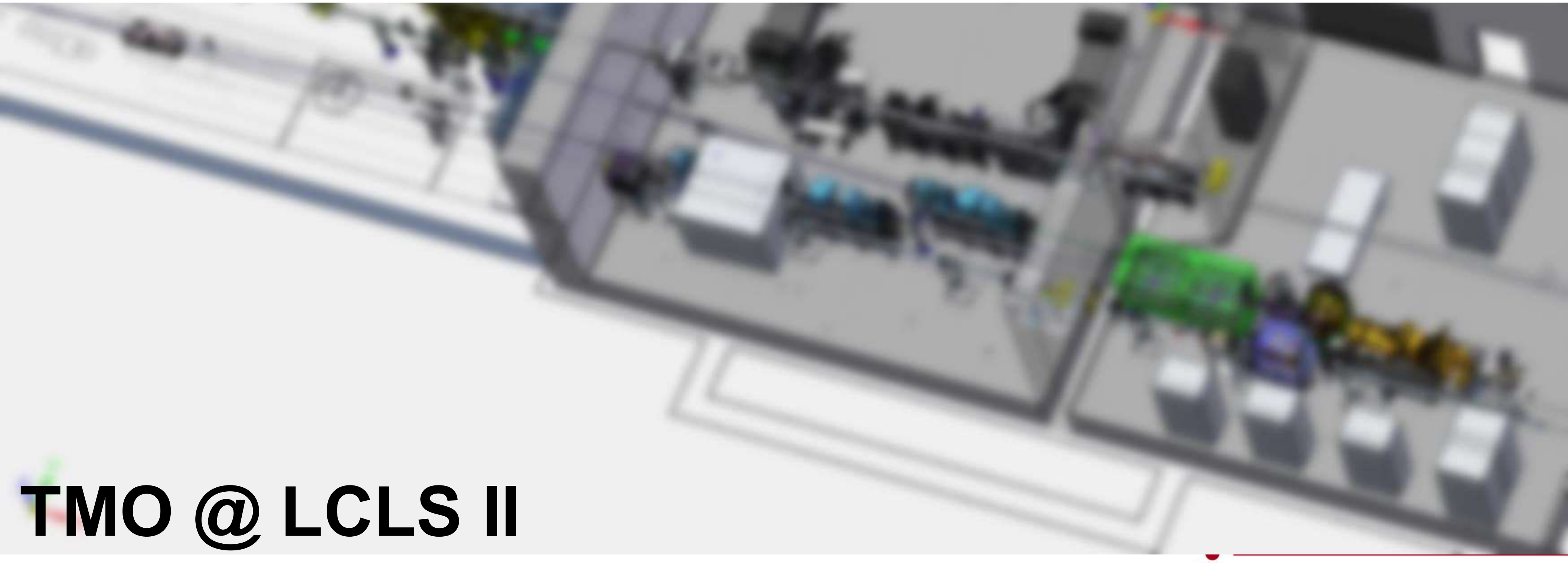


TMO @ LCLS II

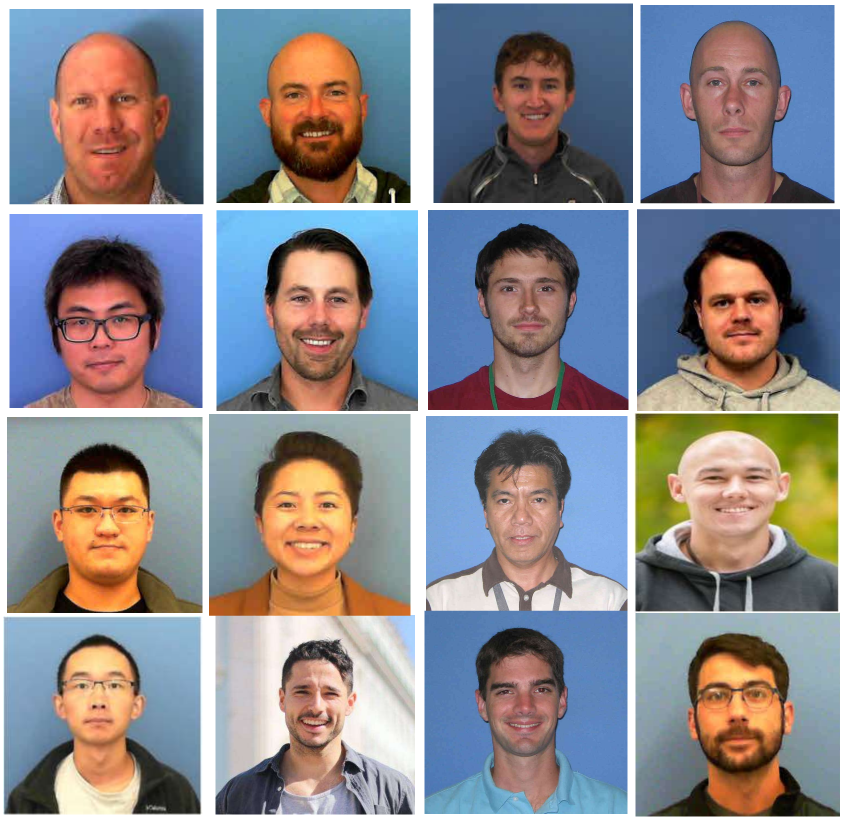
Overview, Capabilities & Plans for TMO

Peter Walter

Non-Linear Multidimensional Methodologies for Studying
Chemical Sciences

Acknowledgement

The AMO / TMO Team:



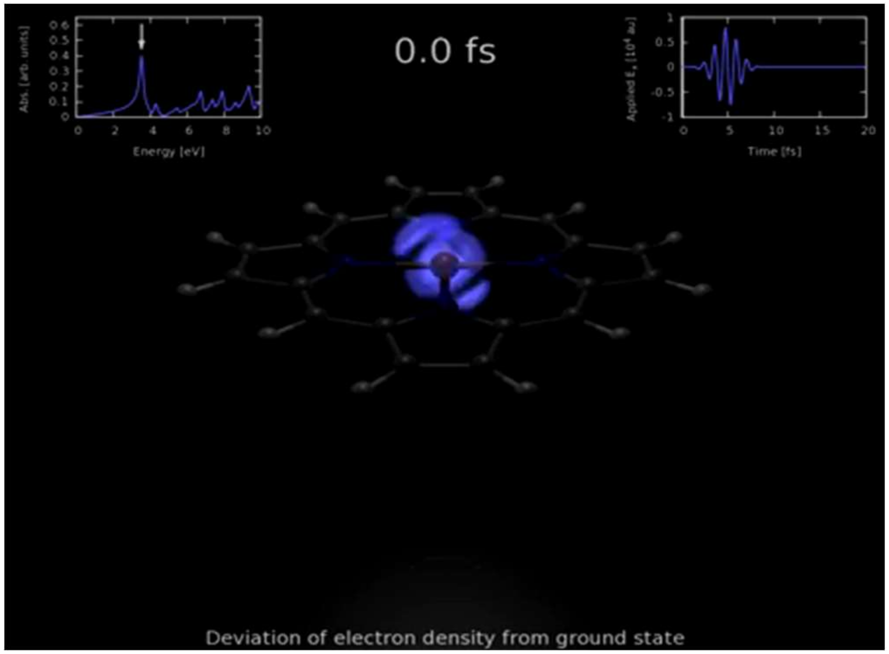
Jean-Charles Castagna, Timur Osipov, Michael Holms, Lope Amores, Niranjan Shivaram, Averell Gatton, Dileep Kumar, Xianchao Cheng, Hongliang Shi, Daniel Morton, Corey Hardin, Daniele Cocco, Matthew Church, Matthew Seaberg, Ed Newman, Jing Yin, Alan Pai, Alex Wallace, Nolan Brown, Jackson Sheppard, Yunus Sameen, Kayla Ninh, Lin Zhang, Hengzi Wang, Ian Evans, Jana Thayer, Christopher O’Grady, Clemens Weniger, Kingston Chan, Kai LaFortune, Joseph Robinson, David Fritz, Alan Conder.

Advisory Panel:

Christoph Bostedt - PSI, ETH Zurich
Reinhard Dörner - Frankfurt
Gilles Doumy – Argonne
Oliver Gessner - LBNL - CSD
Markus Guehr - U. Potsdam
Daniel Rolles - KSU
Thorsten Weber - LBNL - CSD
Nora Berrah - U. Conn
Adrian Cavalieri - PSI
Jon Marangos - ICL
Artem Rudenko - KSU

TMO Science Motivation, SLAC

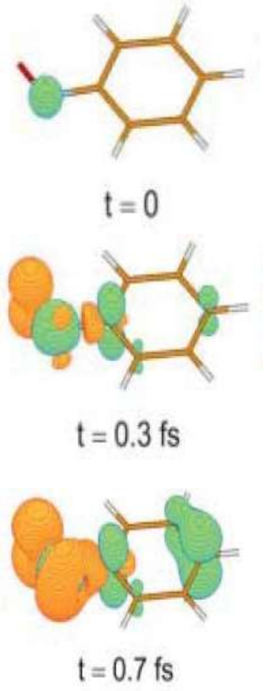
"From attosecond charge migration involving electronic dynamics and correlation to femtosecond charge transfer involving nuclear rearrangement"



Attosecond Electron Dynamics

- Electron motion is responsible for all chemistry
- Our goal is to track the evolution of electrons on their natural time scales
- We want to determine what role attosecond scale electronic coherence has on longer timescale, femtosecond motion (Chemistry).

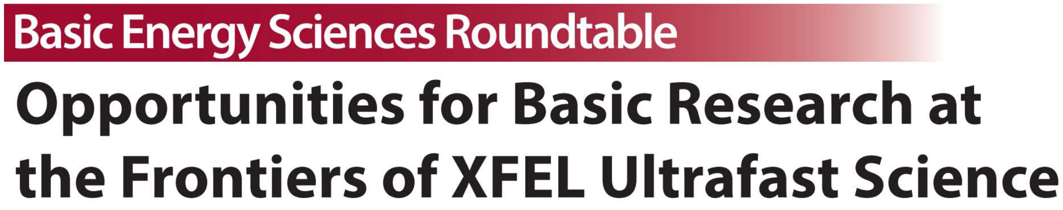
Environmental Molecular Sciences Laboratory (EMSL) @ PNNL: https://www.youtube.com/watch?v=ZYsktRlhMOg
J. Chem. Theory Comput. **7**, 1344–1355 (2011)



Kuleff at al. 2016

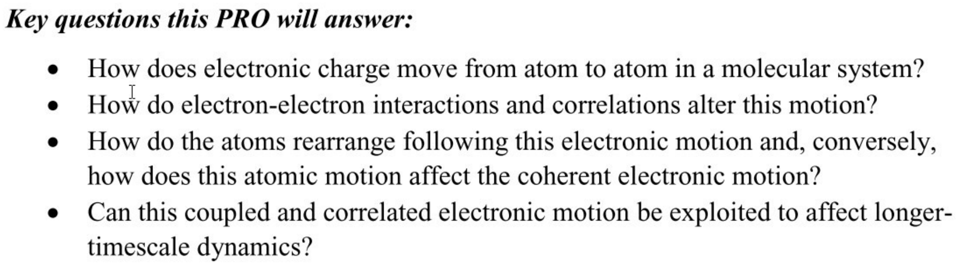
Important for all photo-induced processes in chemistry and biology like energy conversion and storage, but also photosynthesis, metabolism, oxidation, reduction and light driven charge transfer and charge injection in materials

AMO Science Motivation, Community



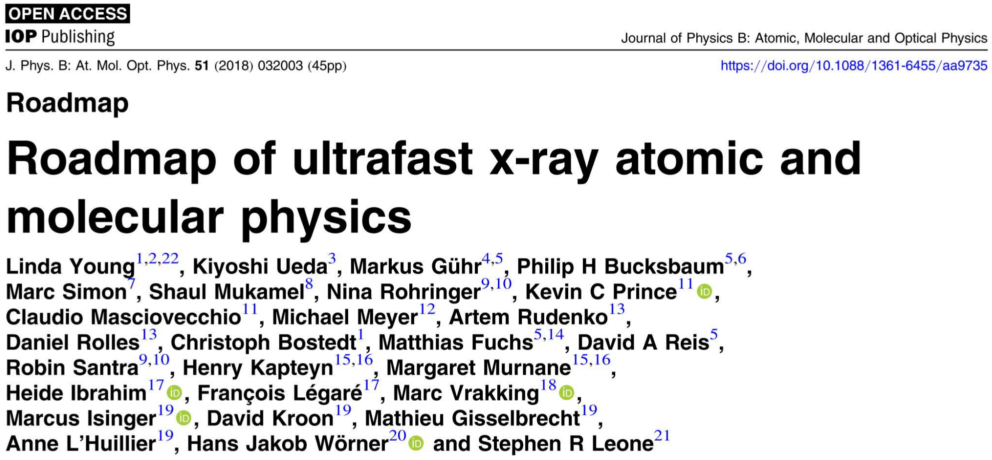
Basic Energy Sciences Roundtable

Opportunities for Basic Research at the Frontiers of XFEL Ultrafast Science



Key questions this PRO will answer:

- How does electronic charge move from atom to atom in a molecular system?
- How do electron-electron interactions and correlations alter this motion?
- How do the atoms rearrange following this electronic motion and, conversely, how does this atomic motion affect the coherent electronic motion?
- Can this coupled and correlated electronic motion be exploited to affect longer-timescale dynamics?



