LCLS
L2SI, LCLS-HE and Petawatt

Alan Conder LCLS Chief Engineer
Frank O'Dowd NEH2.2 Project Engineer

SLAC NATIONAL ACCELERATOR LABORATORY

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U.S. DEPARTMENT OF ENERGY
Office of Science

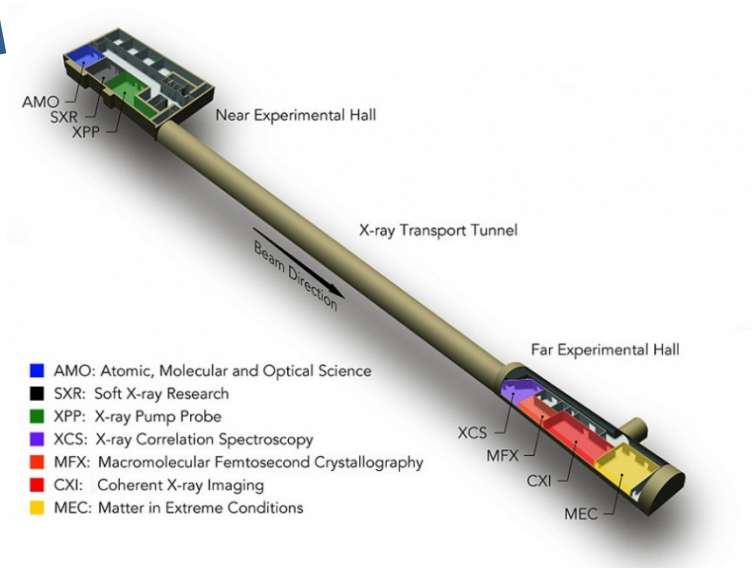
LCLS-I brought new capabilities to X-ray science, enabling new frontiers of research not available with synchrotrons

LCLS-I world's 1st X-ray Free Electron Laser

- Became operational in 2009
- X-ray Range: 0.25 to 13.8 keV
- FEL Pulse Length: 5 – 500 fs
- FEL Pulse Energy: ~ 6mJ
- FEL Rep Rate: 120 Hz
- Fixed gap undulator
- Seven experiment stations

Experiment stations

- AMO: Basic nature of matter
- SXR: Imaging and scattering
- XPP: Transient states of matter
- XCS: Dynamic changes of condensed matter
- MFX: Macromolecular crystallography
- CXI: Imaging of non-periodic nano-objects
- MEC: Matter at extreme temp and pressure



LCLS-II will push X-ray FEL science further into new frontiers with higher rep rates and finer control of energy tuning

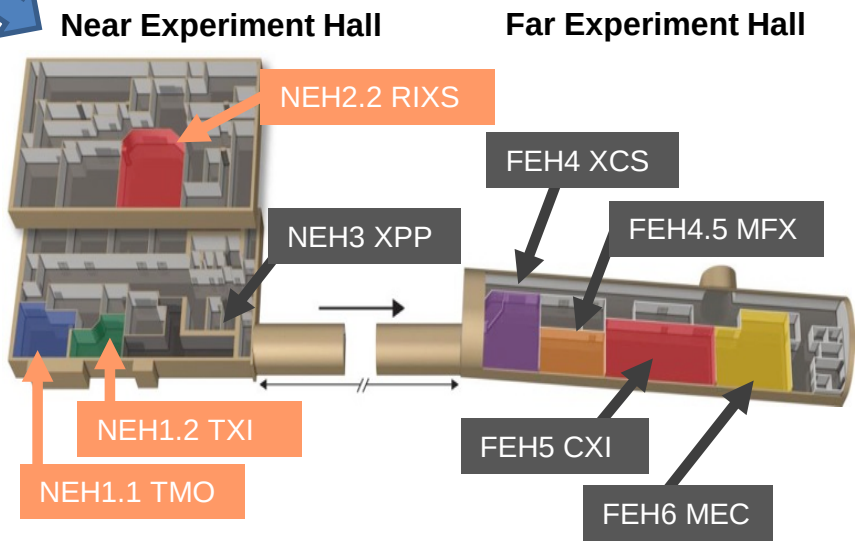
LCLS-II adds super conducting cryomodules

- Planned operations in 2021
- X-ray Range: 0.25 to 5 keV (SCRF)
- FEL Pulse Length: 5 – 500 fs
- FEL Pulse Energy: ~ 3mJ
- FEL Rep Rate: 120 Hz → 1 MHz
- Two variable gap undulators (energy tuning) HXR CuRF ~ 25keV and SXR
- Three new experiment stations (L2SI)

Experiment stations

- TMO: Time resolved AMO
- TXI: Tender X-ray imaging and scattering
- RIXS: Resonant inelastic X-ray spectrometer
- XPP: Transient states of matter
- XCS: Dynamic changes of condensed matter
- MFX: Macromolecular crystallography
- CXI: Imaging of non-periodic nano-objects
- MEC: Matter at extreme temp and pressure

L2SI endstations TTO summer 2020 (CuRF)



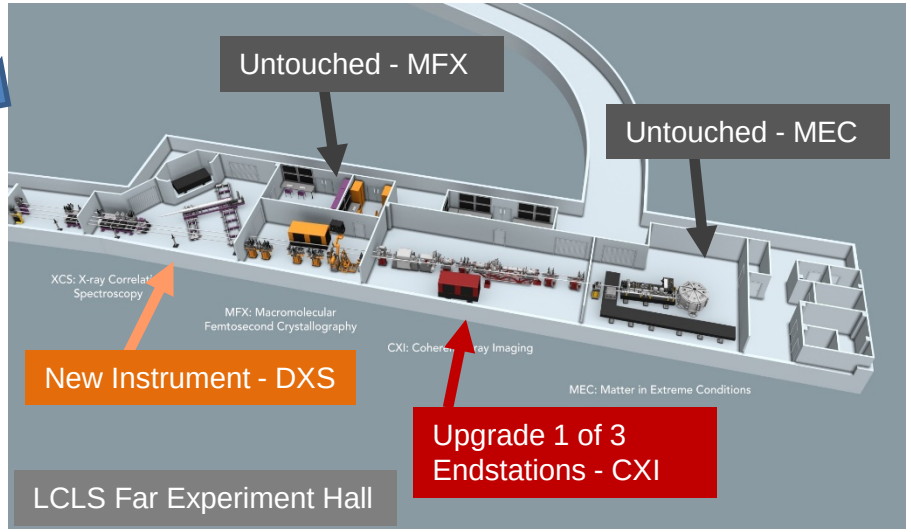
LCLS-HE brings additional cryomodules to produce higher energy X-rays (5 – 12.5 keV) at LCLS-II rep rates (1 MHz)

LCLS-HE additional cryomodules

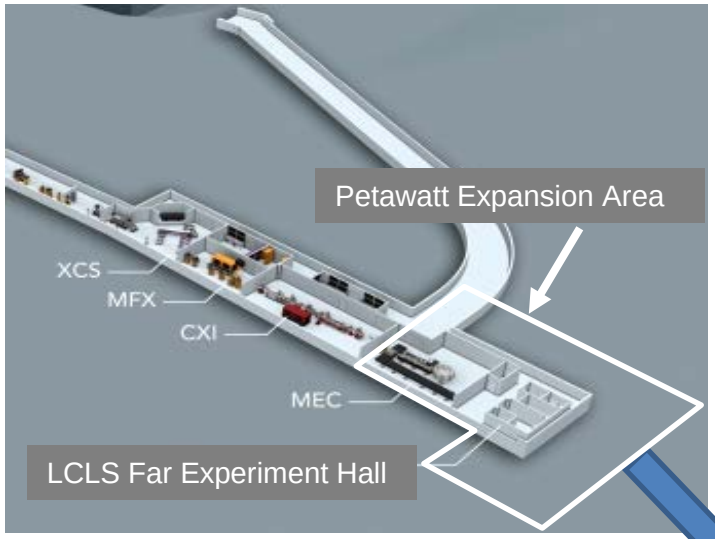
- Planned operations in 2026
- X-ray Range: 5 to > 12.5 keV (SCRF)
- FEL Pulse Length: 5 – 500 fs
- FEL Pulse Energy: ~ 3 mJ
- FEL Rep Rate: 120 Hz → 1 MHz
- Two variable gap undulators (energy tuning) HXR CuRF ~ 25keV and SXR
- One new experiment station + upgrades

Experiment stations

- TMO: Time resolved AMO
- TXI: Tender X-ray imaging and scattering
- RIXS: Resonant inelastic X-ray spectrometer
- XPP: New detector and upgraded diagnostics
- DXS: Dynamic X-ray scattering
- MFX: Macromolecular crystallography
- CXI: New optics, detector and DAQ
- MEC: Matter at extreme temp and pressure



