γmc^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
Nominal pulse duration (FWHM)	$\Delta\tau_f$	20			fs
Max Pulse Energy*	U	0.06	0.05 - 0.14	0.16	mJ
Photons per pulse*	N_γ	0.28	0.4 - 1.1	5.0	10^{12}
Peak brightness*	$B_{pk, SASE}$	20	8.6 - 24	1.7	10^{30} §
Average brightness* (@33 kHz)	$\langle B \rangle$	137	57 – 161	12	10^{20} §
SASE bandwidth (FWHM)	$\Delta\omega/\omega$	4	3	3	eV
Photon source size (rms)	σ_s	TBD			µm
Far field divergence (FWHM)	$\Theta_{FWHM,x}$ ∞	TBD			µrad
Max. Beam Rate	φ_{FEL}	1,000 – 40,000 **			Hz
Avg. x-ray beam power (@33kHz)	P_x	2.0	1.7-4.6	5.3	W
Linear Polarization (100%)	$\langle P \rangle$	Horizontal			

Pulse energies of >100 µJ in 30 fs for Early Access Science

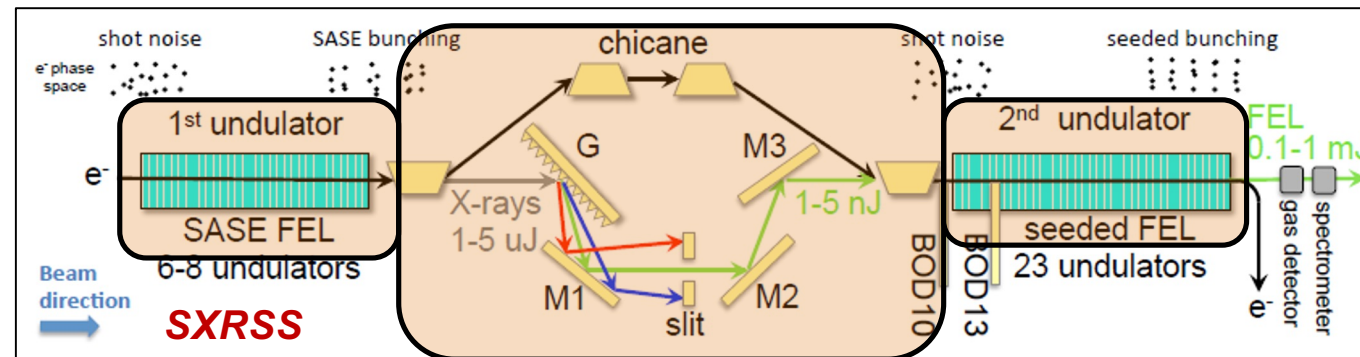
* Assuming nominal duration and undulator strength

§ Brightness units are photons/sec/mm²/mrad²/0.1%-BW

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

Soft X-ray Self-Seeding (SXRSS)

- Commissioning with NC Linac being completed now
- Capability to be extended to SC linac after performance is established, and charge increased (50 pC)

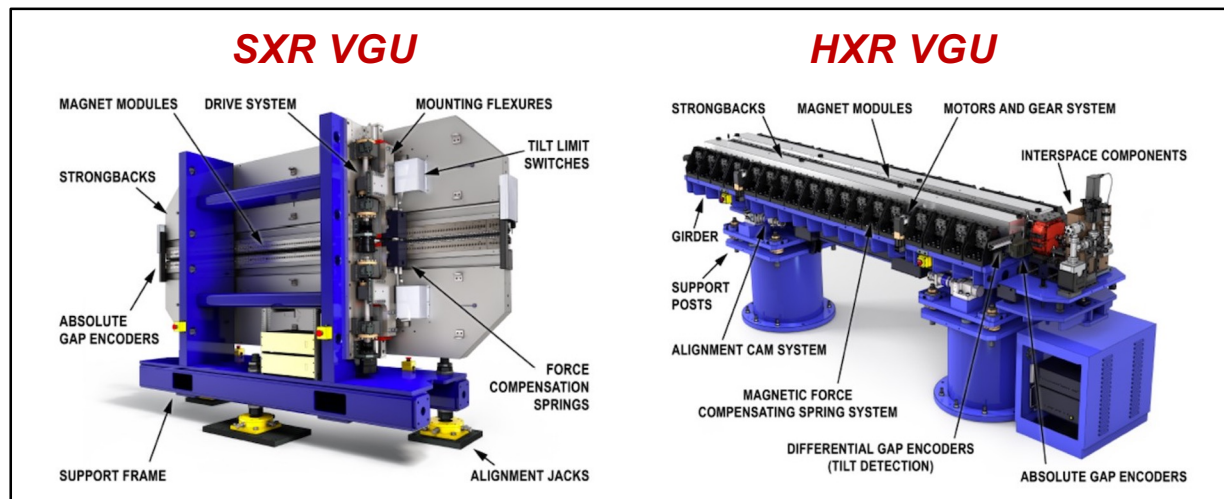


Photon energy	400-1200 eV
Bandwidth (FWHM)	0.1-0.2 eV
Max pulse energy	20 – 50 μ J @ 50 pC
Duration	20 – 50 fs