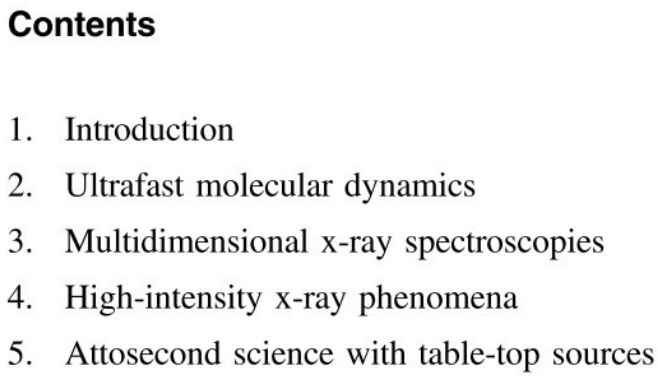
OPEN ACCESS
IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. **51** (2018) 032003 (45pp) https://doi.org/10.1088/1361-6455/aa9735

Roadmap

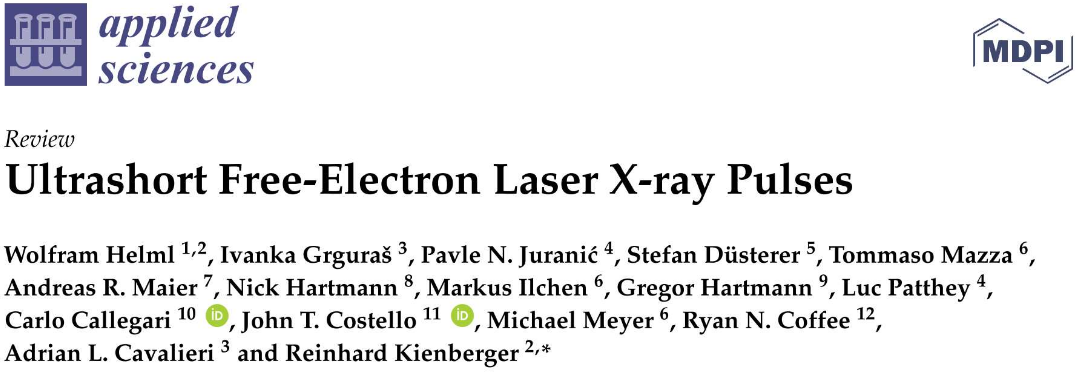
Roadmap of ultrafast x-ray atomic and molecular physics

Linda Young[1,2,22], Kiyoshi Ueda[3], Markus Gühr[4,5], Philip H Bucksbaum[5,6], Marc Simon[7], Shaul Mukamel[8], Nina Rohringer[9,10], Kevin C Prince[11], Claudio Masciovecchio[11], Michael Meyer[12], Artem Rudenko[13], Daniel Rolles[13], Christoph Bostedt[1], Matthias Fuchs[5,14], David A Reis[5], Robin Santra[9,10], Henry Kapteyn[15,16], Margaret Murnane[15,16], Heide Ibrahim[17], François Légaré[17], Marc Vrakking[18], Marcus Isinger[19], David Kroon[19], Mathieu Gisselbrecht[19], Anne L'Huillier[19], Hans Jakob Wörner[20] and Stephen R Leone[21]



Contents

1. Introduction
2. Ultrafast molecular dynamics
3. Multidimensional x-ray spectroscopies
4. High-intensity x-ray phenomena
5. Attosecond science with table-top sources



applied sciences MDPI

Review

Ultrashort Free-Electron Laser X-ray Pulses

Wolfram Helml [1,2], Ivanka Grguraš [3], Pavle N. Juranić [4], Stefan Düsterer [5], Tommaso Mazza [6], Andreas R. Maier [7], Nick Hartmann [8], Markus Ilchen [6], Gregor Hartmann [9], Luc Patthey [4], Carlo Callegari [10], John T. Costello [11], Michael Meyer [6], Ryan N. Coffee [12], Adrian L. Cavalieri [3] and Reinhard Kienberger [2,*]

Development of ultrafast capabilities for X-ray free-electron lasers at the linac coherent light source

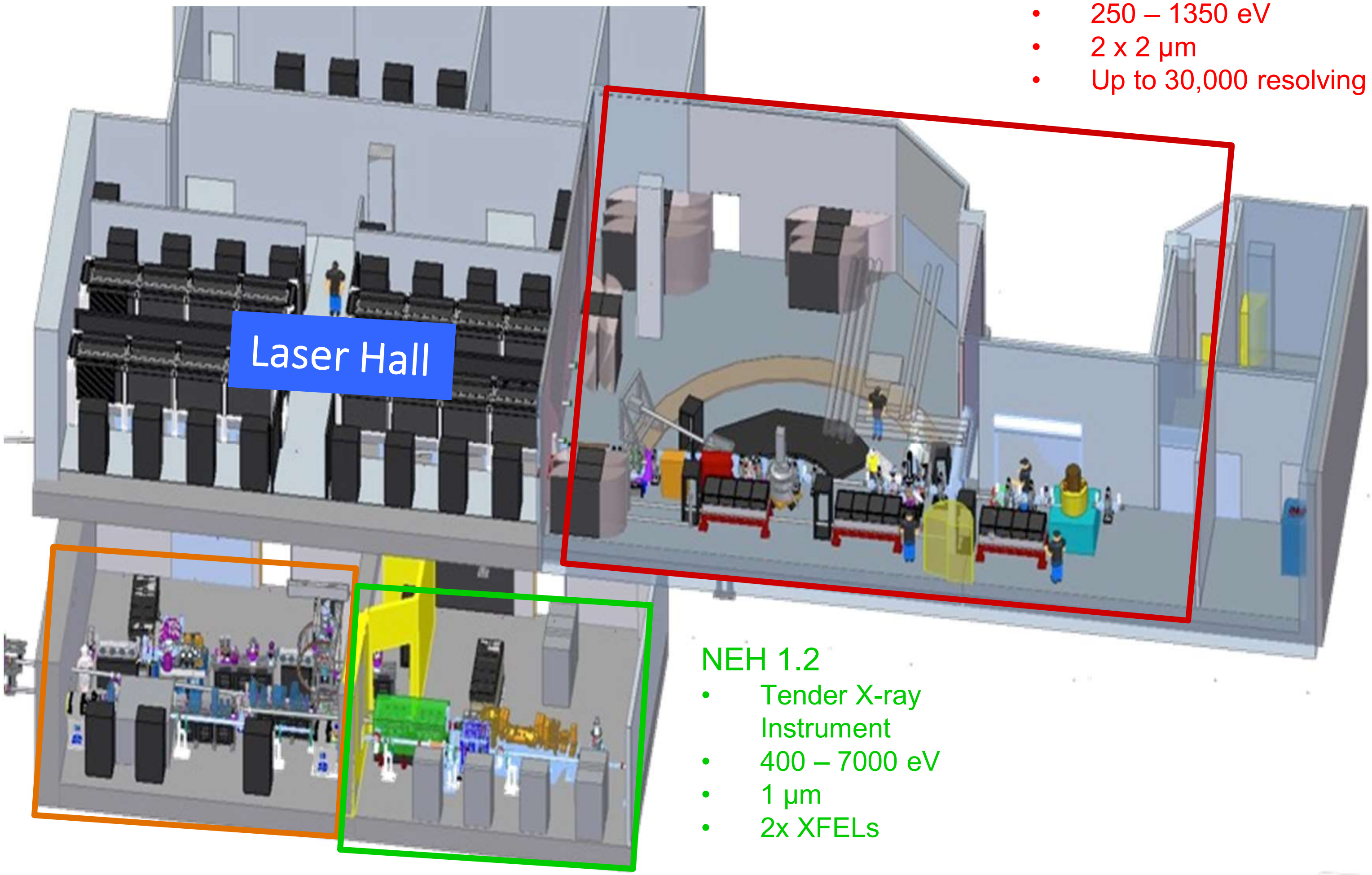
PHILOSOPHICAL TRANSACTIONS A

Ryan N. Coffee[1,2], James P. Cryan[1,2], Joseph Duris[3], Wolfram Helml[4,5], Siqi Li[3,6] and Agostino Marinelli[3]

L2S-I Hutches

- 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

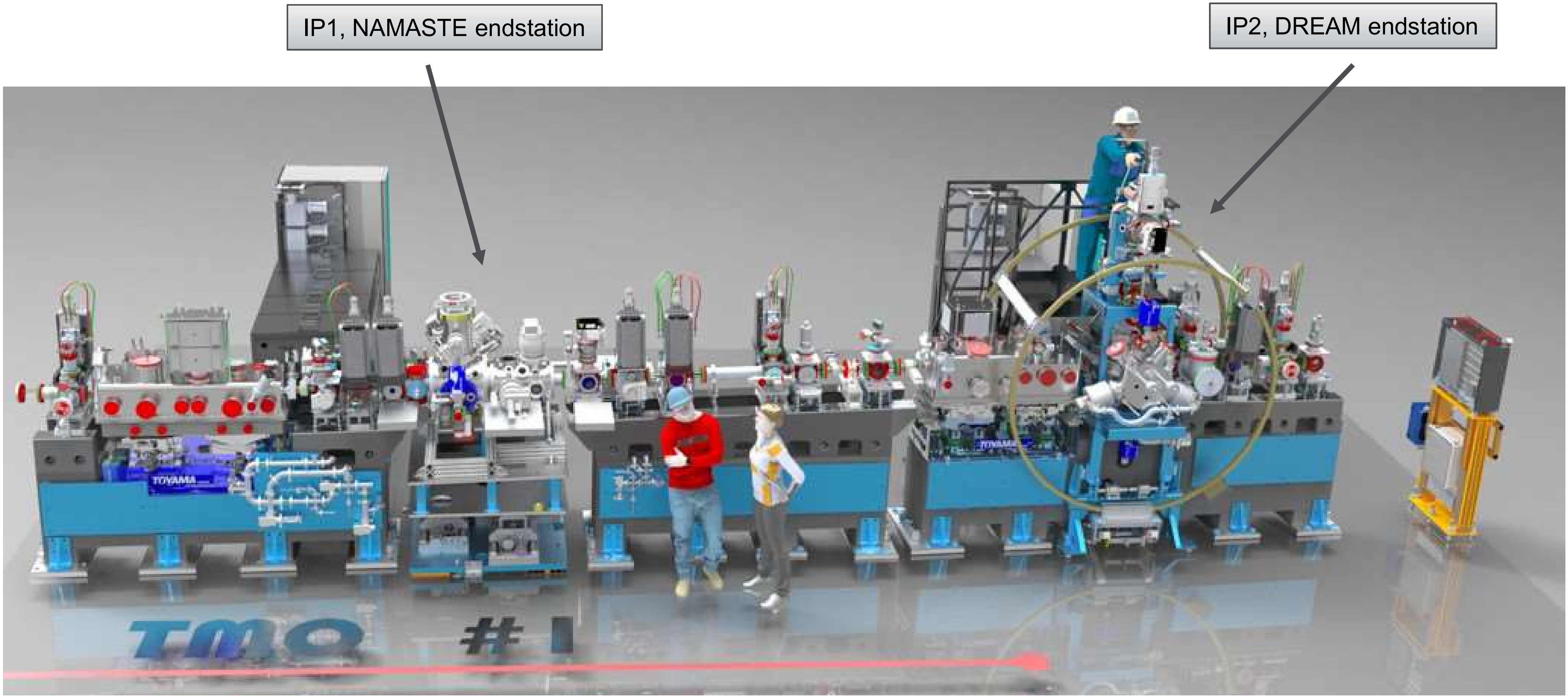


NEH 2.2
- qRIXS & chemRIXS
- 250 – 1350 eV
- 2 x 2 µm
- Up to 30,000 resolving power

NEH 1.1
- **High Flux Soft X-ray**
- **250 – 2000 eV**
- **<1 µm / <0.3 µm**
- **Minimal Optics**

NEH 1.2
- Tender X-ray Instrument
- 400 – 7000 eV
- 1 µm
- 2x XFELs

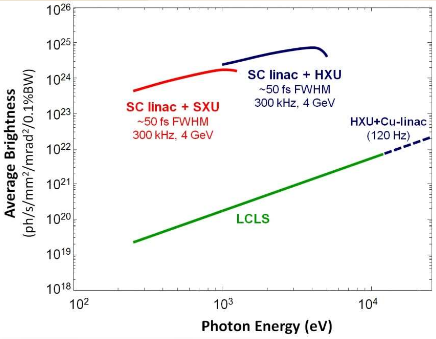
TMO, NAMASTE (IP1) and DREAM (IP2) Endstations

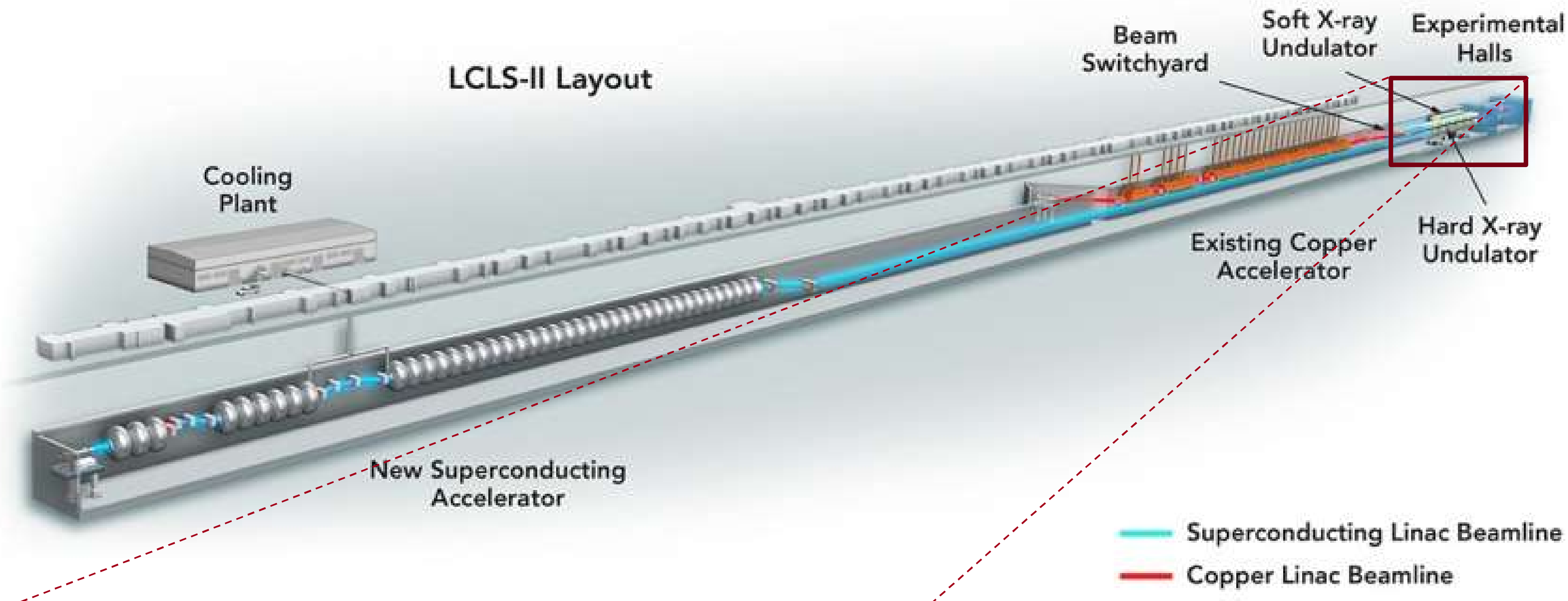

IP1, NAMASTE endstation

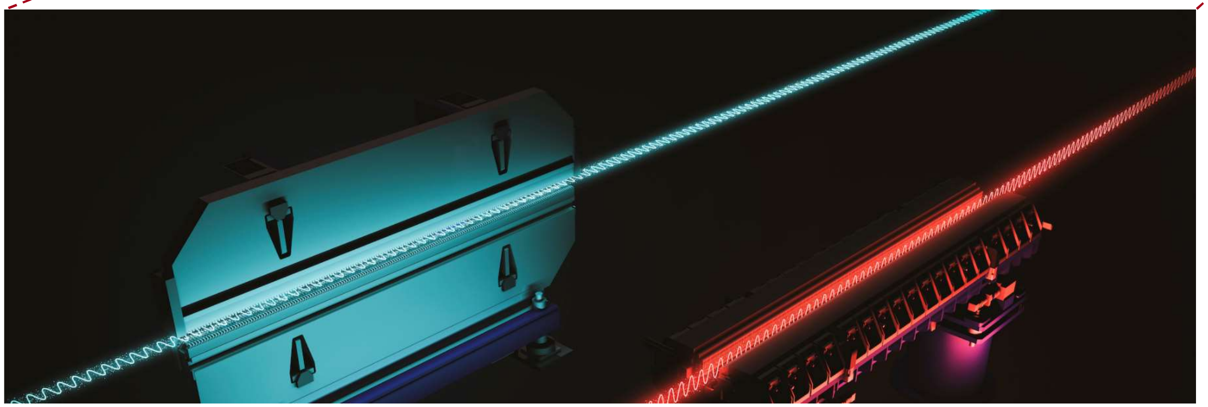
IP2, DREAM endstation

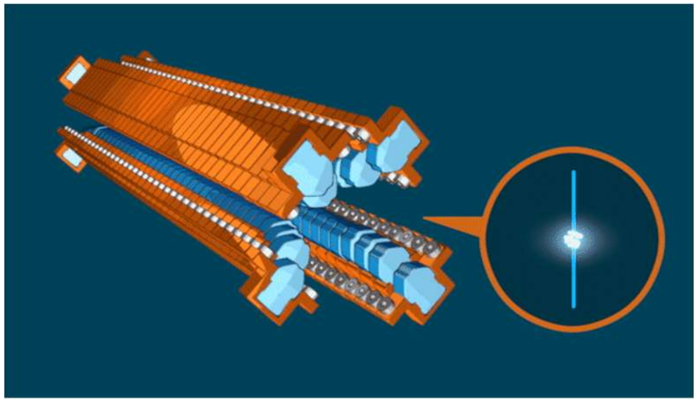
The new designed **T**ime-resolved Atomic, **M**olecular and **O**ptical Science end station (TMO), will be configured to take full advantage of both the high per pulse energy from the copper accelerator (120 Hz) as well as high average intensity and high repetition rate (1 MHz) from the superconducting accelerator. TMO will support many experimental techniques not currently available at LCLS and will locate two experimental endstations. Thereby, TMO will support AMO science, strong-field and nonlinear science and a new dynamic reaction microscope.