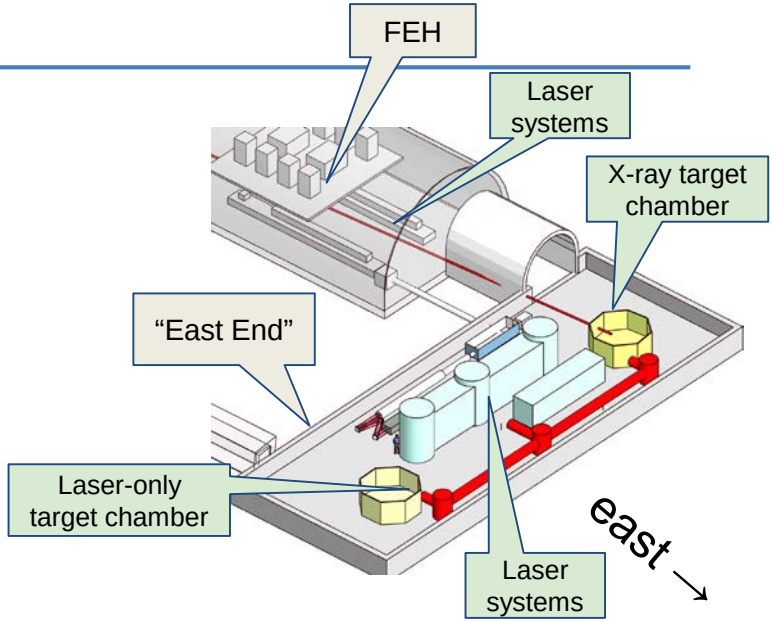
Petawatt is a new project from DOE's office of fusion energy science that upgrades the capabilities of MEC



Petawatt brings upgraded capability

- Planned operations in 2025
- Wavelength Range: 1050 – 1063 nm
- Pulse Length: < 150 fs
- Peak Optical Power: 1 – 10 PW
- Rep Rate: every 5 minutes (20 Hz goal)
- Two new target chambers

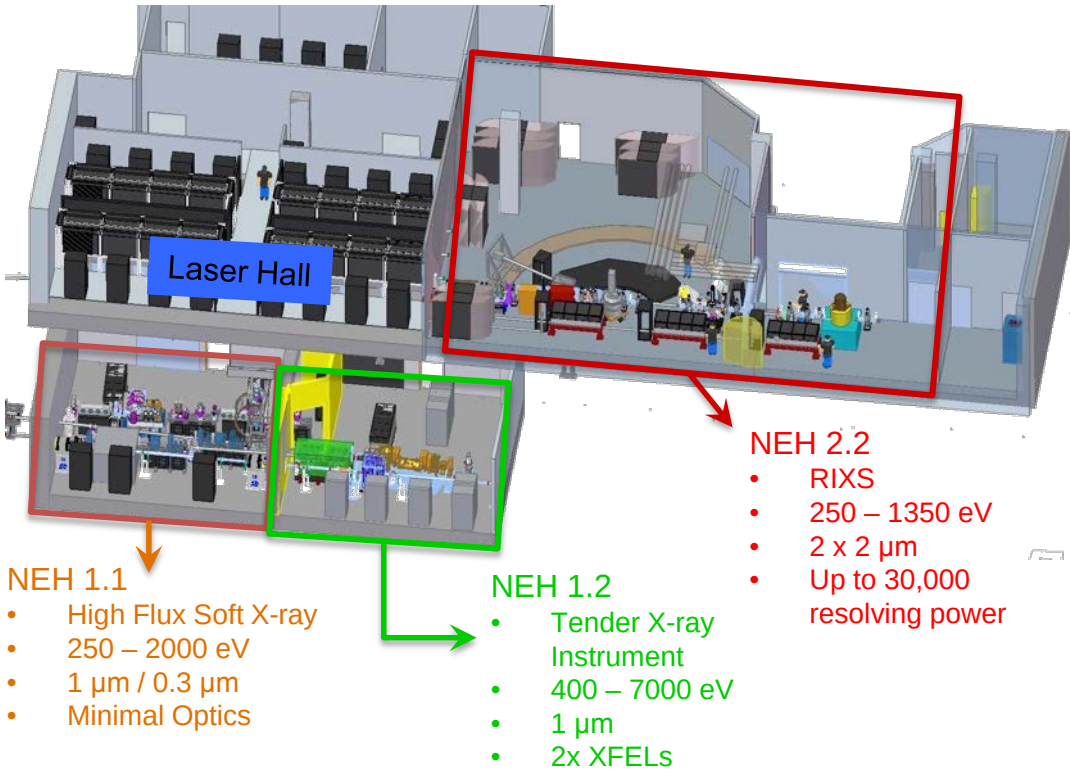
Pushing the envelope on material properties under extreme pressure and temperature. This will be the only Petawatt facility that enables coupling the HXR FEL beam into the sample to probe material properties under extreme conditions.



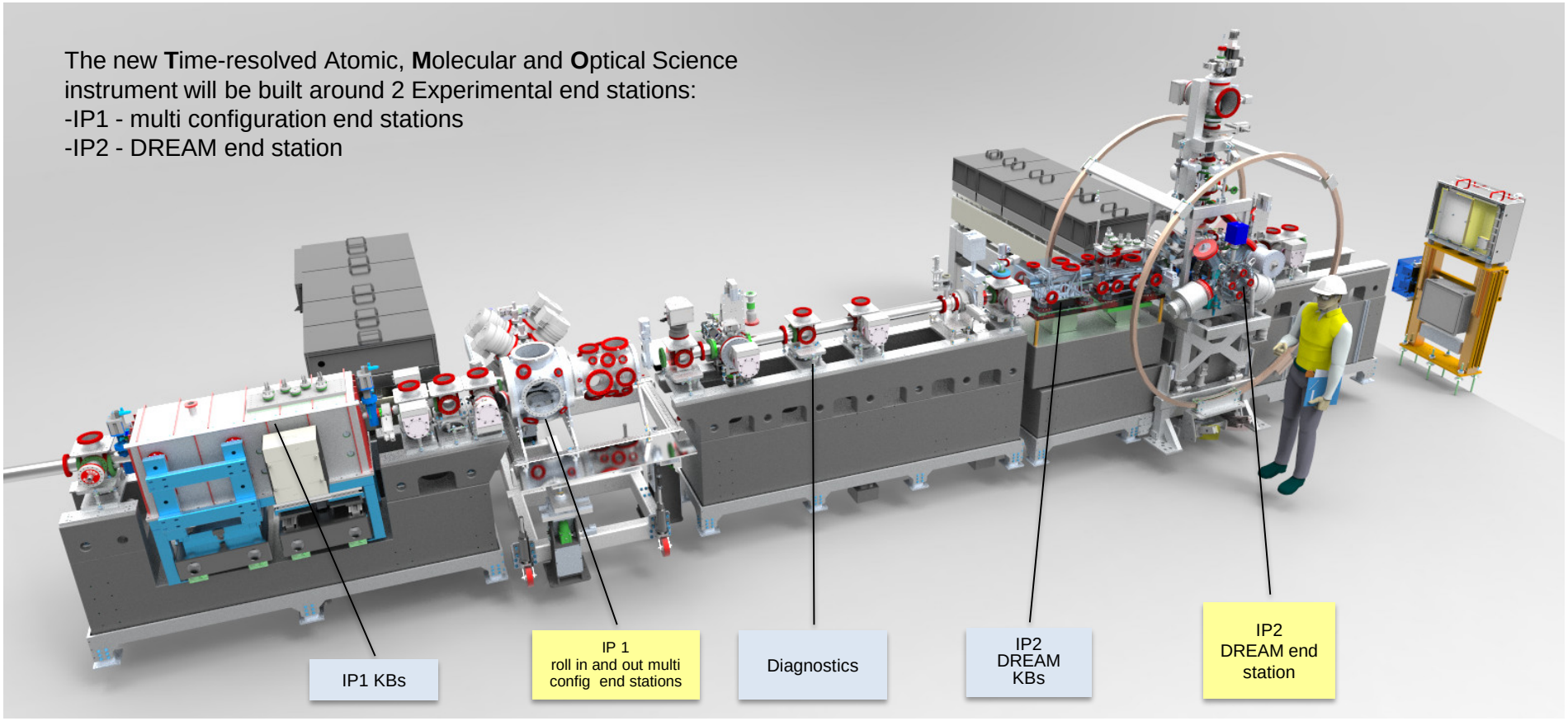
LCLS-II Scientific Instruments (L2S-I)

- The L2S-I scope includes:
  - 3 new instruments (5 endstations)
    - X-ray optics, diagnostics, detectors, controls
  - A central high-power optical laser complex
  - A high throughput data complex

- Program is focused on ensuring first two instruments (NEH 1.1, NEH 2.2) are delivered on time for LCLS-II operations