SXRSS to be demonstrated w/ SC linac toward end of Run 21 (At Risk)

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	TBD end of Run 21



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

SC Linac Summary

Will deliver for Early Access science to the SXU for Run 21

- **Rate:** Ramp from 1 kHz to 33 kHz delivery over Run 21
- **Intensity/quality:** Ramp intensity/ph. energy first 1-2 months
- Special capabilities:
 - **Photon energy scans** ready beginning Run 21
 - **Short pulses** (fs to sub-fs) – End of Run 21 (At Risk)
 - **SXRSS** – End of Run 21 (At Risk)

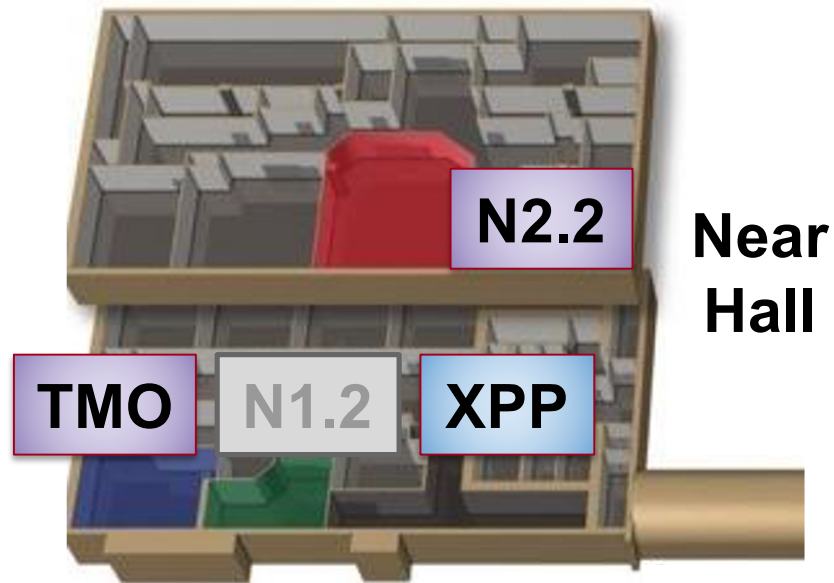
Provisional X-ray and Laser Parameters for high repetition-rate operation



X-ray Parameters			
Repetition rate (Hz)	Up to 50 kHz		
Energy Range (eV)	250 - 1800		
Pulse Duration	20 fs (nominal)	Under Development (increased risk)	
		Tunable to 5 fs	< 1 fs (XLEAP-II)
Energy per pulse	~ 50 μJ	Scales linear with pulse energy	2-3 μJ
Bandwidth (FWHM)	2 eV	2 eV	4-8 eV
Spot Size, FWHM (range)	1.0 - 200 (um) diameter		
Polarization	Linear, Horizontal		
Two Pulse Mode (icryan@stanford.edu for more information)	Under development, offered at risk < 10 μJ / pulse with tunable delay via split undulator method. This provides a minimum delay of ~10 fs for arbitrary wavelength. For harmonic operation ($\omega/2\omega$, $\omega/3\omega$) the minimum delay ~200 as.		

Laser Parameters				
Repetition rate (Hz)	Synchronized up to 33 kHz			
Wavelength	800 nm	400 nm	High Risk	ES Only
			266 nm	1300-2400 nm
Pulse Duration	< 25 fs	< 50 fs	< 50 fs	< 100 fs
Energy per pulse (on target)	100 μJ	> 10 μJ	~ 1 μJ	< 10 μJ
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.			