LCLS II LINAC CONFIGURATION



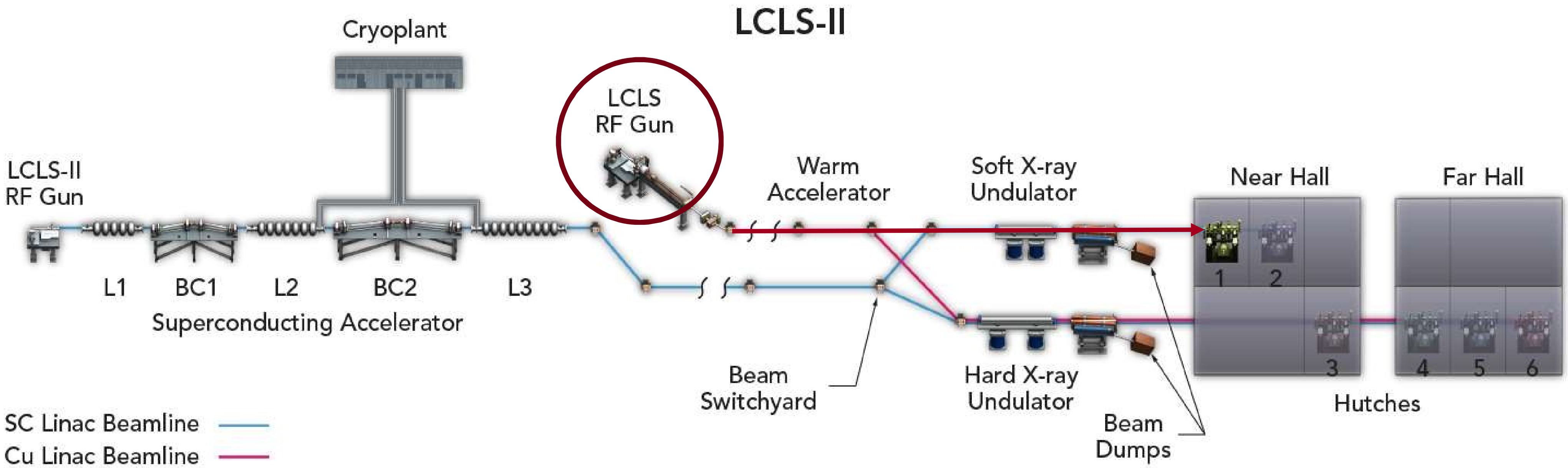






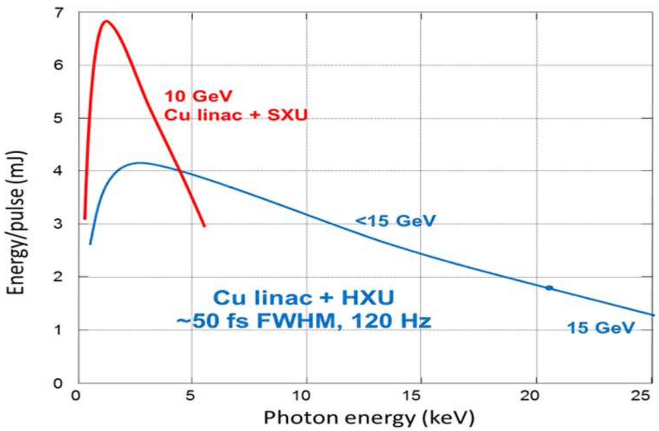
DELTA2, polarization control

CuRF + SXU

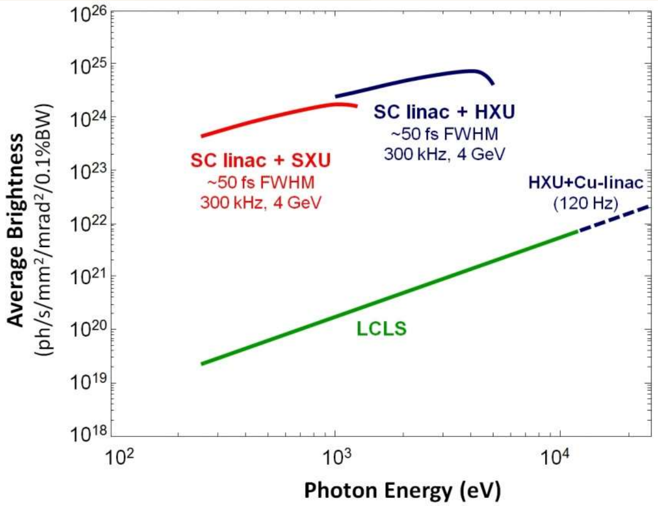


CuRF (LCLS I) + Soft X-ray Variable Gap Undulators

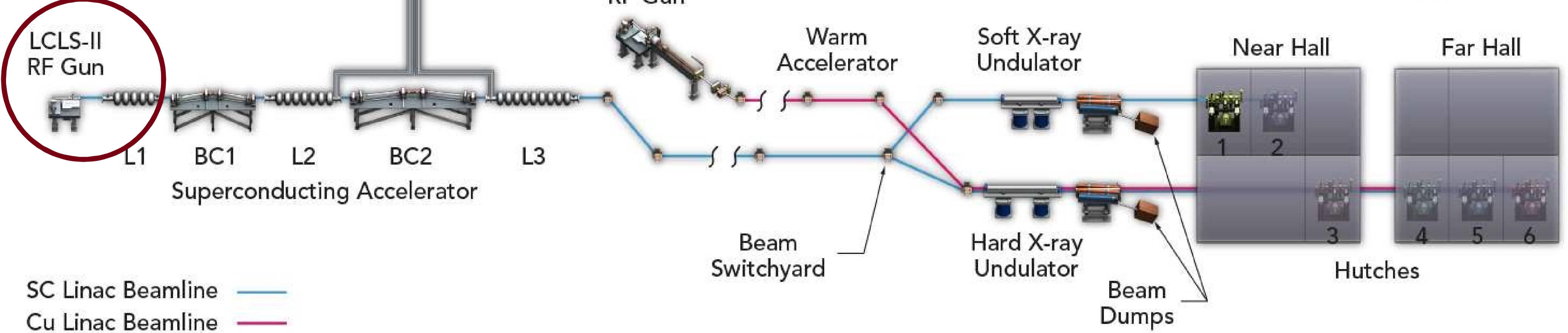
Experimental Technique with CuRF FEL source (high FEL Pulse Energy, low Rep Rate)	**FEL Pulse Duration**	**Rep Rate**	**Pulse Energy[1]**	**Average Power**	**Photon Energy Range**
NAMSTE: Strong field charged multi-hit / multi-particle spectroscopy, ARPES (TOF, VMI)	0.5 - 100 fs	120 Hz	> 5 mJ	1.5 W	250-2000 eV
DREAM: Coincidence charged particle spectroscopy	< 100fs	120 Hz	> 0.2 mJ	> 0.2 W	250-1500 eV



SCRF + SXU

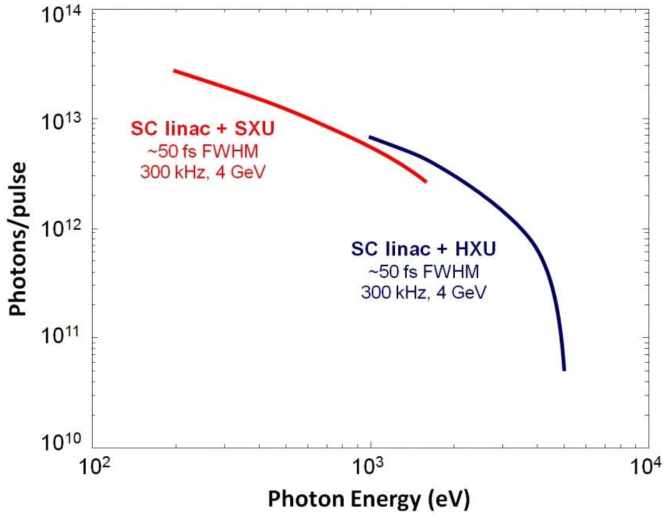


LCLS-II

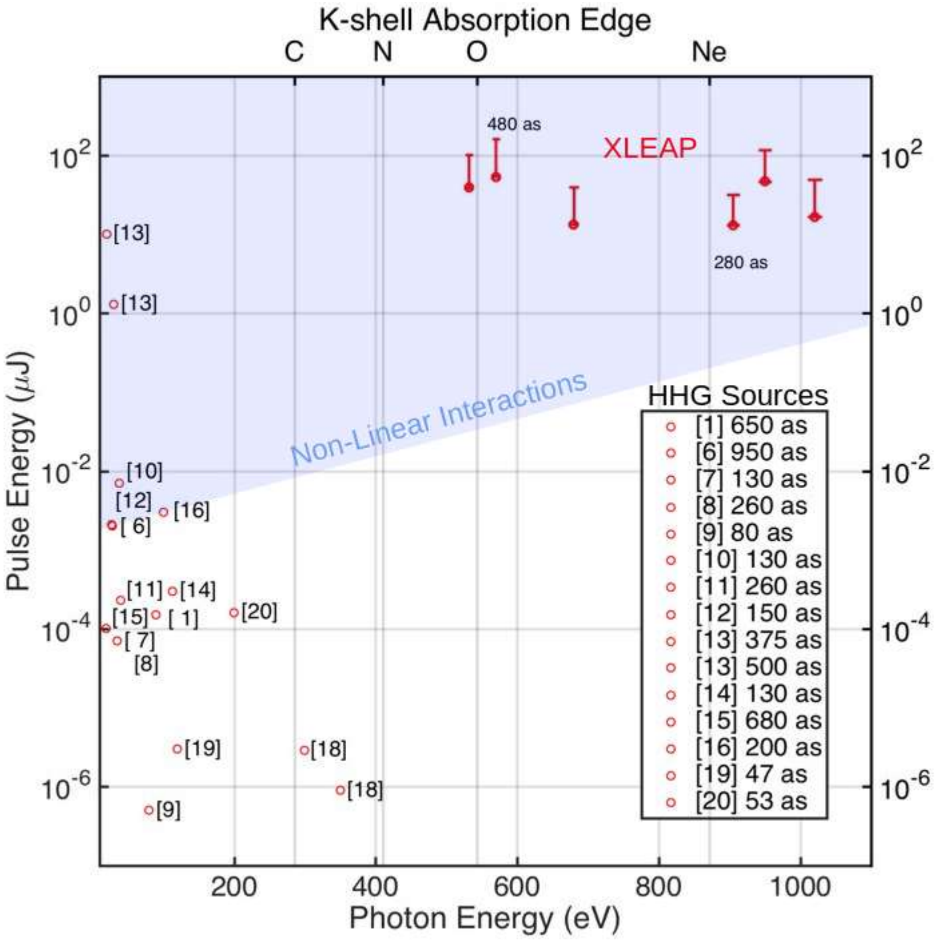


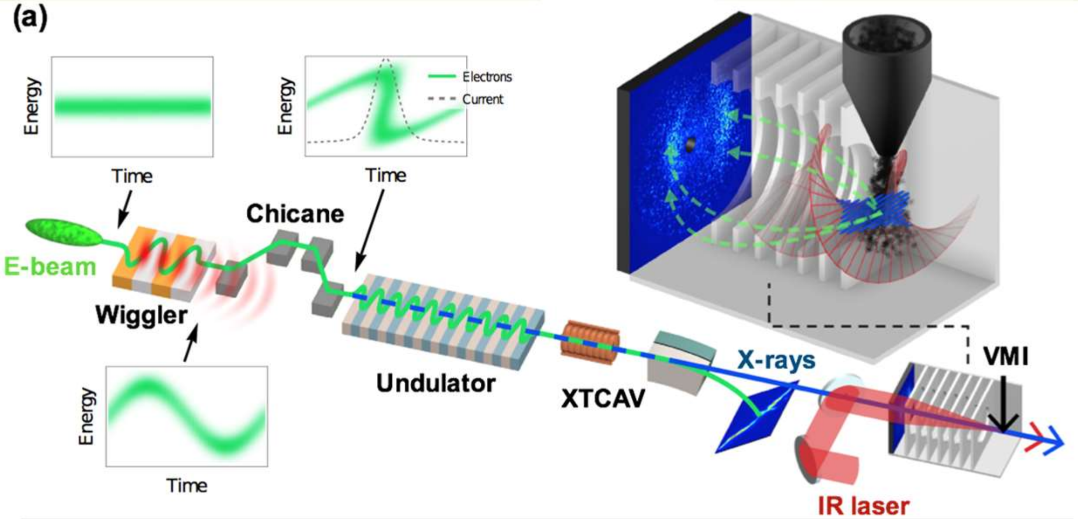
SCRF (LCLS II) + Soft X-ray Variable Gap Undulators