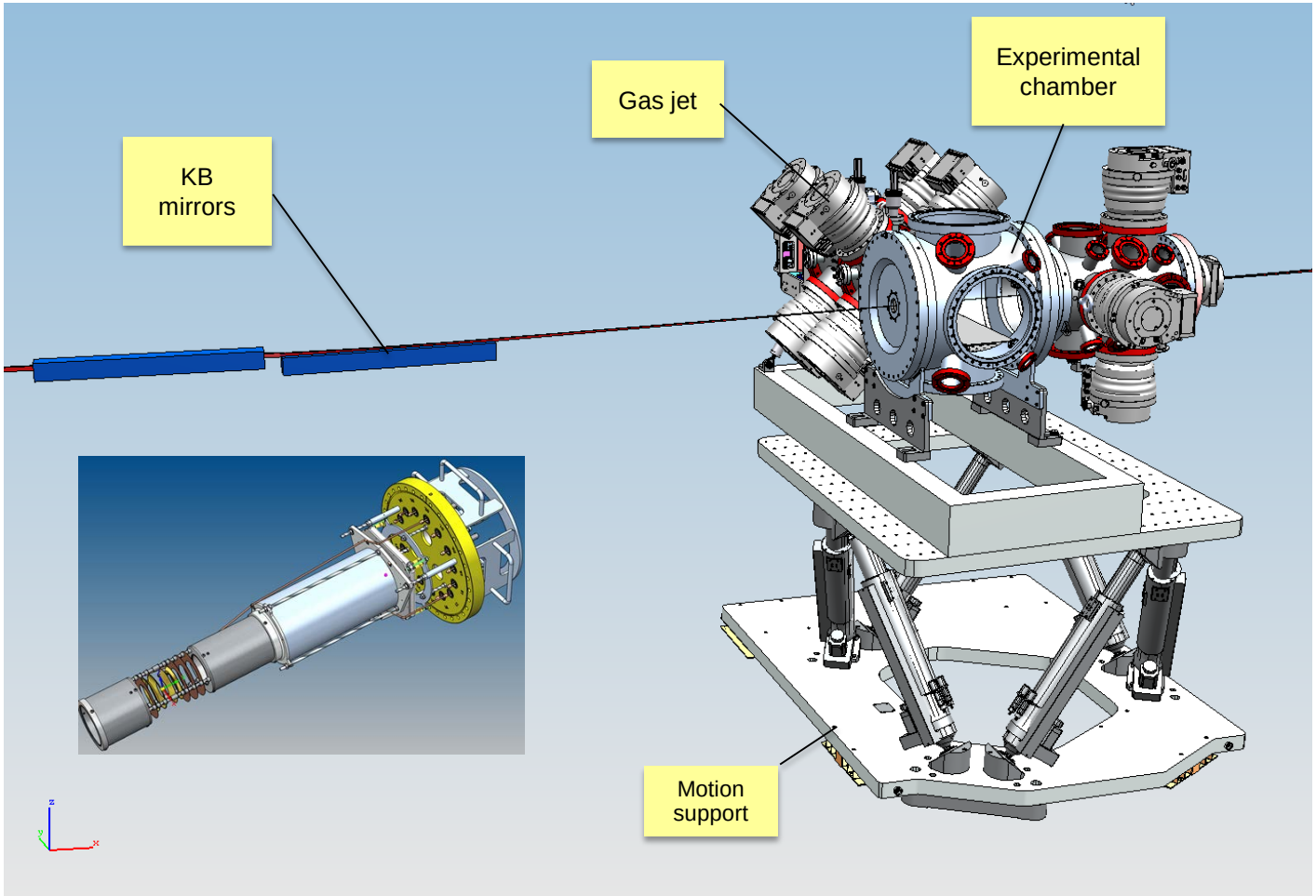


TMO Beamline Overview



TMO beamline will offer the possibility to install modular stations (roll in and out) which can be set up, aligned and commissioned outside the hutch and installed at the first IP1 focus spot.

TMO Beamline IP1

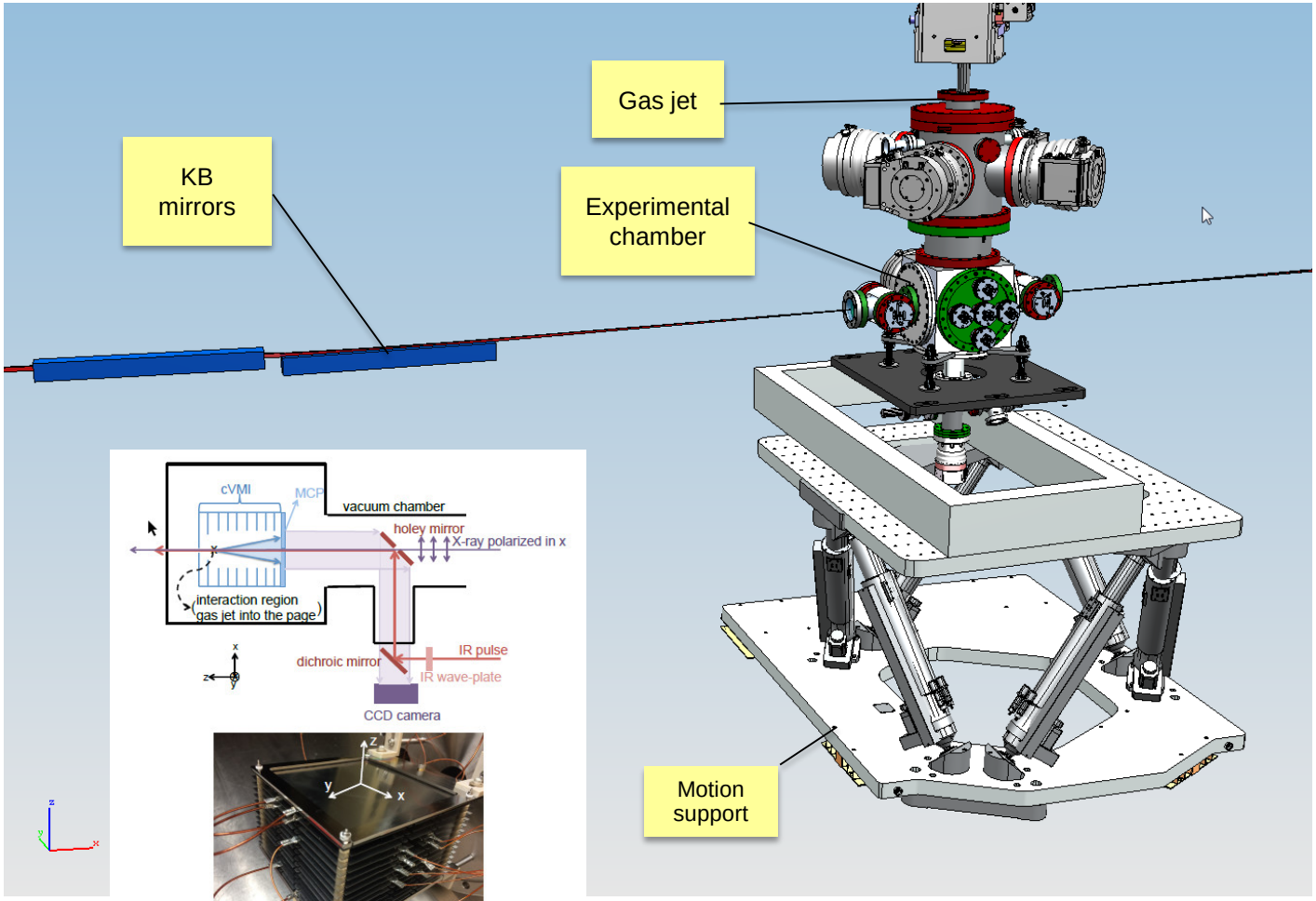


LAMP end station

Time-resolved multi-edge photoelectron-photo ion coincidence spectroscopy

- Vacuum: 10-9 and up to 10-5 Torr
- Accommodate gas, clusters, aerosols with X, Y, Z manipulation
- Spot size ⌀ 1-50µm

TMO Beamline IP1



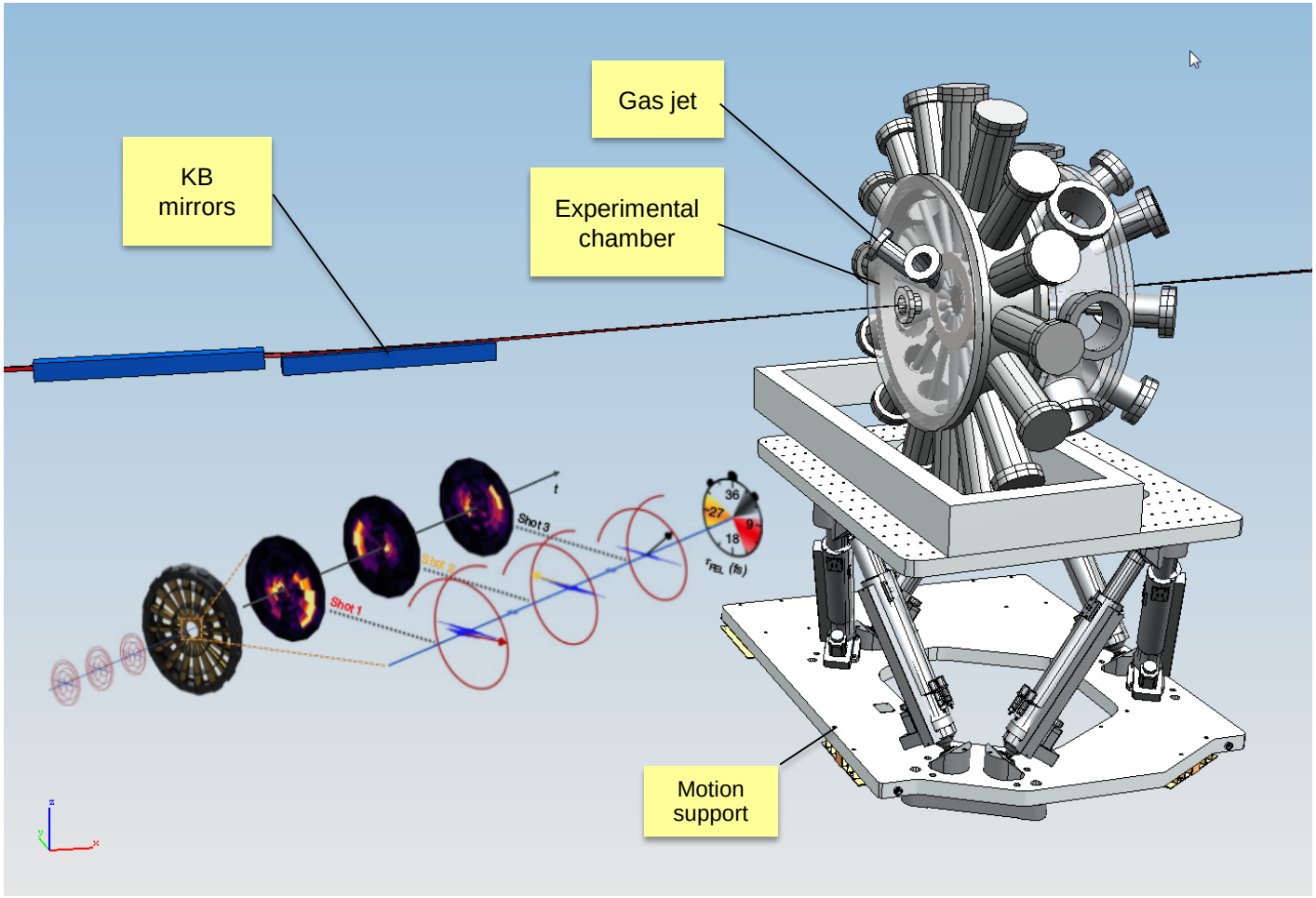
CVMI end station

Attosecond Photophysics and Photochemistry

- Vacuum: 10-9 and up to 10-5 Torr
- Spot size ⌀ 1-50µm

TMO Beamline IP1

MRCOFFEE end station



Multi **R**esolution **C**ookiebox **O**ptimized for **F**uture **F**ree **E**lectron Laser **E**xperiments