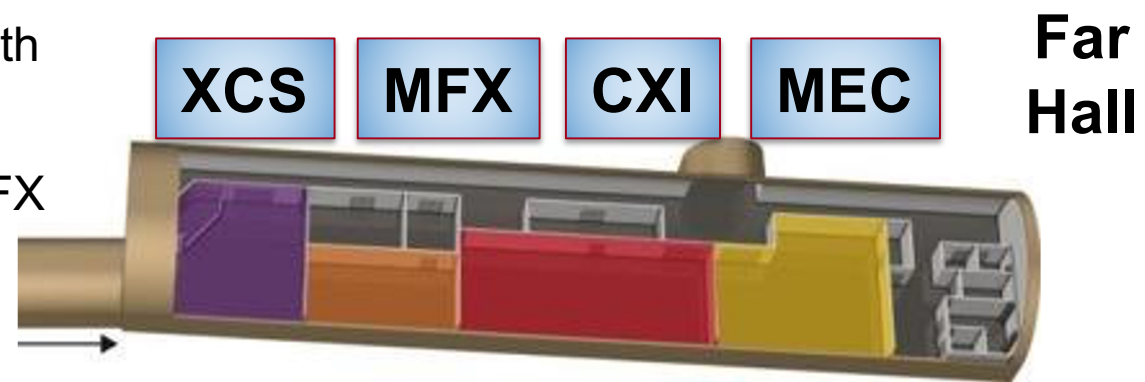
Ultrafast lasers available at all instruments for Run 21



**Near
Hall**

- TMO and 2,2 will share the high rep-rate OPCPA system, running at 33 kHz for Early Science
 - Limited wavelengths available - see more later
- XPP will continue to use the 120 Hz Ti:S laser systems in the NEH Laser Hall
 - Maintains previous broad range of laser capability

- All FEH hutches have ultrafast laser capability with Ti:S regen now commissioned in MFX
- High-energy OPO also available (primarily) at MFX
- Tunable UV capability under development at CXI



**Far
Hall**

Laser capabilities at high rep rate

- High rep rate OPCPA system will be available, for the first time, for commissioning and Early Science experiments in TMO and Hutch 2.2
- OPCPA system will operate at 800nm, 33kHz, <25fs and ~35W output power
- Anticipated on-target parameters (include losses in transport and conversion efficiencies). Availability varies by instrument - check web pages for details
 - 800nm, <25fs, ~300 μ J
 - 266nm, <50fs, ~3 μ J
 - 400nm, <50fs, ~30 μ J
 - 1300-2400 nm, <100fs, <30uJ (signal), >10uJ (idler)
- Laser repetition rate can be picked down to some sub-harmonics of 33 kHz (maintaining the same pulse energy)
- Time-tool will initially be at lower rate (through averaging), and progress towards shot-to-shot through the run
- Pulsed fiber timing system will be incorporated to reduce timing drift and improve overall temporal resolution of experiments

Laser capabilities for hard X-ray hutches (not MEC)

- XPP, XCS, MFX, CXI primarily use femtosecond Ti:S systems:
 - 800nm, 120Hz, ~40fs, <20mJ with MPA, ~3mJ with regen
 - Programmable pulse-train to delay shots on demand for X-ray only background shots (“Goose trigger”)
 - Time-tool available for shot-to-shot arrival time tagging (dependent on the X-ray parameters at the time-tool!)
- Wavelength generation from UV-THz. Specific capabilities and geometries are hutch dependent, based on local laser infrastructure and typical need
- Few-cycle pulses have now been generated and used in XPP, XCS. Talk to POCs for more information
- Tunable ns OPO or ns 527nm lasers can be moved between MFX, CXI and XPP. OPO will be limited to high-energy, 10Hz operation in run 21
- Tunable UV capability under development at CXI. Details on instrument web pages.

LCLS laser capability varies between instruments



Y	Typically available. Depends on specifics of the experiment
~	May be available depending on specifics and interest
N	Not available at this time

See instrument webpages for details and standard configs

* Some flexibility in CXI UV wavelengths

Contact the laser POC for the instrument with questions

Instrument	MPA	800	Harmonics 200 nm	Harmonics 400, 266 nm	OPA 480- 1200 nm	OPA 1.2-2.4 μ m	MIR	THz	<10fs (800 nm)	527 nm (ns)	OPO (ns)	Time- Tool
1.1 IP1	N/A	Y	N	Y	N	~	N	N	N	N	N	Spatial
2.2 chemRIXS	N/A	Y	N	Y	N	N	N	N	N	N	N	Spatial
2.2 qRIXS	N/A	Y	N	N	N	N	N	N	N	N	N	Spatial
XPP	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	~	Spectral
XCS	N	Y	~	Y	Y	Y	N	N	Y	N	N	Spectral
MFX	N	Y	N	Y	Y	Y	N	N	N	Y	Y	Spectral
CXI	~	Y	Y*	Y*	Y	Y	~	~	N	Y	Y	Spectral
MEC	Substantially different laser capabilities. Covered in the MEC instrument slides in the breakout.											