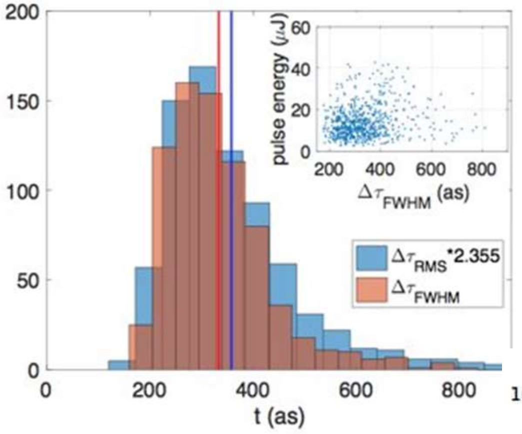
Experimental Technique with CuRF FEL source (high FEL Pulse Energy, low Rep Rate)	FEL Pulse Duration	Rep Rate	Pulse Energy[1]	Average Power	Photon Energy Range
NAMSTE: Strong field charged multi-hit / multi-particle spectroscopy, ARPES (TOF, VMI)	0.5 - 100 fs	Up to 1 MHz	0.1-2 mJ	Up to 100 W	250-2000 eV
DREAM: Coincidence charged particle spectroscopy	0.5 - 100 fs	Up to 1 MHz	1-10 μJ, <1mJ	Up to 100 W	250-1500 eV



Attosecond XFEL - A New Regime

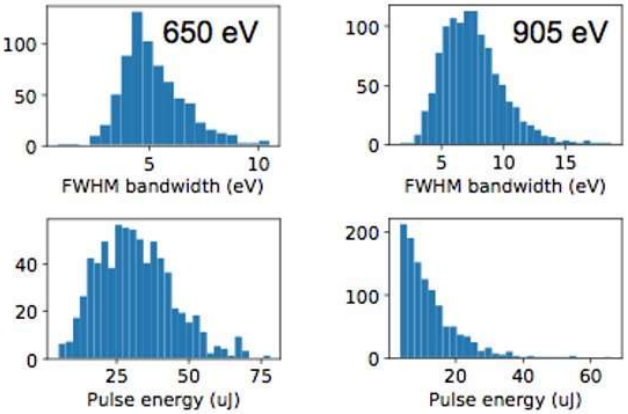






Duris *et al.* Nature Photonics accepted

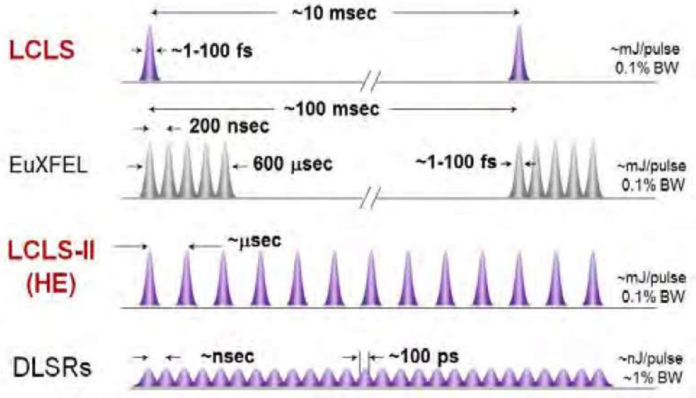
- Brightest source of sub-femtosecond SXR pulses by 6 orders of magnitude
- Enables nonlinear X-ray techniques.



Courtesy of J. Cryan

Long Term Key Requirements, TMO

Beamline Requirements
Focus spot < 1μm (HxV)
High repetition rate (>100kHz)
Sub femto second pulses to few femto second pulses
Thru Zero Delay Scans
High Intensity Pulses (>5mJ)
X-ray Energy 250 – 2000 eV
Polarization Control
Automation



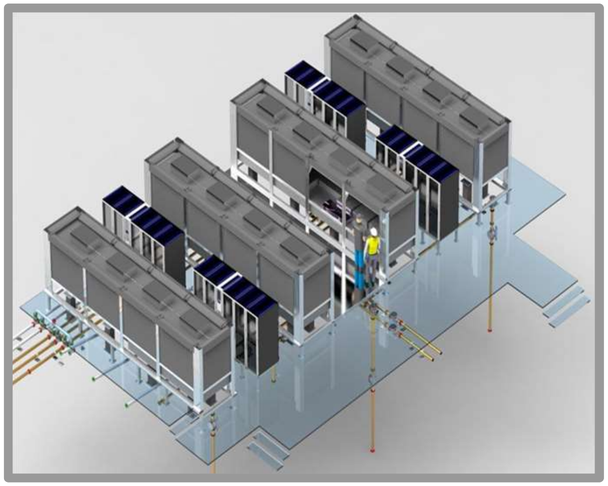
Detector/ Experiment Requirements
High resolution e^- -Detector
High resolution ion Detector
Large TOF window (>100eV)
Position and Time resolution (delay-line)
Gas phase ARPES capability

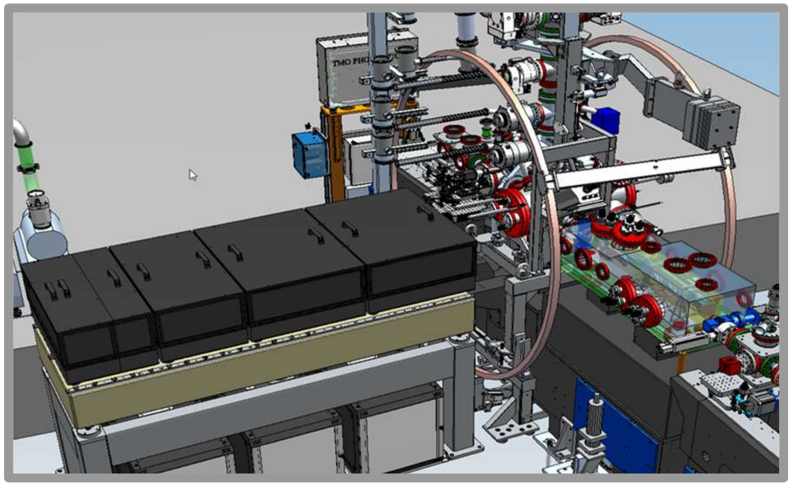
Diagnostics
Attosecond capability
Focus Optimization (WFS in-situ)
<10 fs rms timing resolution

Optical Laser, TMO

Laser specs
OPCPA
Short focus in-coupling
Colinear in-coupling
>10 mJ/cm^2 fluence
>100 kHz, <100 fs
<10 fs rms timing resolution
1-5 J/cm2, <10 fs pulses for strong-field experiments

	NAMASTE	DREAM
Turn-on date	4/2020	10/2021
Mid-IR	X	(x)
NIR	X	(x)
800	X	X
400	X	X
266	X	X
200	(x)	(x)
< 20 fs	(x)	(x)





TMO optical LASER (800 – 266)

TMO Priority: Shorter > rep rate > tuneability > pulse energy

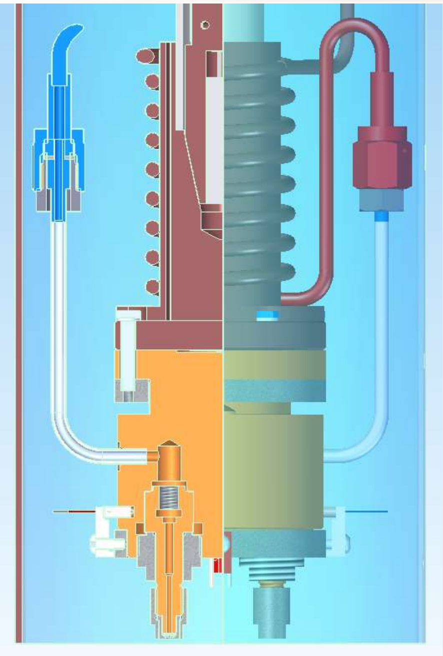
	IP1	IP2
800 nm		
duration	<20 fs	<20 fs
Energy	200 uJ [50 um]	130 uJ
Spot Size (diameter)	20-50 um	< 10 um
Intensity/Fluence	few 10^14 W/cm^2	10^15 W/cm^2
Rep. Rate (kHz)	100 kHz	100 kHz
Harmonics (400/266)		
duration	<10 fs	<10 fs
Pulse Energy	2.5 uJ (50 um dia)	0.5 uJ
Spot Size	20-50 um	< 10 um
Fluence	> 100 mJ/cm^2	500 mJ/cm^2 10^13 W/cm^2
Rep. Rate	100 kHz	100 kHz

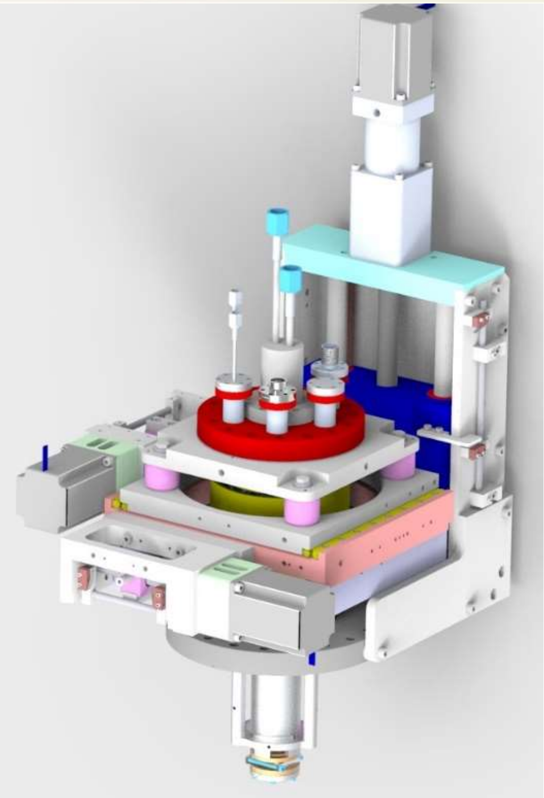
TMO optical LASER (>800 - MIR)

TMO Priority: Shorter > rep rate > tuneability > pulse energy

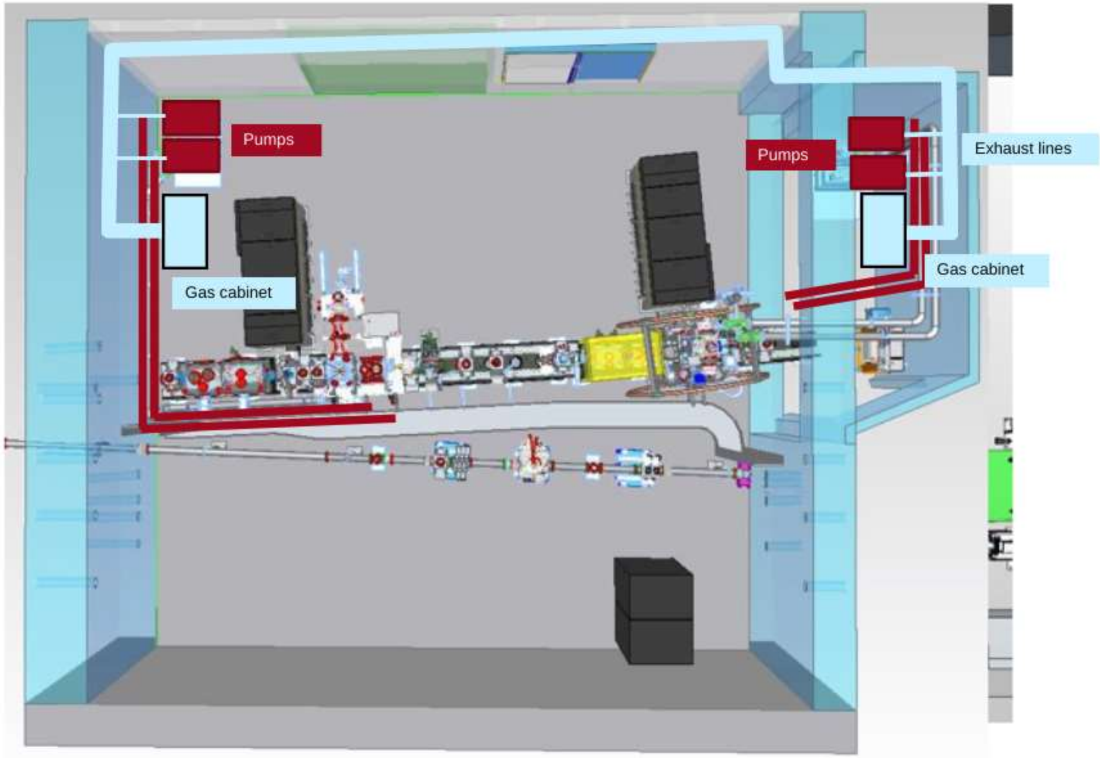
	IP1	IP2
Tunable IR (1300-2400)		
duration	<25 fs	<25 fs
Pulse Energy	140 uJ [100 um]	60 uJ
Spot Size (diameter)	20-100 um	< 50 um
Fluence	10^14 W/cm^2	10^14 W/cm^2
Rep. Rate	100 kHz	100 kHz
Tunable MIR (2400-17000)		
duration	< 100 fs	
Pulse Energy	flexible	
Spot Size	flexible	
Fluence	> 5*10^12 W/cm^2	
Rep. Rate	100 kHz	