Attosecond Resolution

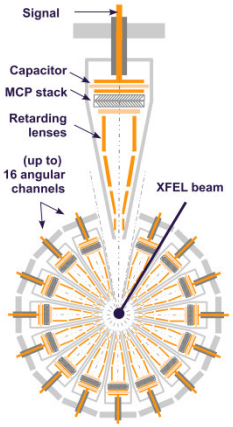
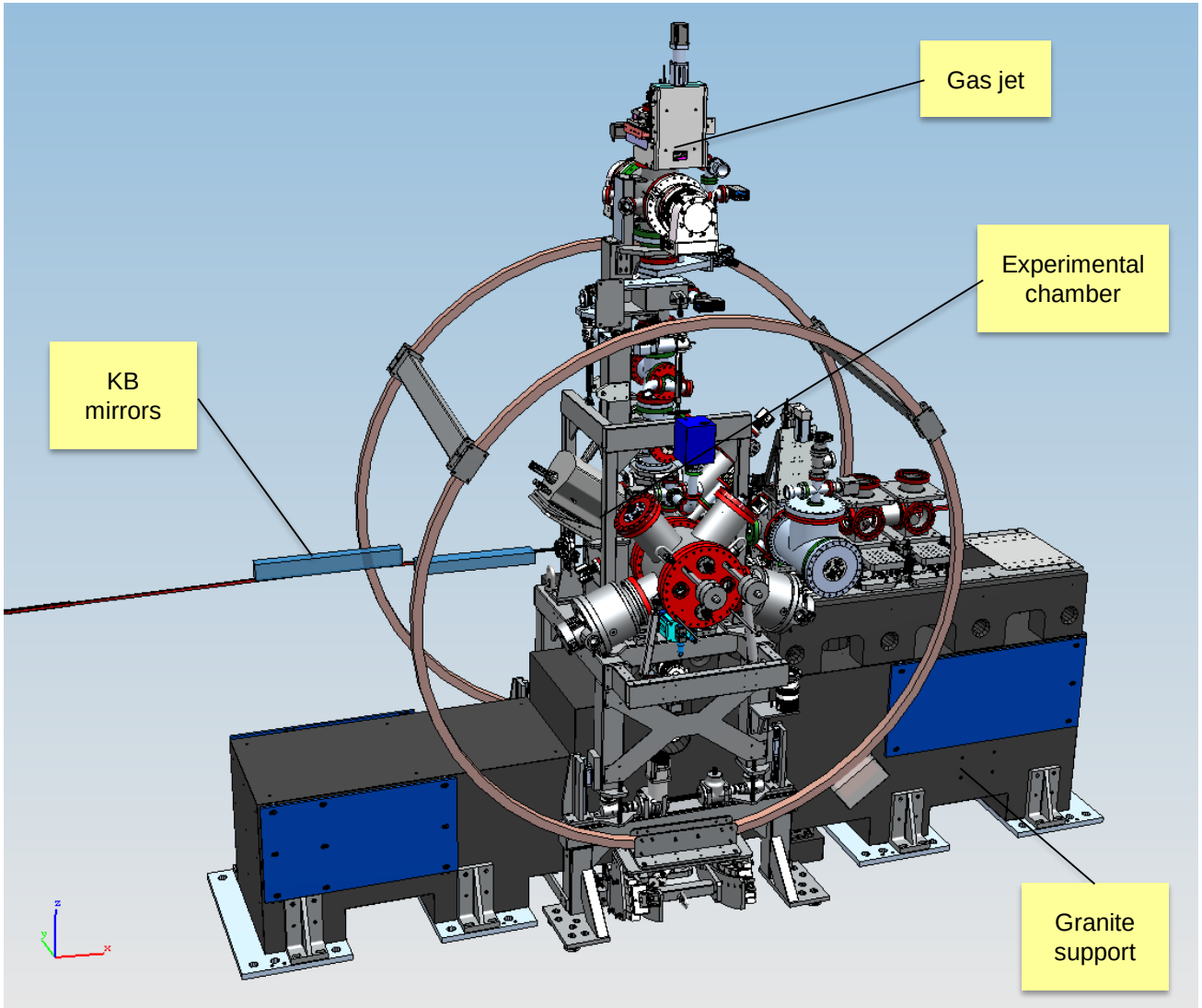


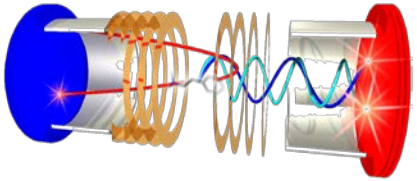
Figure 2: Scheme of a eTOF spectrometer designed in a group P04 at PETRA.

TMO Beamline IP2



DREAM end station

Dynamic REAction Microscope

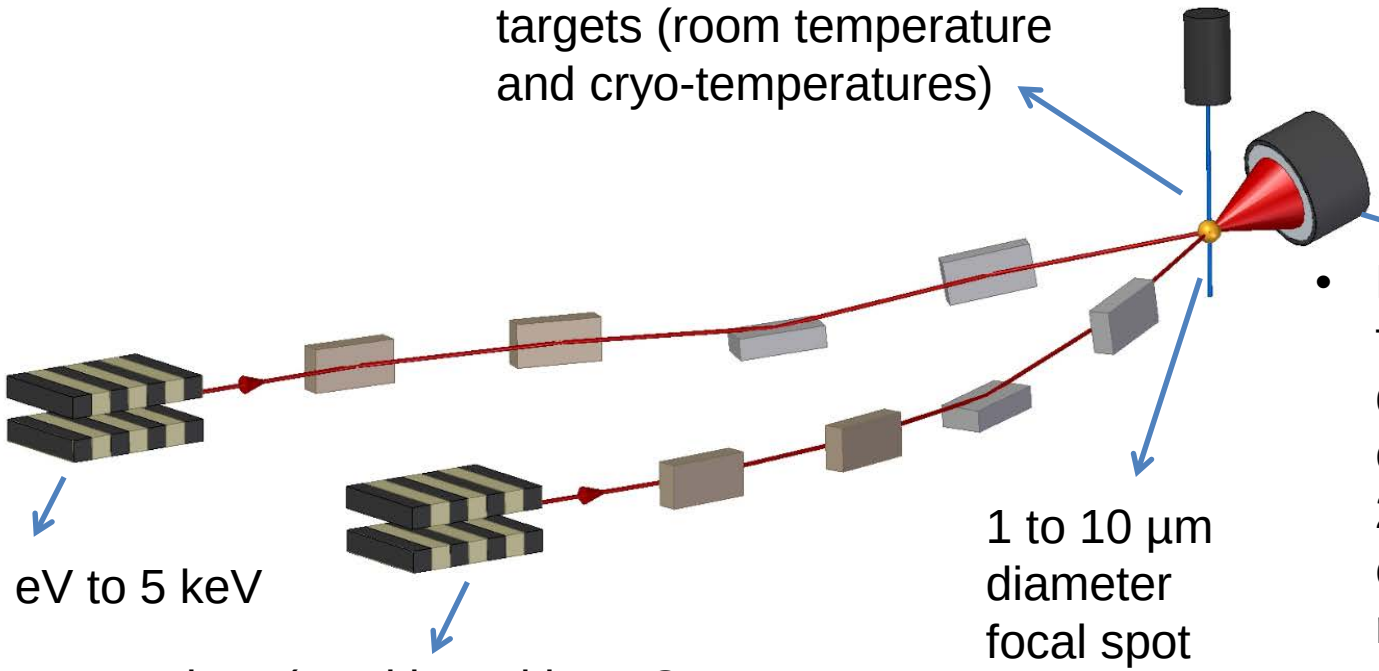


DREAM: coincident electron/ ion 3D momentum imaging,
COLTRIMS type spectrometer as a standard configuration to accommodate extreme vacuum, sub-micron focus spot size, and target purity requirements dictated by the pump-probe class of coincidence experiments, while accumulating data on the event-by-event basis at the rep rates in excess of 100 kHz fully utilizing the LCLS-II capabilities. Photon fluence in DREAM will reach over 1021 photons/cm2 with superconducting Linac X-rays

4pi collection efficiency
(<20eV ions, <100eV electrons)
Spot size ⌀ 0.3-50µm
2-10^{-11} torr vacuum

TXI Beamline Conceptual Layout

The instrument will support, liquid jets, aerosols & fixed targets (room temperature and cryo-temperatures)



200 eV to 5 keV

1 to 7 keV (Working with D. Cocco to extend up to 10 keV)

1 to 10 µm diameter focal spot

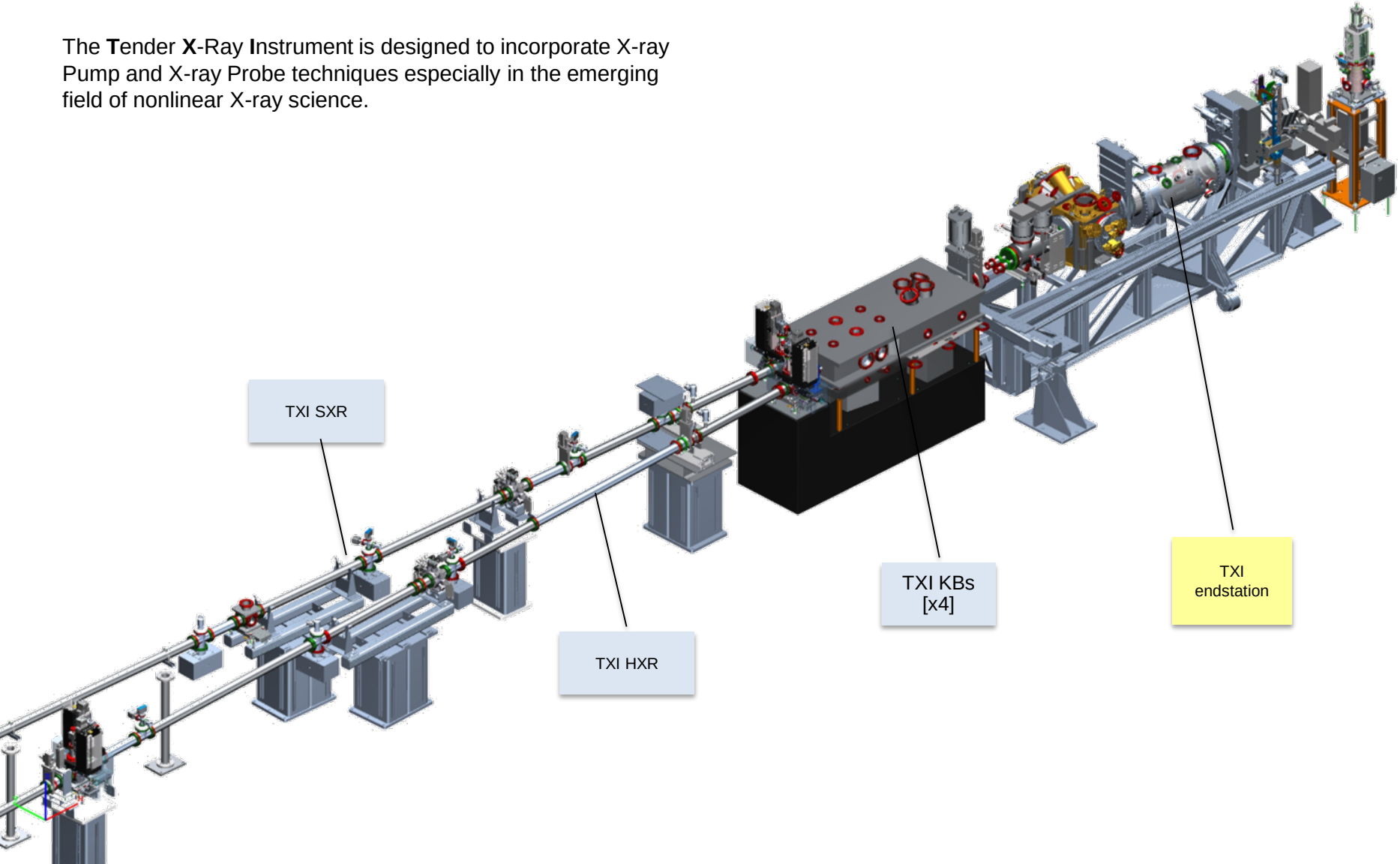
- Multi megapixel forward scattering detector with collection angles, 2θ, > 60° & collection repetition rates > 5 kHz

- Additional X-ray spectrometers will support X-ray emission.

Delay times from fs up to 1 ns, using a crystal delay line on the hard X-ray branch line

TXI Beamline Overview

The **T**ender **X**-Ray **I**nstrument is designed to incorporate X-ray Pump and X-ray Probe techniques especially in the emerging field of nonlinear X-ray science.



TXI Beamline Experimental Techniques

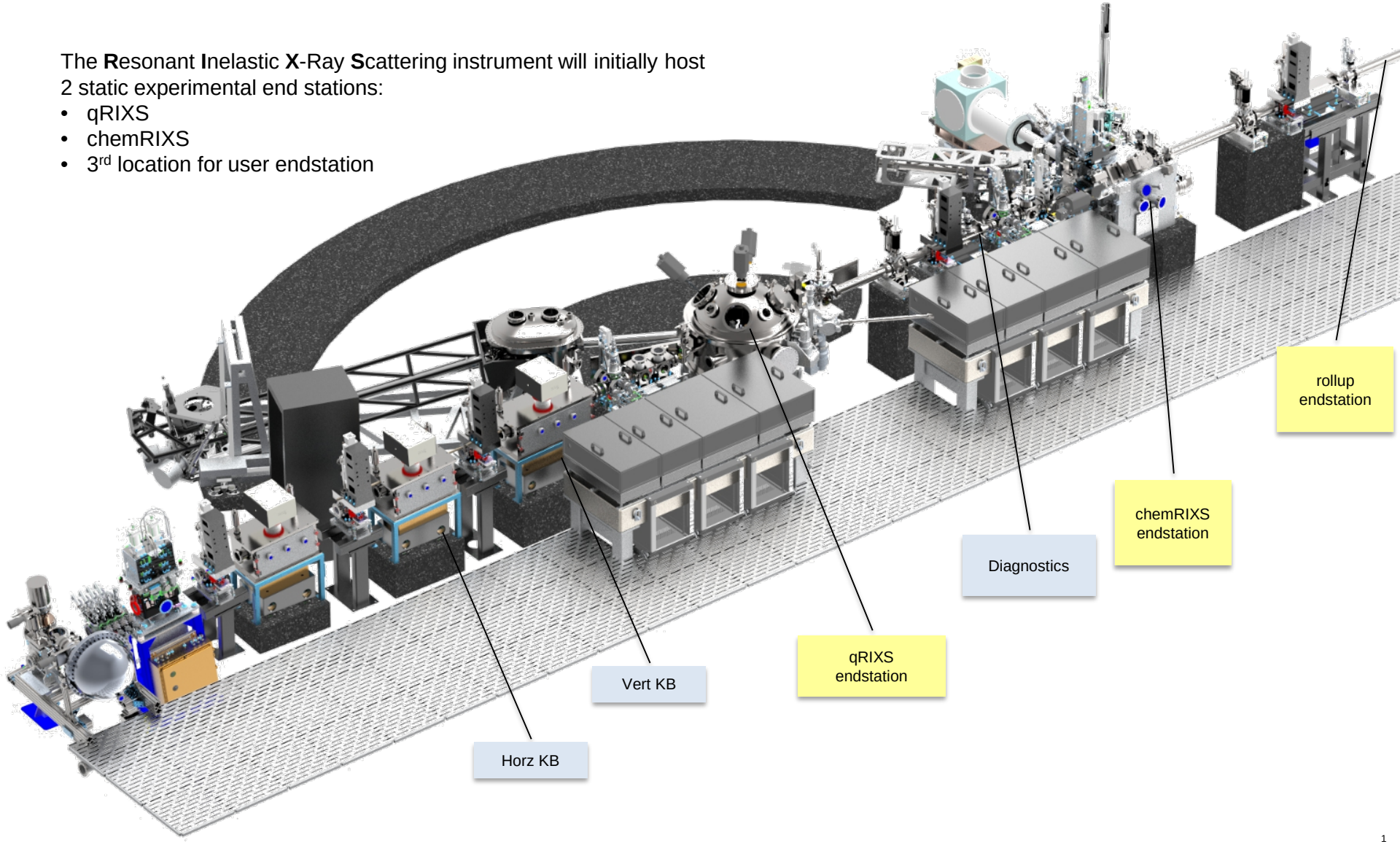
Experimental Technique	Rep Rate	Pulse Energy	Average Power	Photon Energy Range
1. X-ray pump / X-ray probe	100 kHz 100 kHz	0.2 mJ 0.2 mJ	20 W 20 W	250 –1300 eV 1000 – 5000 eV
1a. Nonlinear X-ray physics (including Stimulated Raman)	10 kHz 10 kHz	0.2 mJ 0.2 mJ	20 W 20 W	700 –1300 eV 1000 – 5000 eV
1b. Phonon Dynamics (including FT Inelastic X-ray Scattering)	10 kHz[1] 10 kHz[1]	0.2 mJ 0.2 mJ	20 W 20 W	250 –1300 eV 1000 – 5000 eV
1c. Coincidence Catalysis (including Enzymatic reactions dynamics)	10 kHz 10 kHz	0.2 mJ 0.2 mJ	20 W 20 W	700 –1300 eV 1000 – 5000 eV
2. Coherent scattering & imaging (including time resolved)	10 kHz	3 mJ	30 W	2000 – 5000 eV
2a. Fluctuation X-ray Scattering	10 kHz	3 mJ	30 W	2000 – 5000 eV
2b. Single particle Imaging	10 kHz 120 Hz	3 mJ 8 mJ	30 W 1 W	2000 – 5000 eV 250 - 5000 eV
3. Tender X-ray spectroscopy	100 kHz	0.2 mJ	20 W	1900 – 5000 eV
3a. X-ray emission spectroscopy (time resolved is a future upgrade)	100 kHz	0.2 mJ	20 W	2000 – 5000 eV
3b. Absorption spectroscopy (time resolved is a future upgrade)	100 kHz	30 μJ[2]	3 W	1900- 4500 eV