Sample Delivery



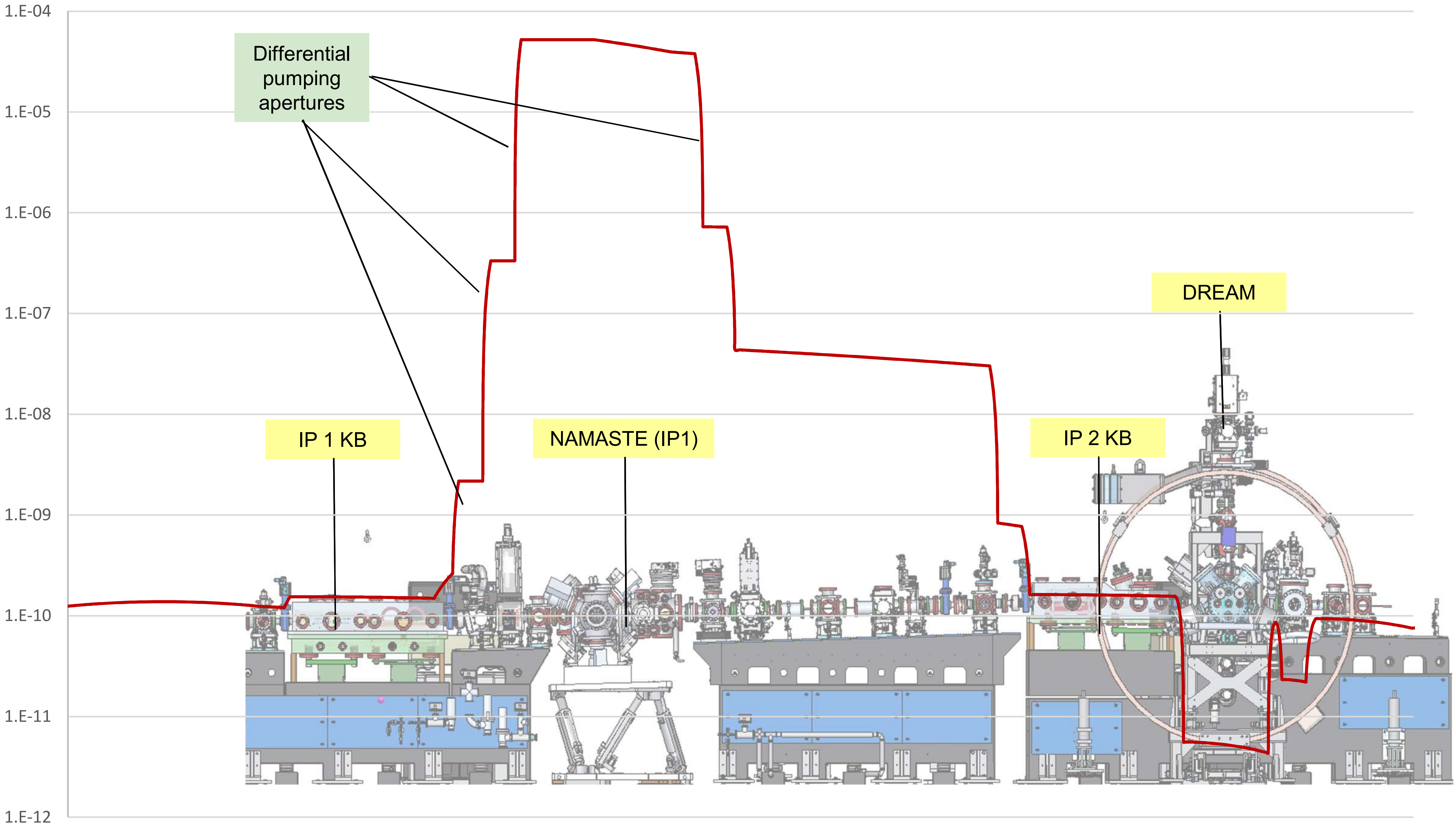


Cryo Jet Option	Parameter
Cooling	L-He and L-N2
Temperature range	5 – 650K
Nozzle	2x
Nozzle size	20-200μm (variable)

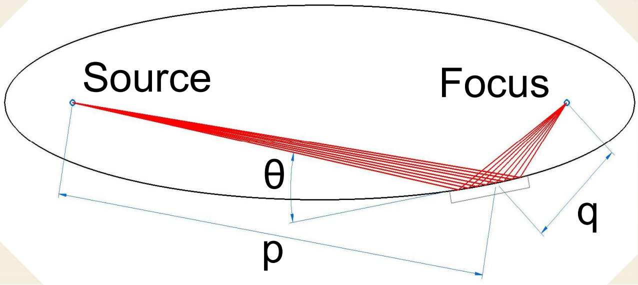


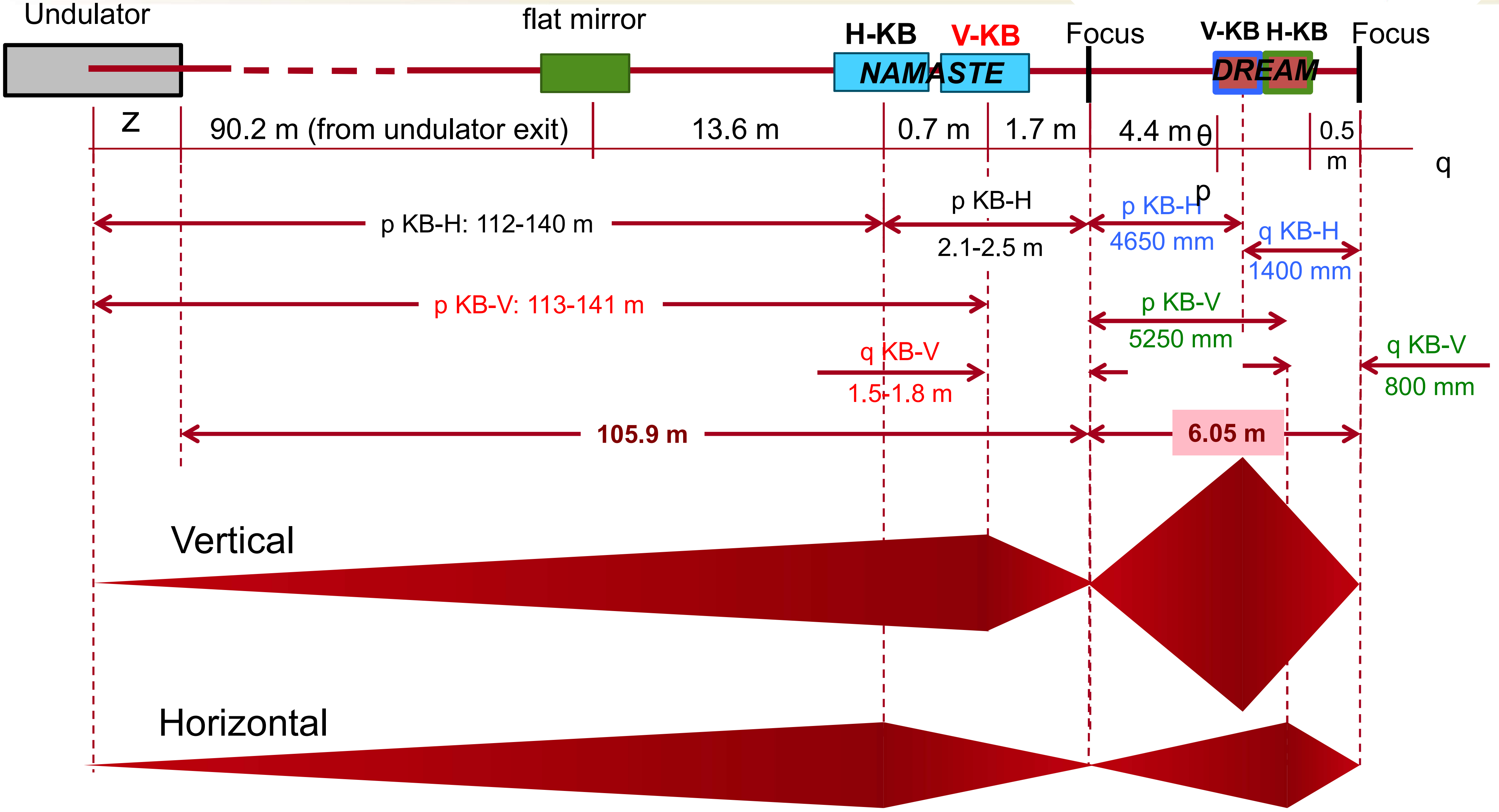
JET	Operation Mode
Cryo CW Jet	continuous
Even-Lavie	pulsed
Parker Valve	pulsed

Beamline vacuum profile NEH1.1



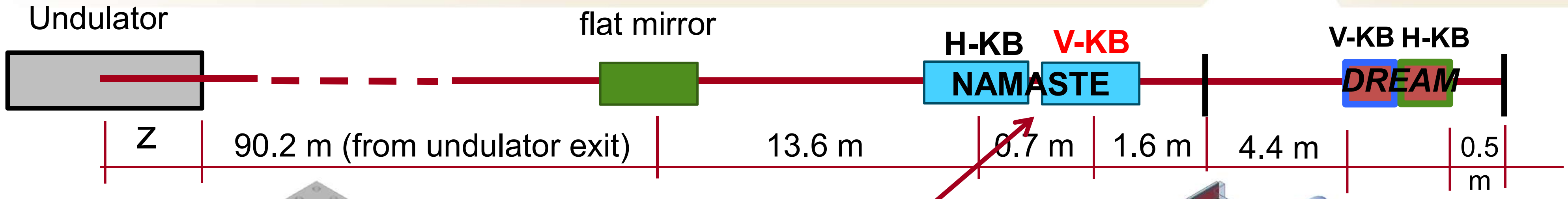
TMO Optics

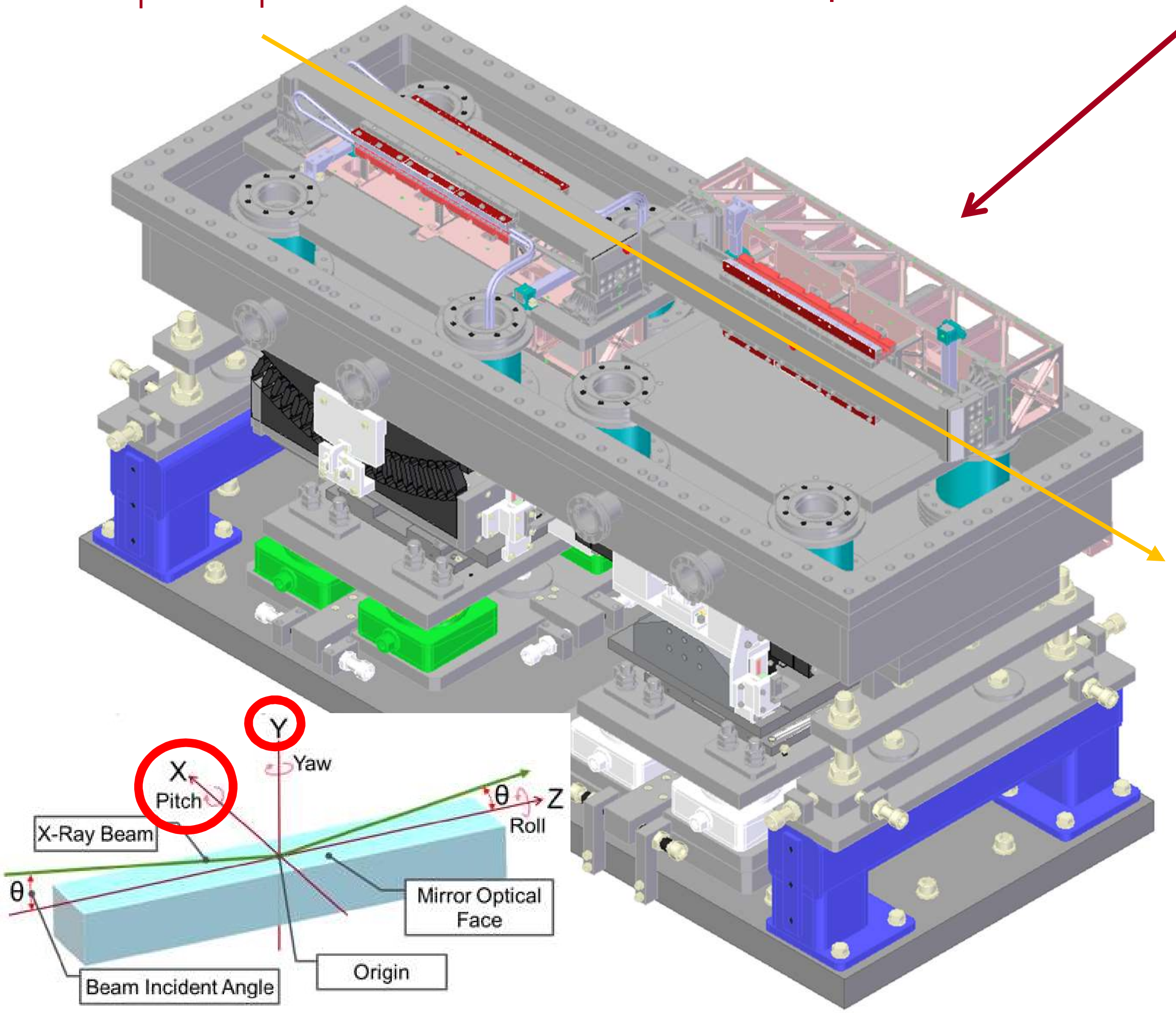


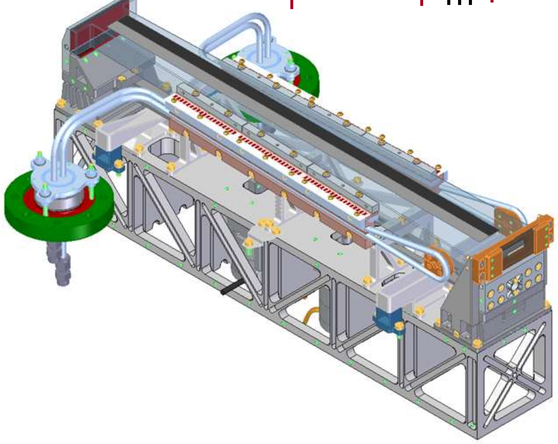


$$\text{ellipse}(p,q,\theta,x)=\frac{(p+q)(p-q)x\cos\theta+2\left(-pq+\sqrt{pq(pq-x^2-px\cos\theta+qx\cos\theta)}\right)\sin\theta}{-(p+q)^2+(p-q)^2\sin^2\theta}$$

IP 1, KB System (NAMASTE)



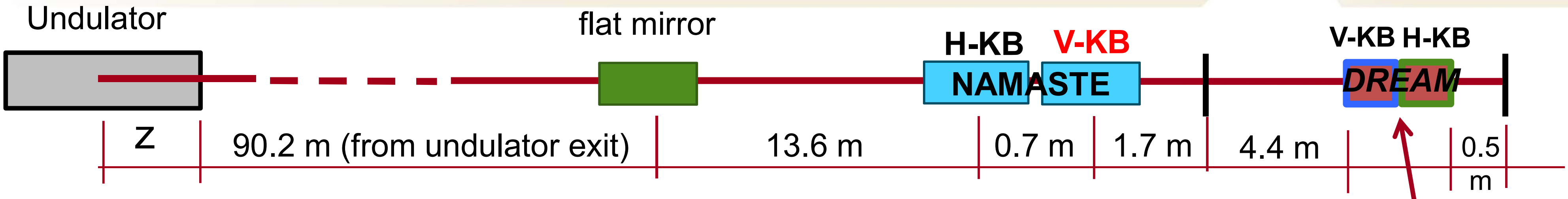


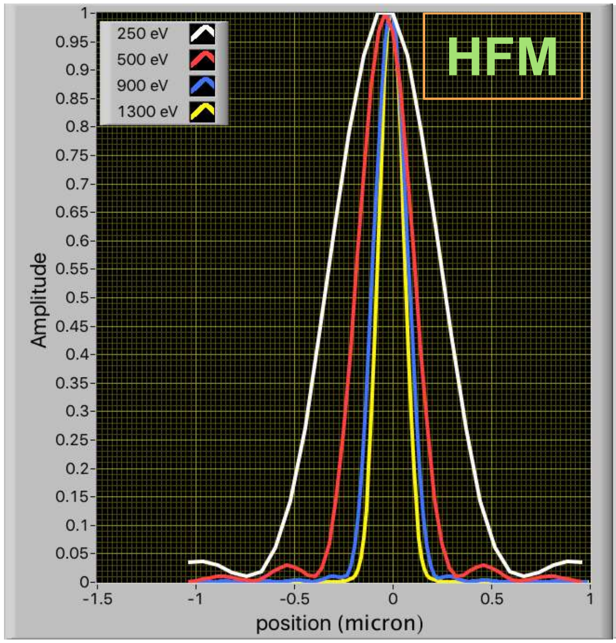


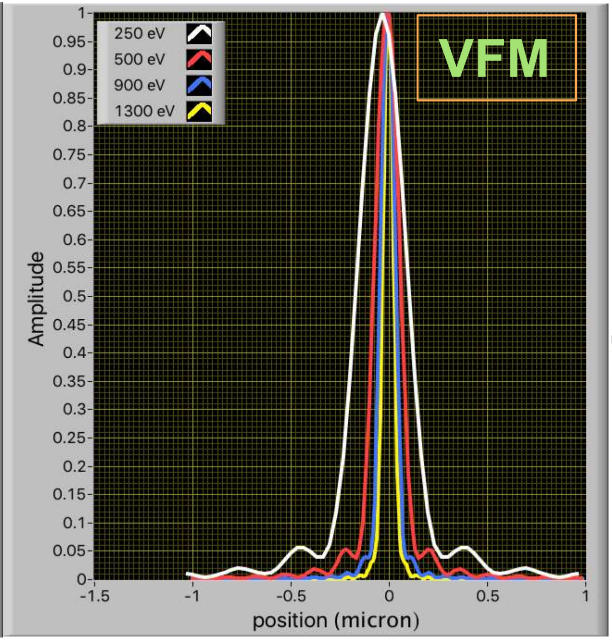
Beam Energy [eV]	HFM [um]	VFM [um]
250	1.25	0.83
500	0.79	0.56
900	0.69	0.47
1300	0.67	0.45