[1] The maximum rep rate will be determined by the fast kicker (currently 10 kHz).
[2] Through a 4-bounce crystal delay line (bandwidth ~500 meV)

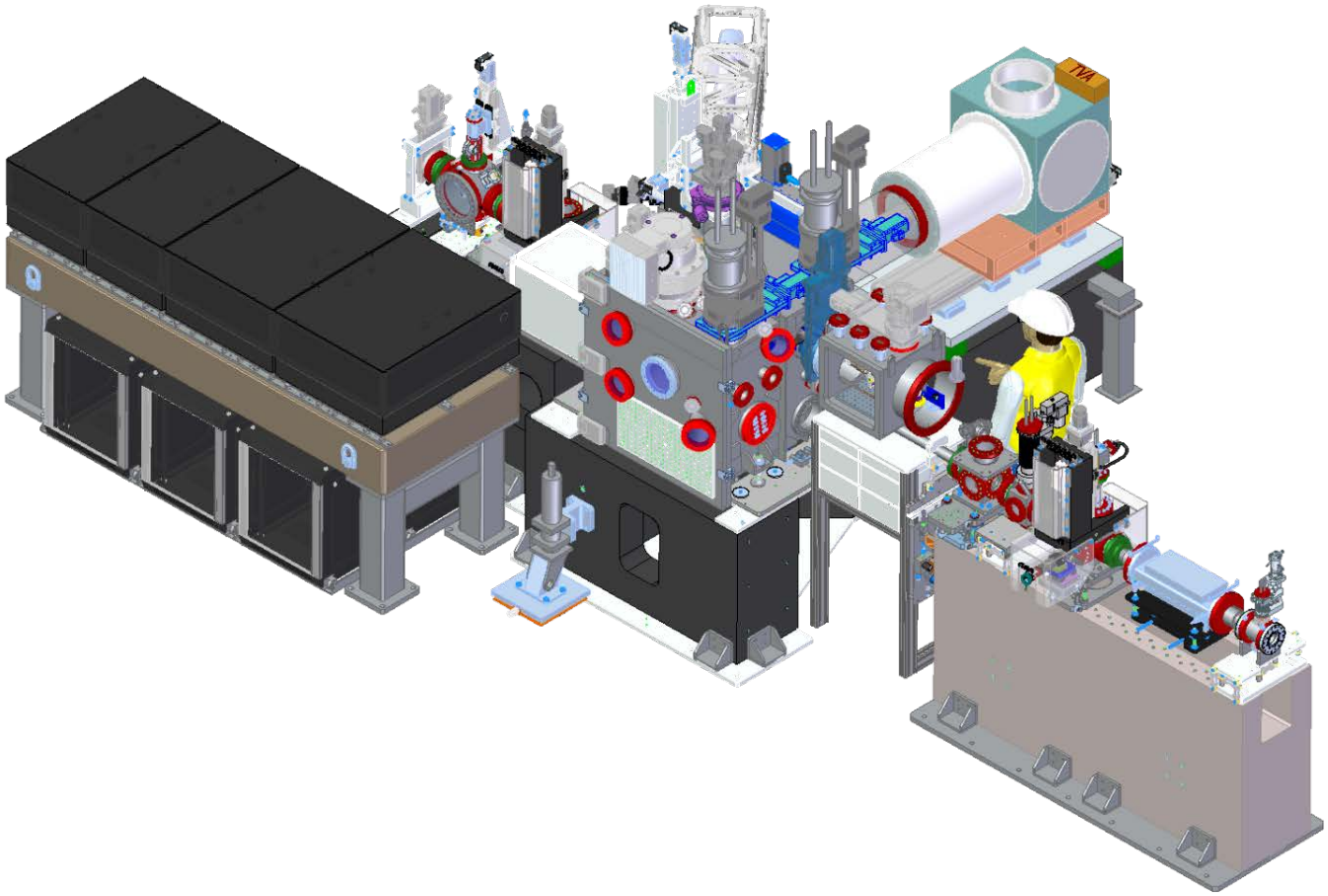
RIXS Beamline Overview

The **R**esonant **I**nelastic **X**-Ray **S**cattering instrument will initially host 2 static experimental end stations:

- qRIXS
- chemRIXS
- 3rd location for user endstation

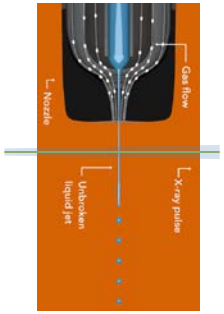


chemRIXS



chemRIXS end station

Liquid Jet

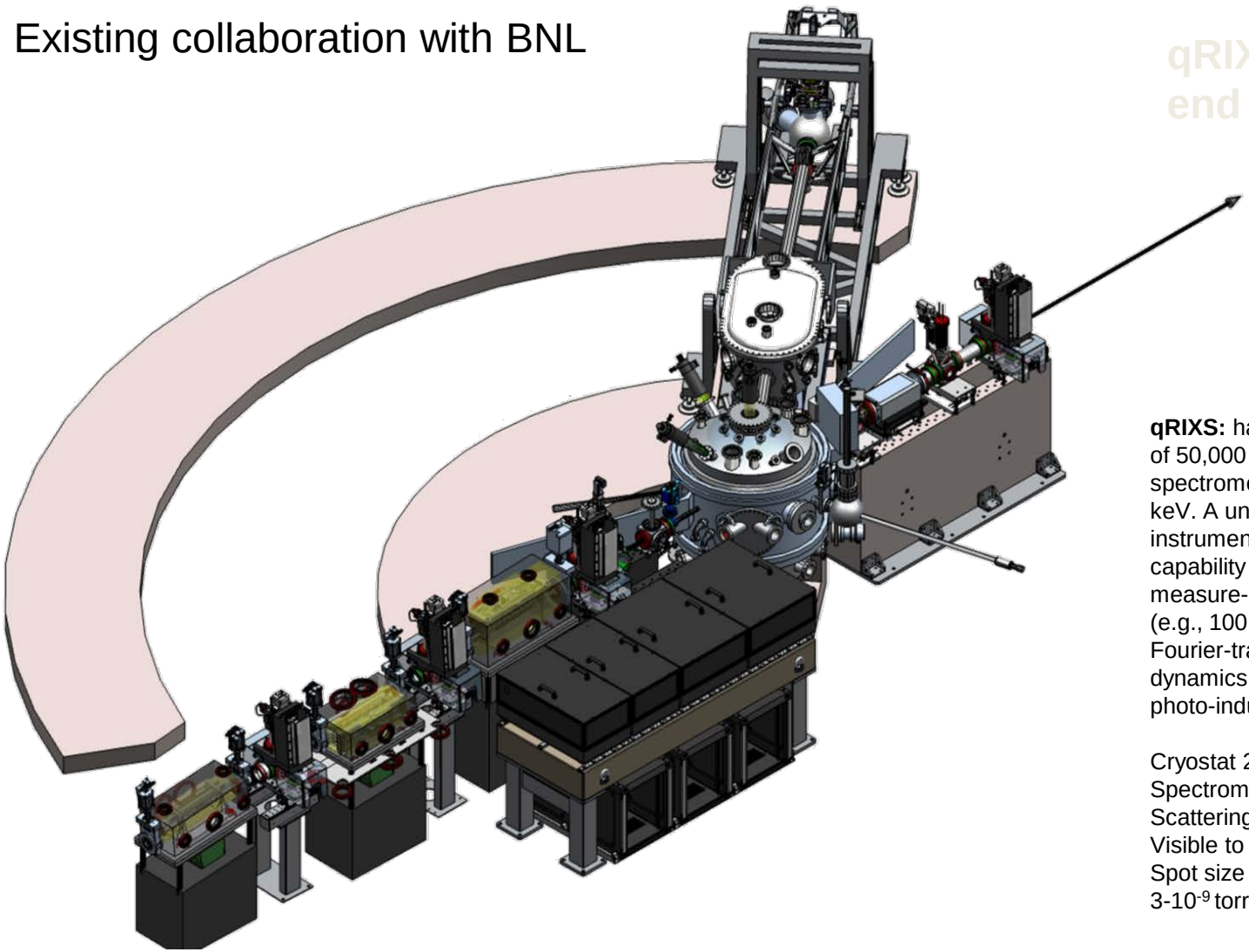


chemRIXS: designed for soft X-ray spectroscopy experiments on liquid samples, using two X-ray emission spectrometers, the Varied Line Spacing (VLS) portable spectrometer and the Transition Edge Sensor (TES) spectrometer, sub-micron focus spot size, and target purity requirements dictated by the pump-probe class of experiments.

Cylindrical / Sheet Jet
XAS / XES / RIXS
Ultra-fast time resolution
Spot size 3-1000µm
4-10^{-6} torr vacuum

qRIXS

Existing collaboration with BNL



qRIXS
end station

qRIXS: has a a target resolving power (RP) of 50,000 and a combined (beam-line + spectrometer) RP of better than 30,000 at 1 keV. A unique aspect of the RIXS instrument enabled by LCLS-II is the capability of performing time-resolved measure-ments with high energy resolution (e.g., 100 fs correspond to 18 meV at the Fourier-transform limit) to study the dynamics of these collective excitations and photo-induced non-equilibrium states.

Cryostat 20K
Spectrometer RP 50,000 / 10,000
Scattering Angle 40-150˚
Visible to THz Lasers
Spot size 3-1000µm
3-10^{-9} torr vacuum

L2S-I Timeline

FEL Source	Inst.	Commissioning	Early Science (LCLS + users)	Standard Operations (via PRP)
CuRF	XCS MFX CXI MEC XPP*	N.A.	N.A.	3/2020
CuRF	NEH 1.1 (LAMP/cVMI)	4/2020	6/2020	8/2020
CuRF	NEH 2.2 (ChemRIXS)	6/2020	8/2020	10/2020
SCRF	NEH 1.1 (LAMP/cVMI)	3/2021	6/2021	12/2021
SCRF	NEH 2.2 (ChemRIXS)	3/2021	6/2021	12/2021
SCRF	NEH 1.1 (DREAM)	3/2021	6/2021	12/2021
SCRF	NEH 2.2 (qRIXS)	1/2022	5/2022	10/2022
SCRF	NEH 1.2 (TXI)	1/2023	5/2023	10/2023

* Optical pump laser not available first few months

Tied to LCLS-II early finish

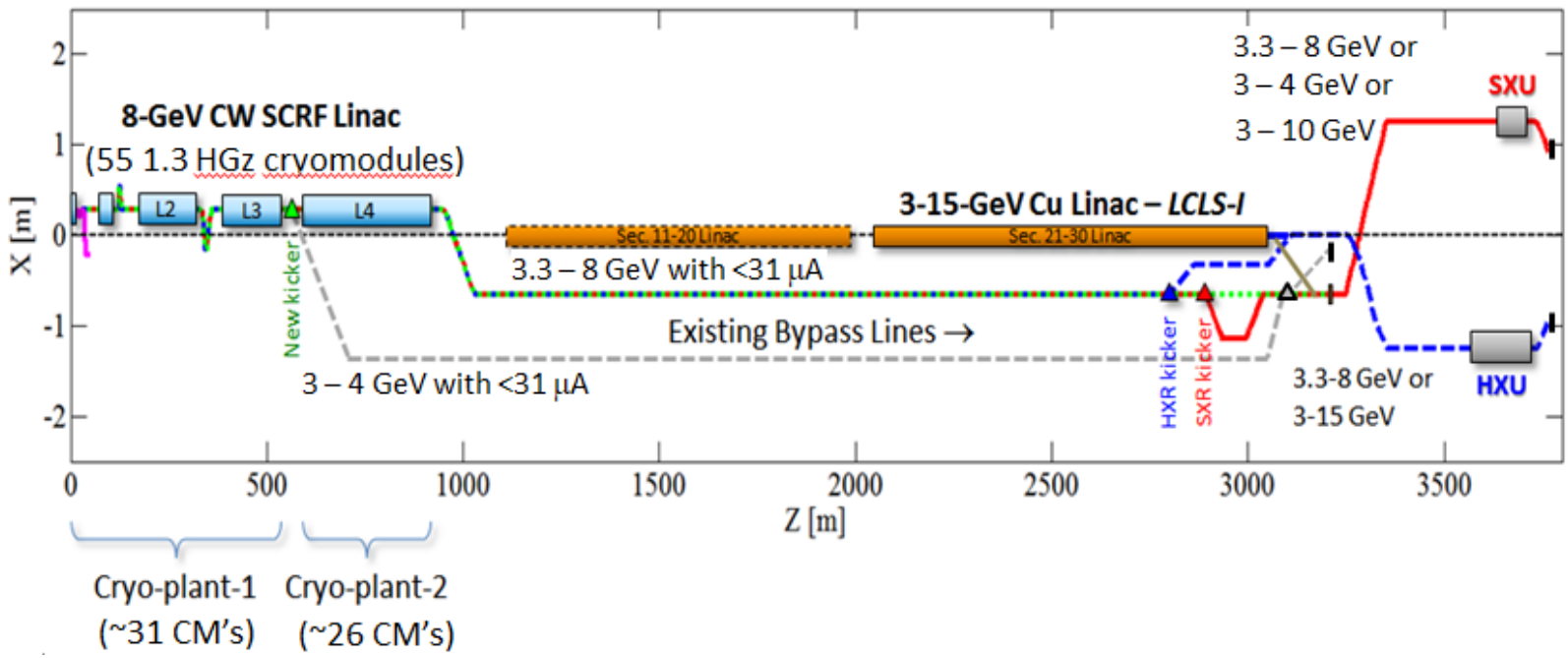
Backup

LCLS-II High Energy Upgrade
LCLS-II extension to go from 5 keV → 12.8 keV or more

Left space in the LCLS-II for additional cryomodules

→ Add 20 additional cryomodules and 2nd bypass

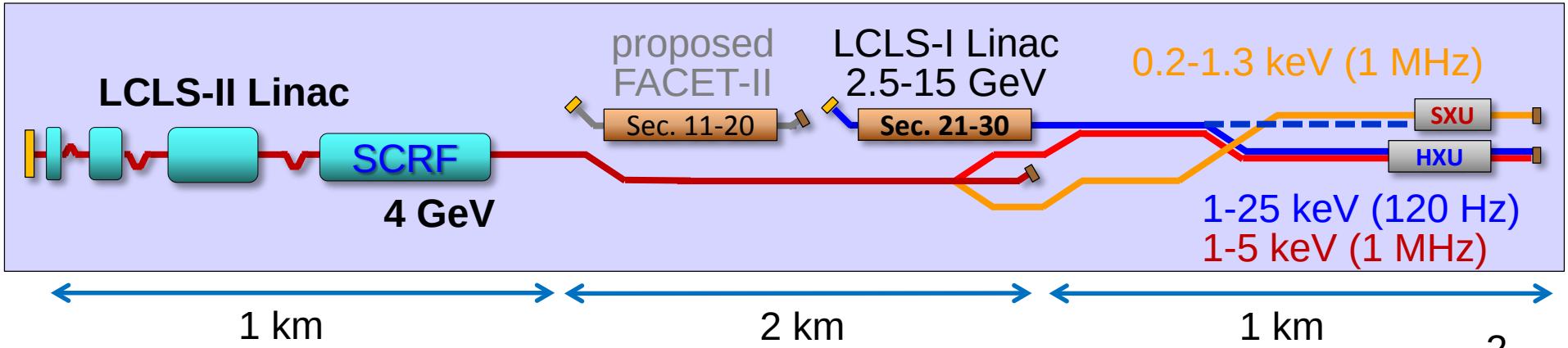
Three independent sources: CuRF 2-15 GeV, 120 Hz; LCLS-II: 3-4 GeV, 31 μA; LCLS-II-HE: 3-8 GeV, 31 μA



LCLS-II Accelerator Layout
New Superconducting Linac → LCLS Undulator Hall

- Two sources: MHz rate SCRF linac and 120 Hz Cu LCLS-I linac
- Hard and Soft X-ray undulators can operate simultaneously in any mode
- SCRF beam destination controlled with fast (μs) magnetic deflector

Undulator	SC Linac (up to 1 MHz)	Cu Linac (up to 120Hz)
Soft X-ray	0.20 - 1.3 keV with >> 20 Watts	
Hard X-ray	1.0 - 5.0 keV with > 20 Watts	1 - 25 keV with mJ-class X-ray pulses



New and upgraded instruments will address science needs and take advantage of the capabilities of LCLS-II-HE

Instr.	Upgrade Plan	Science Opportunities
XPP	New detector Upgraded diagnostics	• Understand coupled dynamics of molecular structure and charge & their role in energy flow • Characterize materials heterogeneity, fluctuations & link to function
DXS	Repetition rate enhancement IXS capability	• Map collective excitations & understand their relation to emergent phenomena in complex materials • Characterize materials heterogeneity, fluctuations & link to function
CXI	New optics & detector, Enhanced DAQ	• Reveal the role of structural dynamics in biological function • Catalysis: Reveal the correlation between chemical reactivity & structural dynamics

Key Performance Parameter
3 upgraded endstations

Objective KPP
5 upgraded endstations

LCLS-II-HE Science : Upgrade X-ray Pump-Probe (XPP)

Parameter	Value
Photon energy range	2.5-25 keV (Higher energy range with harmonics)
ΔE / E	10^{-3} (SASE), <10^{-4} with C* (111), 10^{-5} with C* (333), <10^{-6} with high resolution mono.
Repetition rate	Single pulse to >100 kHz
X-ray spot size	1-500 µm
Detector arm	1.5 m between 0 and 100º
Optical laser	100 kHz, 1 mJ, OPCPA system with wavelength conversion
Temporal resolution	0.2 – 50 fs dependent on mode of operation
Primary X-ray techniques	Time-resolved X-ray diffraction/scattering Time-resolved absorption/emission Resonant Inelastic X-ay Scattering spectroscopy

Major Modifications for LCLS-II-HE

- Upgrade diagnostics and optics to hard x-ray capabilities
- Upgrade beam sharing monochromator (cooling)
- High repetition rate detector

Science Opportunities

- Understand coupled dynamics of molecular structure and charge & their role in energy flow
- Characterize materials heterogeneity, fluctuations & link to function
- High repetition rate, versatile, atmospheric pressure instrument using mono beam, complementing tender x-ray capabilities

LCLS-II-HE Science: New Dynamic X-ray Scattering (DXS)