Mirrors decoupled from the chambers. Benders with in-vacuum motors

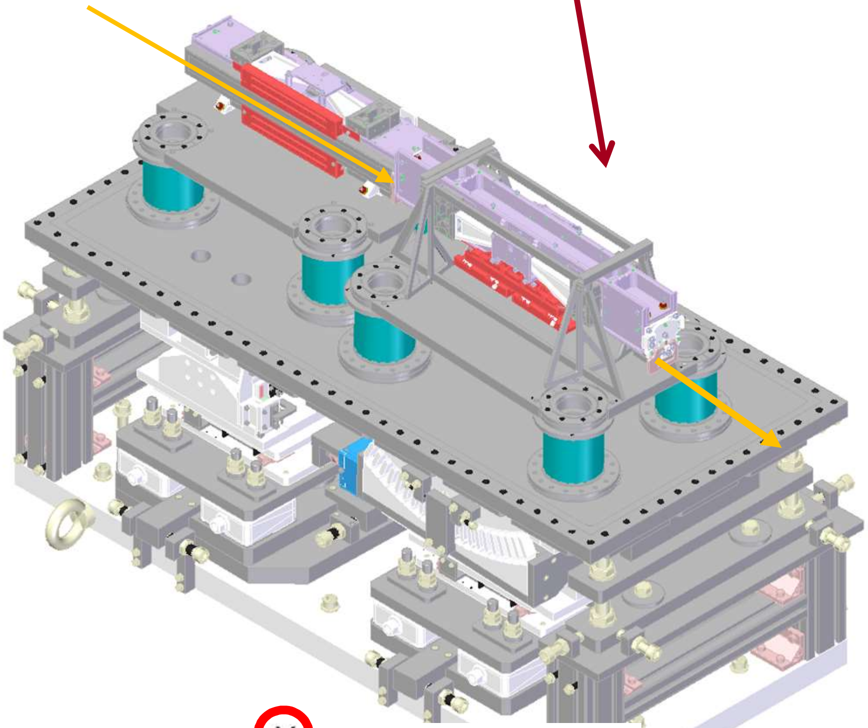
IP 2, KB System (DREAM, no bender)

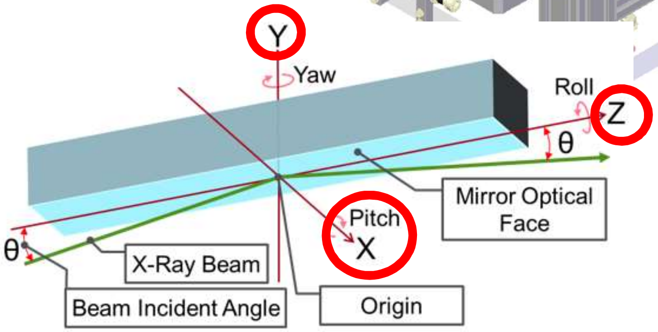




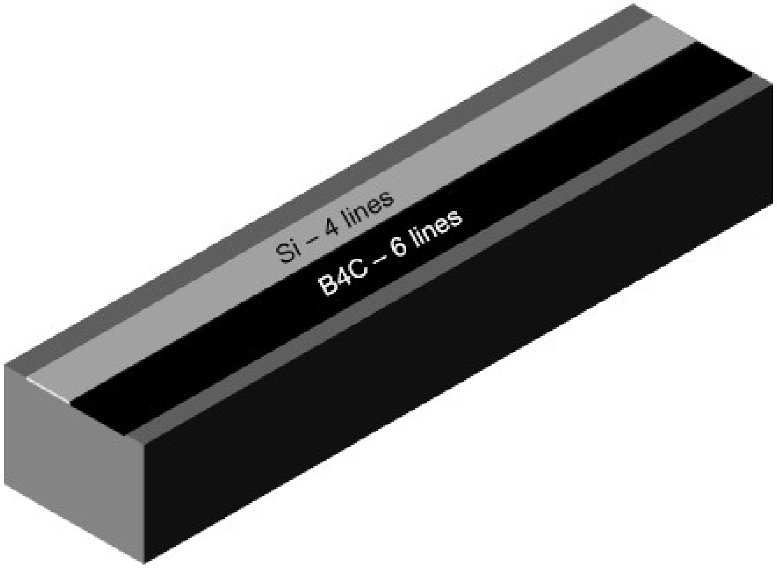


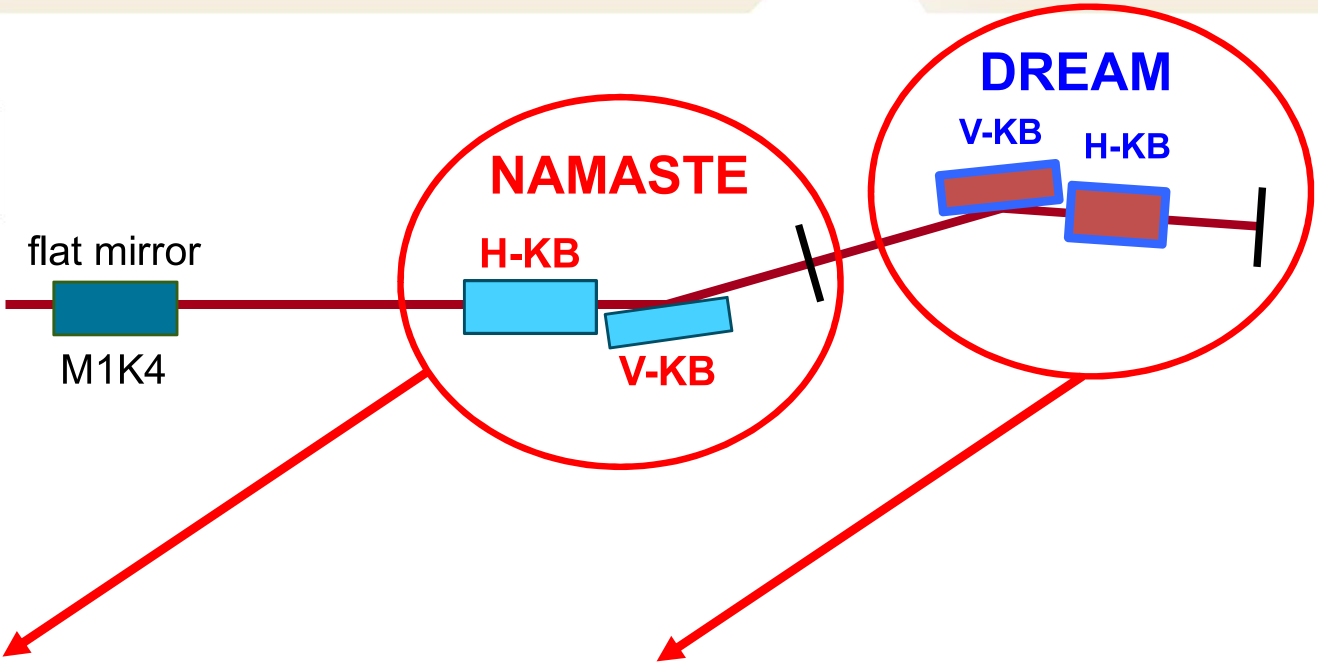
Beam Energy [eV]	HFM [um]	VFM [um]
250	0.58	0.27
500	0.31	0.14
900	0.08	0.19
1300	0.06	0.15

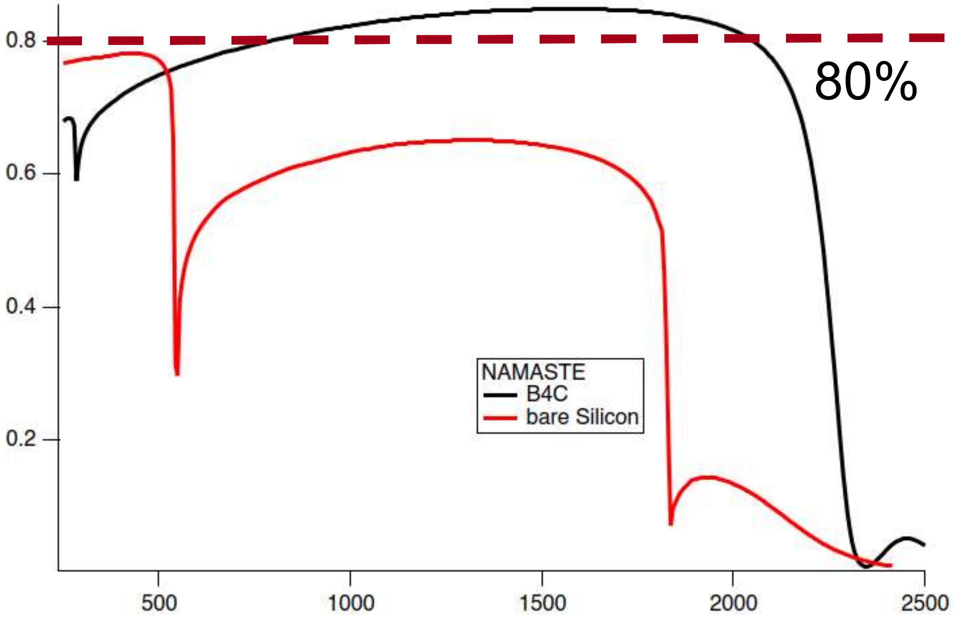


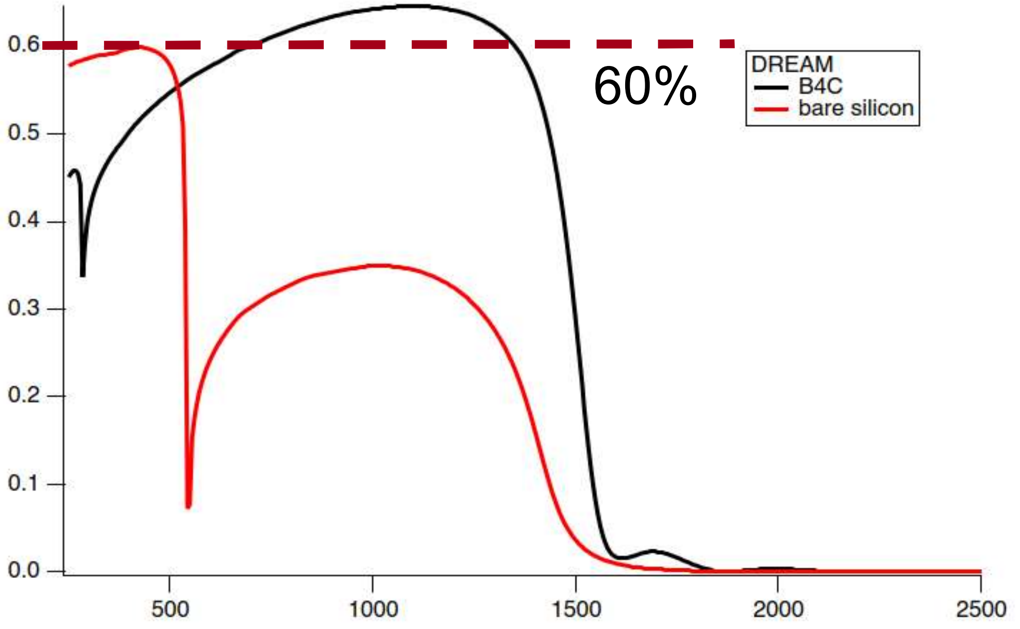


Optics, Transmission (incl. M1K4)



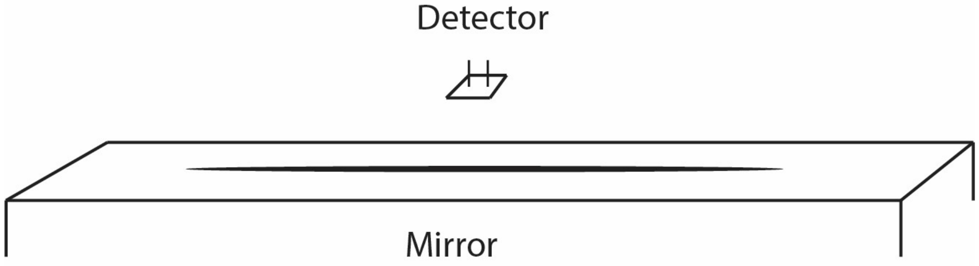


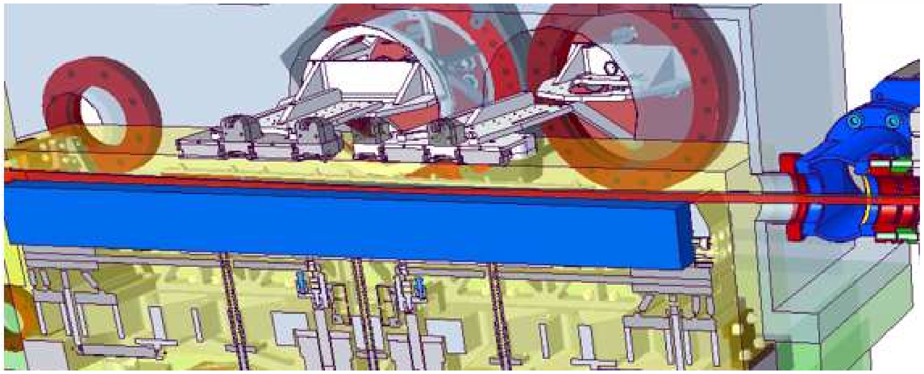


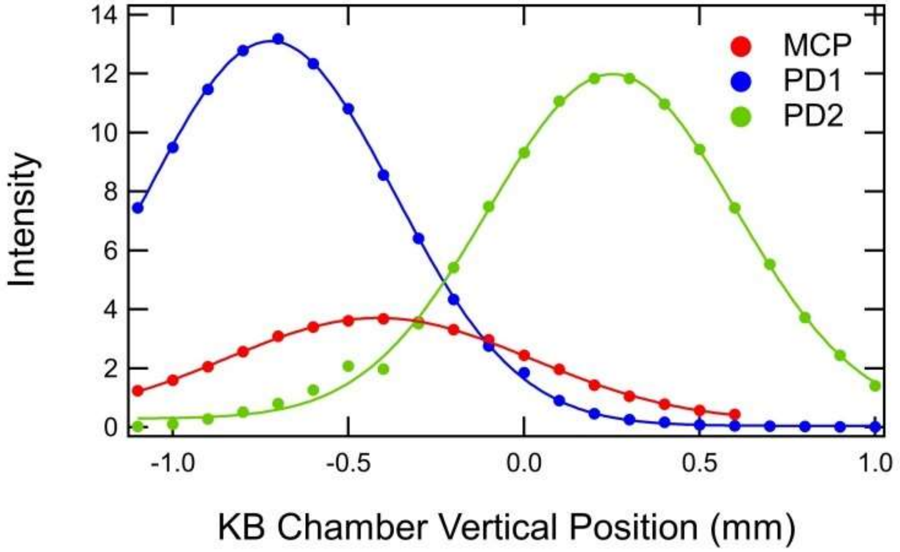


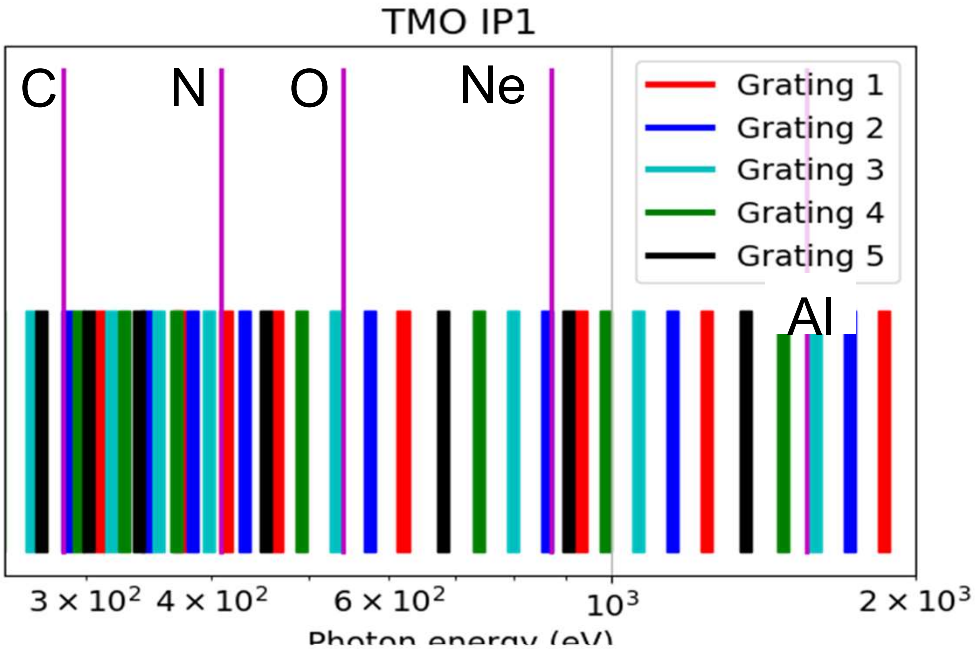
TMO, Diagnostic and WFS

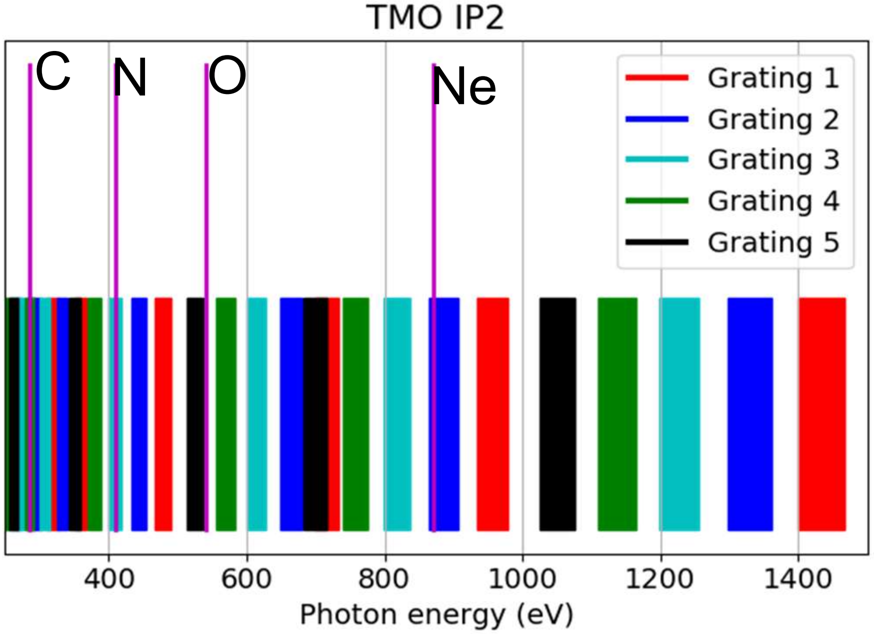
Fluorescence Intensity Monitor











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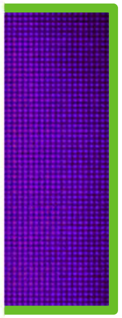
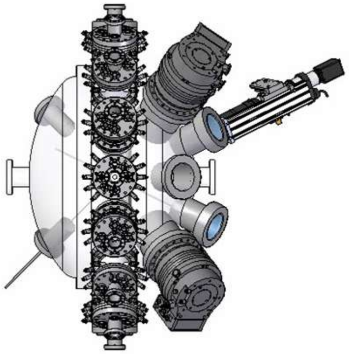


Express

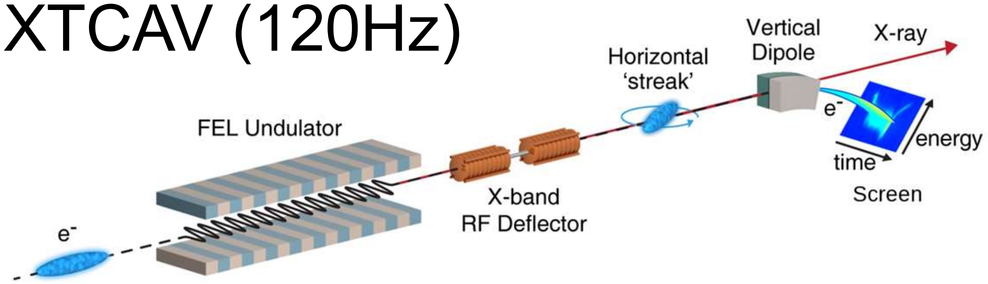
TMO, Diagnostic

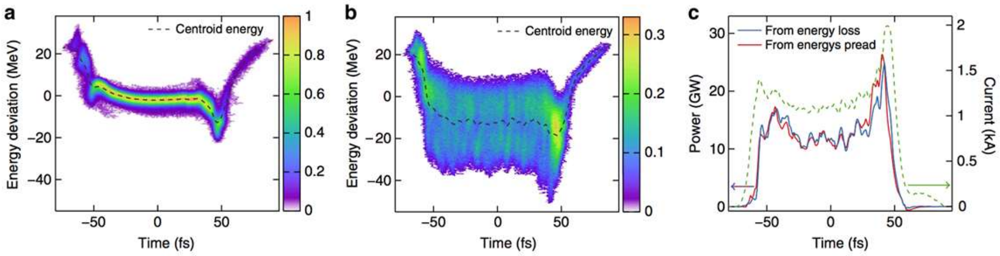
MRCOFEE



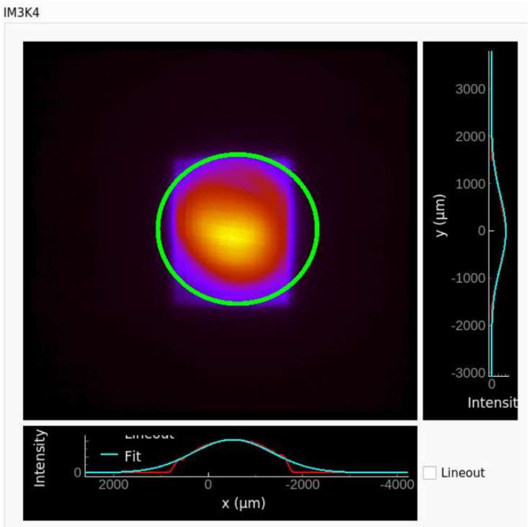
Diagnostic
Polarization
Pulse duration
SASE profile
Rel. Energy, Intensity
Beam position

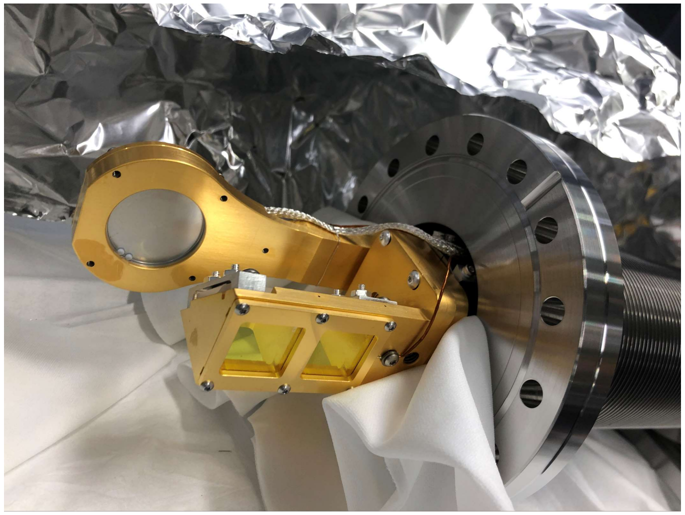
XTCAV (120Hz)

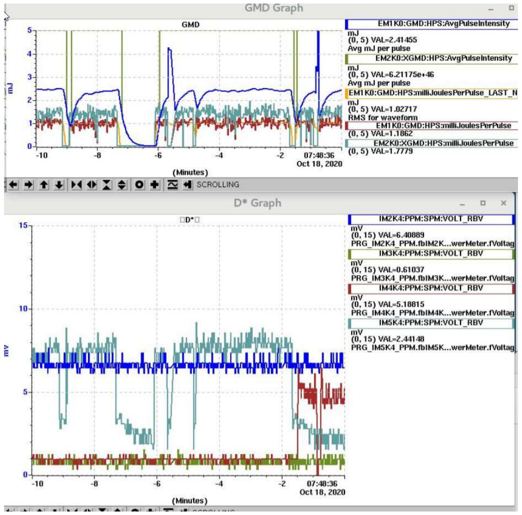




BPM & Power Meter (1Hz)







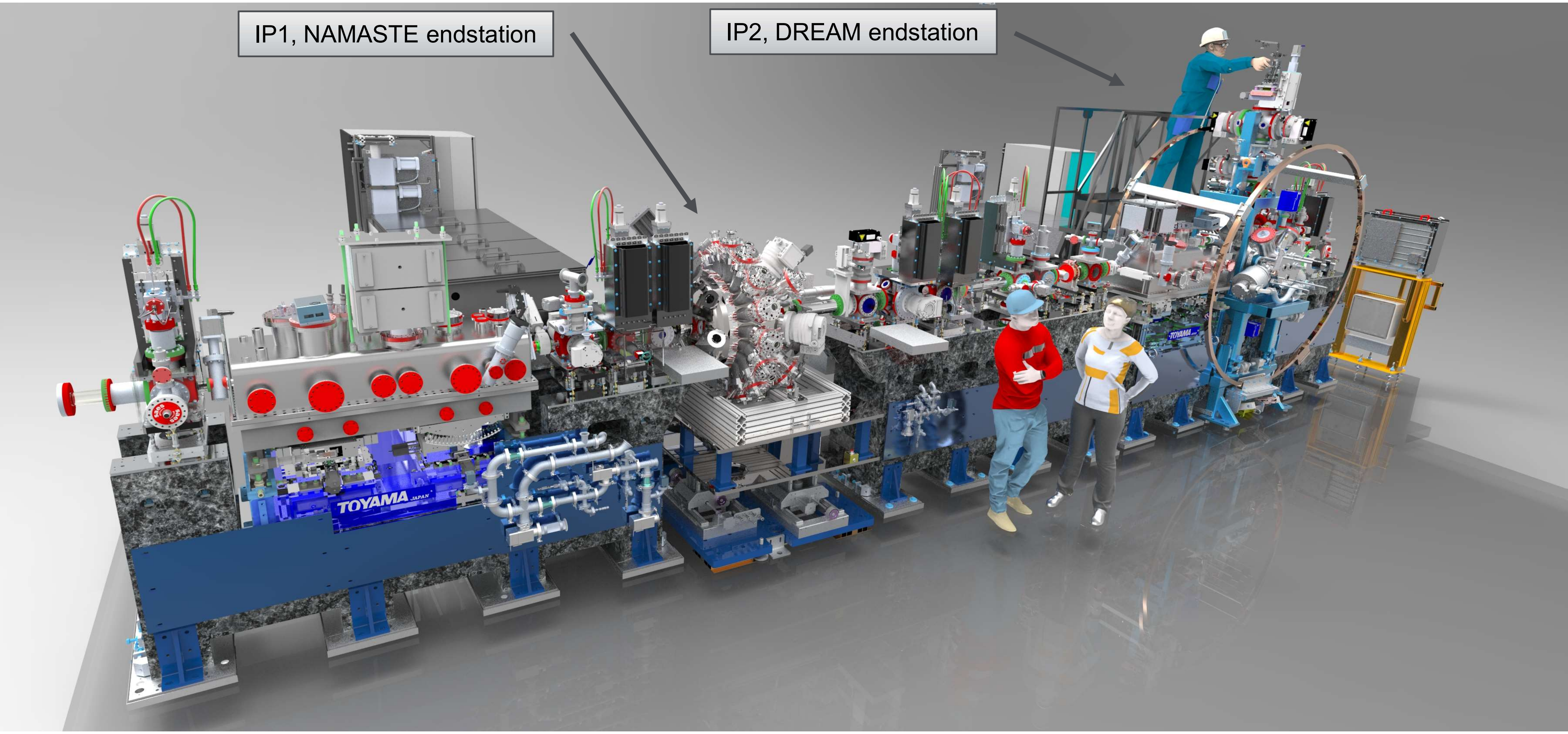
07:48:36
Oct 18, 2020

EM1K0:GMD:HPS:AvgPulseIntensity
mJ
(0, 5) VAL=2.41455
Avg mJ per pulse
EM2K0:XGMD:HPS:AvgPulseIntensity
mJ
(0, 5) VAL=6.21175e+46
Avg mJ per pulse
EM1K0:GMD:HPS:milliJoulesPerPulse_LAST_N
mJ
(0, 5) VAL=1.02717
RMS for waveform
EM1K0:GMD:HPS:milliJoulesPerPulse
(0, 5) VAL=1.1862
EM2K0:XGMD:HPS:milliJoulesPerPulse
(0, 5) VAL=1.7779