Parameter	Value
Photon energy range	11-19 keV (IXS) 4-22 keV (XPCS) (Higher energy range with harmonics)
ΔE / E	SASE, C* (111) or C* (333) mono < 10^{-6} with high resolution mono
Repetition rate	100 kHz to 1 MHz (IXS) Single pulse to >50 kHz (XPCS, detector limited)
X-ray spot size	1-500 µm
Detector arm	8 m between 0 and 55º
IXS energy resolution	1-10 meV (dependent on photon energy)
Optical laser	100 kHz, 1 mJ, OPCPA system with wavelength conversion
Temporal resolution	0.2 – 50 fs dependent on mode of operation
Primary X-ray techniques	Inelastic X-ray scattering X-ray photon correlation spectroscopy

Major Modifications for LCLS-II-HE

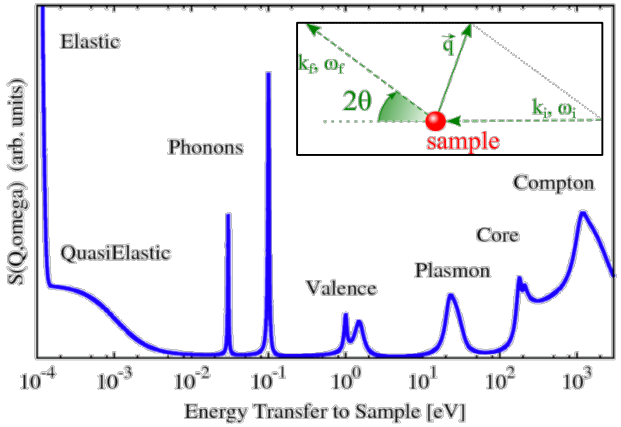
- New high resolution monochromator
- Augment detector arm with inelastic scattering spectrometer
- High repetition rate detector

Science Opportunities

- Map collective excitations & understand their relation to emergent phenomena in complex materials
- Characterize materials heterogeneity, fluctuations & link to function
- High repetition rate high resolution scattering: IXS & XPCS

LCLS-II-HE Science:
Medium-to-high resolution IXS at LCLS-II-HE

- IXS is a photon in/photon out method that is photon hungry
- Critical IXS parameter: High spectral density - # of photons per meV
- HE has unmatched performance (ph/s/meV)
- Time-resolution near the FT limit (200 fs ⇔ 10 meV)
- Lower peak power (1 MHz CW) vs. EuXFEL (~30 kHz burst mode)



	Hard X-ray Flux on Sample	
Resolution	**10 meV**	**~1 meV**
LCLS-II-HE (seeded)	**~10^{15} ph/s**	**~10^{14} ph/s**
LCLS-II-HE (SASE)	**~10^{14} ph/s**	**~10^{13} ph/s**
ESRF	~10^{11} ph/s	~10^{10} ph/s (ID28)
Spring-8	~10^{11} ph/s	~10^{10} ph/s
APS	~10^{11} ph/s	~10^{10} ph/s ~10^{9} ph/s (UHRIXS)
NSLS-II		~10^{10} ph/s

The spectral density of LCLS-II-HE offers the opportunity to significantly impact/improve IXS measurements.

LCLS-II-HE Science: Upgrade CXI Microfocus

Parameter	Value
Photon energy range	4-16 keV
ΔE / E	Source driven
Repetition rate	Single shot to >100 kHz (Detector or Sample Delivery Limited)
X-ray spot size	1 µm
Scattering angle	< 60 degrees
Optical laser	>10 kHz, 6 mJ, Ti:Sapphire system with wavelength conversion
Temporal Resolution	0.2 – 50 fs dependent on mode of operation
Primary X-ray techniques	Crystallography Imaging Diffraction Scattering Emission spectroscopy Absorption Spectroscopy

Major Modifications for LCLS-II-HE

- Upgrade optics and diagnostics (cooling)
- New focusing mirrors (cooled)
- High repetition rate detector

Science Opportunities

- Reveal the role of structural dynamics in biological function
- Catalysis: Reveal the correlation between chemical reactivity & structural dynamics
- High x-ray peak power capabilities, non-linear x-ray physics
- Versatile in-vacuum and in-air instruments optimized for high x-ray power density

1.04 Scope Summary Table

1.04.02		XPP	DXS	CXI	MFX	MEC	TOTAL
Beamline Systems	Arrival Time Monitor	1	1	1			3
	Attenuators		1	2			3
	Diamond Window		1	2			3
	Fluorescence Intensity Monitor			2			2
	Intensity-Position Monitor	3	5	3			11
	Laser In-coupling		1	1			2
	Pre-focusing lenses		1				1
	Profile Monitor		4	3			7
	Power Slits		1	1			2
	Photon Terminator	1	1	1			3
	PPS Collimator		6	3	3	3	15
	PPS Stopper		1	2	1	1	5
	Transfocator		1				1
	Wavefront Sensor	1	1	2			4

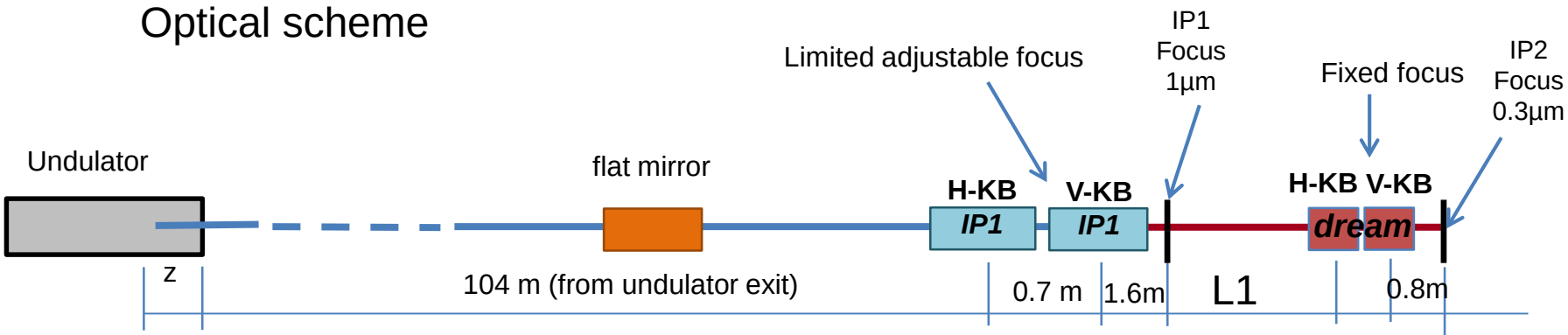
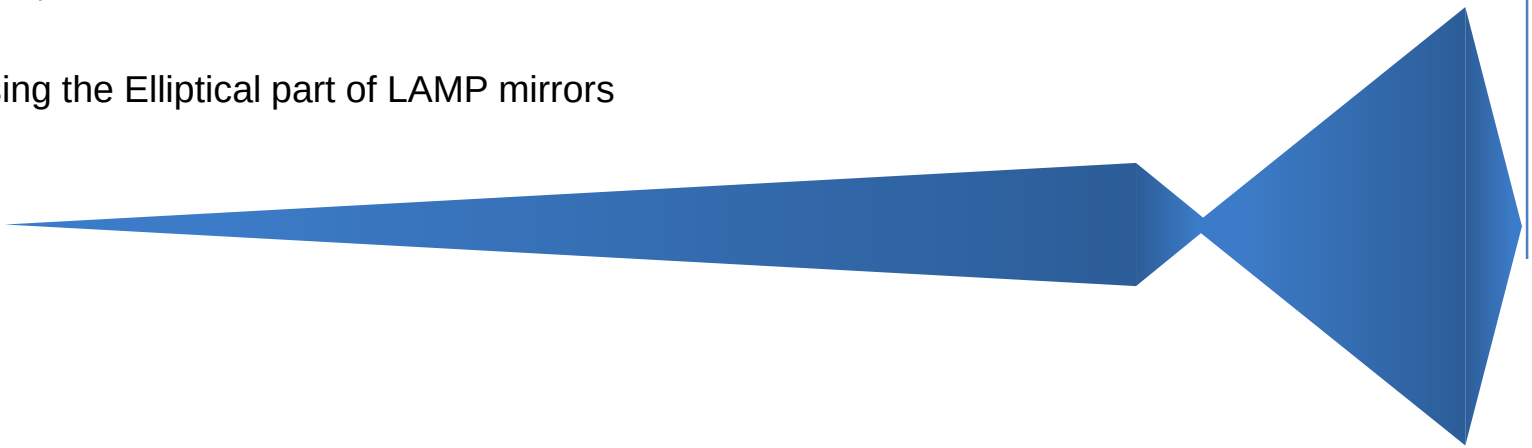
1.04.03		XPP	DXS	CXI	TOTAL
Experimental Systems	Detector: Imaging (2 MPixels)	1		1	2
	Detector: IXS		1		1
	Detector: XPCS				
	DXS Detector Robot		1		1
	DXS High Resolution Mono		1		1
	DXS IXS Spectrometer		1		1
	KB Mirrors			1	1
	Laser Conversion		1		1
	Laser Infrastructure		1		1
	Laser System		1		1
	Laser Transport		1		1
	LODCM	1			1

1.04.04		XPP	DXS	CXI	TOTAL
Data Systems	Data Acquisition		1	1	2
	Data Analysis		1	1	2
	Data Reduction Pipeline		1		1

- 1.04 Scope is defined by these device counts / deliverables
- CDR described a broad spectrum of options
  - Downselection to meet design-to-cost

Optical layout – 2 x KB Mirrors sets

Optical scheme



Using the Elliptical part of LAMP mirrors