07:48:36
Oct 18, 2020

IM2K4:PPM:SPM:VOLT_RBV
mV
(0, 15) VAL=6.40889
PRG_IM2K4_PPM.fbIM2K...werMeter.fVoltag
IM3K4:PPM:SPM:VOLT_RBV
mV
(0, 15) VAL=0.61037
PRG_IM3K4_PPM.fbIM3K...werMeter.fVoltag
IM4K4:PPM:SPM:VOLT_RBV
mV
(0, 15) VAL=5.18815
PRG_IM4K4_PPM.fbIM4K...werMeter.fVoltag
IM5K4:PPM:SPM:VOLT_RBV
mV
(0, 15) VAL=2.44148
PRG_IM5K4_PPM.fbIM5K...werMeter.fVoltag

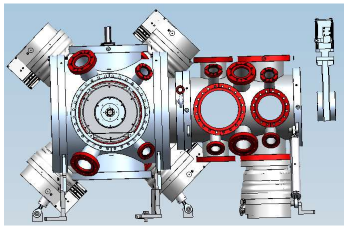
TMO, NAMASTE Endstations (IP1)

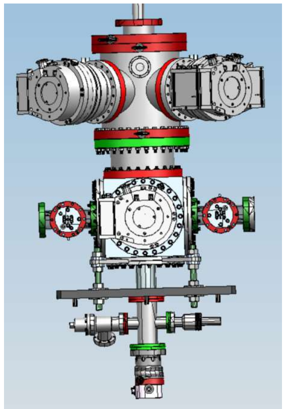

IP1, NAMASTE endstation

IP2, DREAM endstation

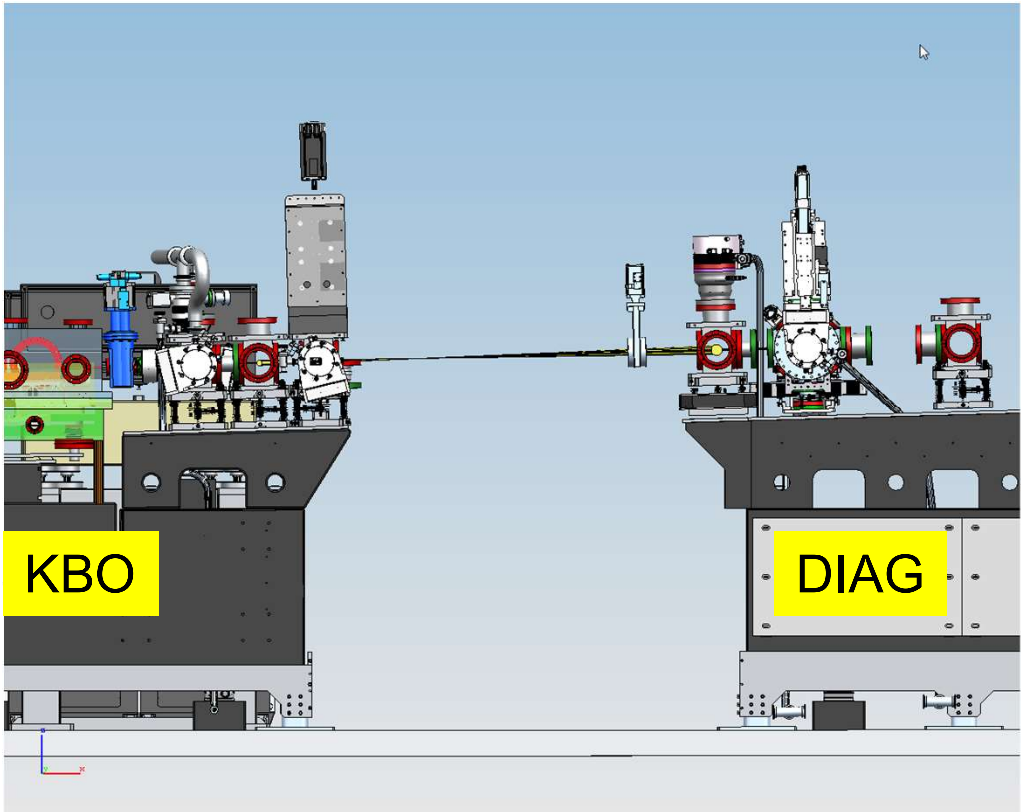
Next generation **A**tomic, **M**olecular, and **A**ccelerator **S**cience and **T**echnology **E**xperiments (NAMASTE).
The NEH 1.1. instrument will offer the possibility to install modular stations (roll in and out) which can be set up, aligned and commissioned outside the hutch and installed at the first TMO focus spot. Therefore, these modules have to be highly standardized by the following parameters. The implementation time needs to be less than 12h (desired 8h) within a reasonable low amount of SLAC manpower (plug and play).

NAMASTE: Roll-in Endstaions



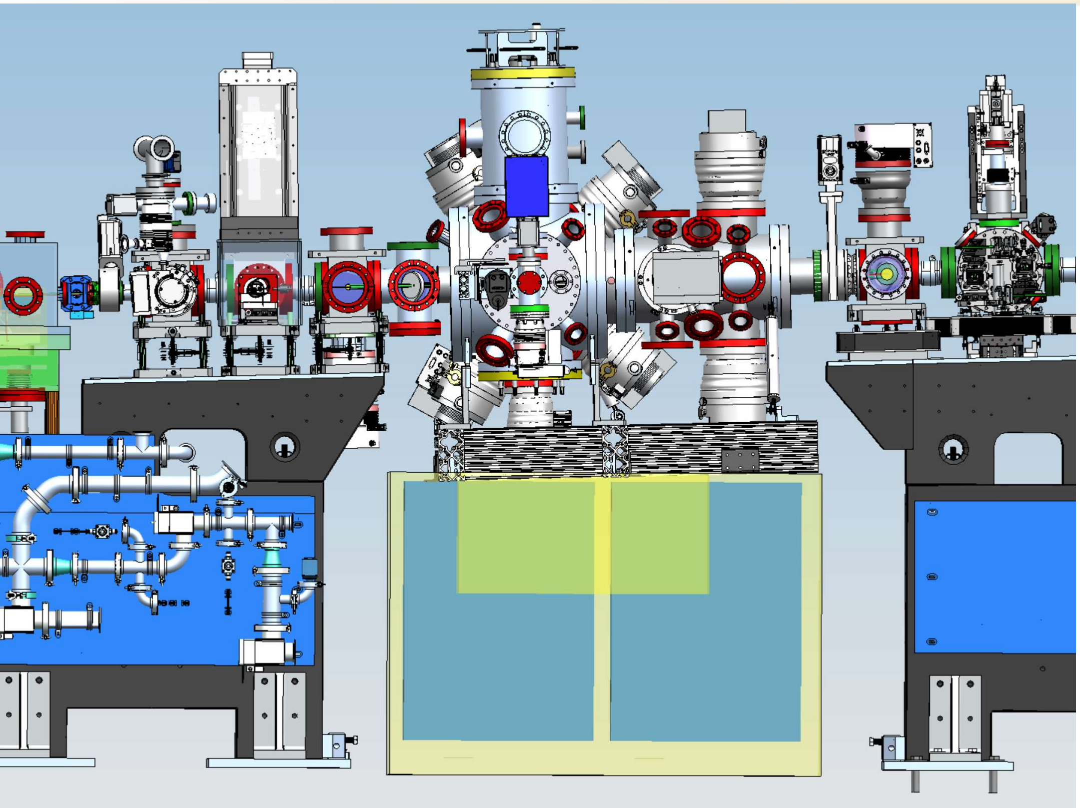


These roll-in Endstation will be highly standardized. The implementation time needs to be less than 12h (desired 8h) within a reasonable low amount of SLAC manpower (plug and play).

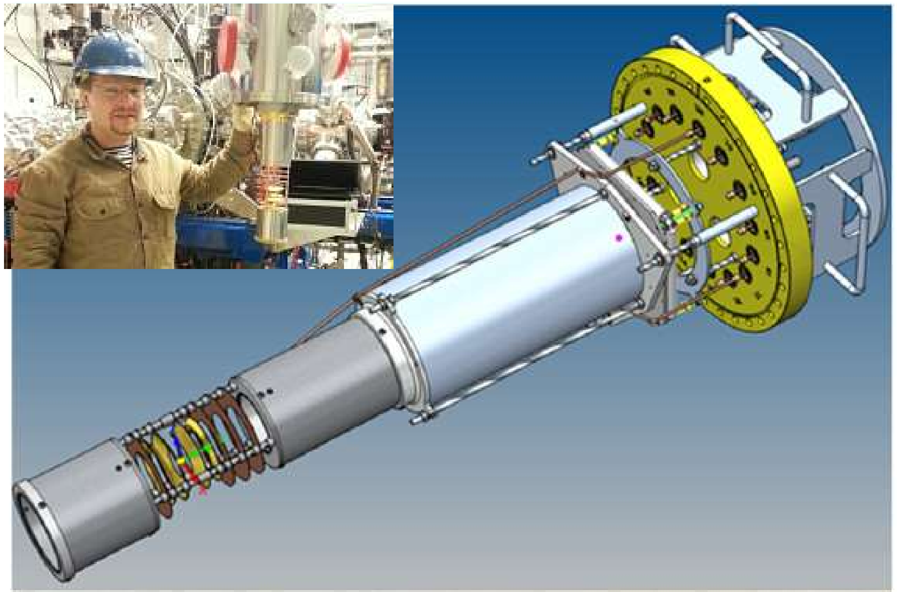


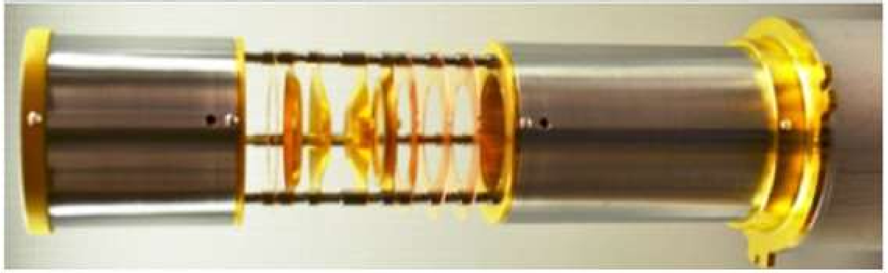
NAMASTE Option: LAMP

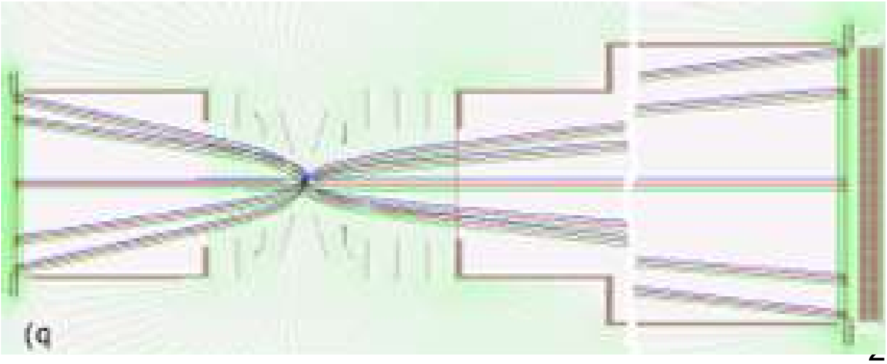
Osipov, T., Berrah, N., et. al. (2018). 035112. https://doi.org/10.1063/1.5017727



Science / Technique	LAMP (OSIPOV VMI)
DAY ONE	**X**
Strong field	X
Ion / e^- covariance	X
XAS	X

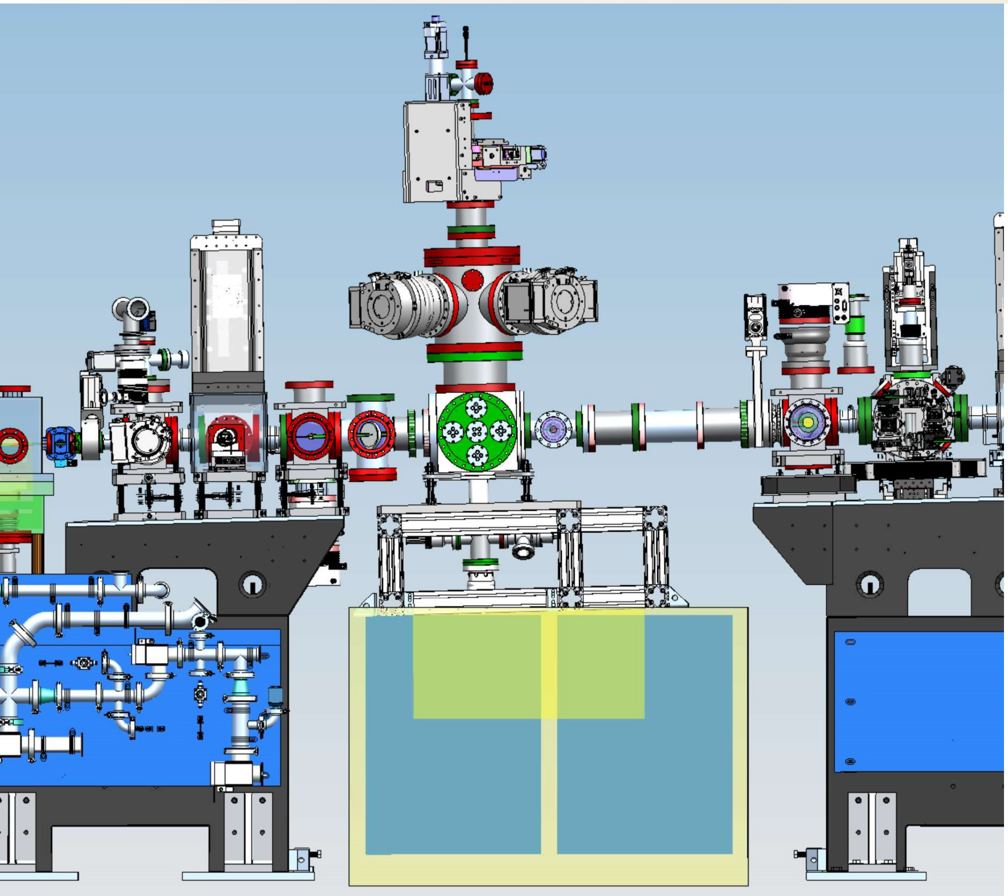


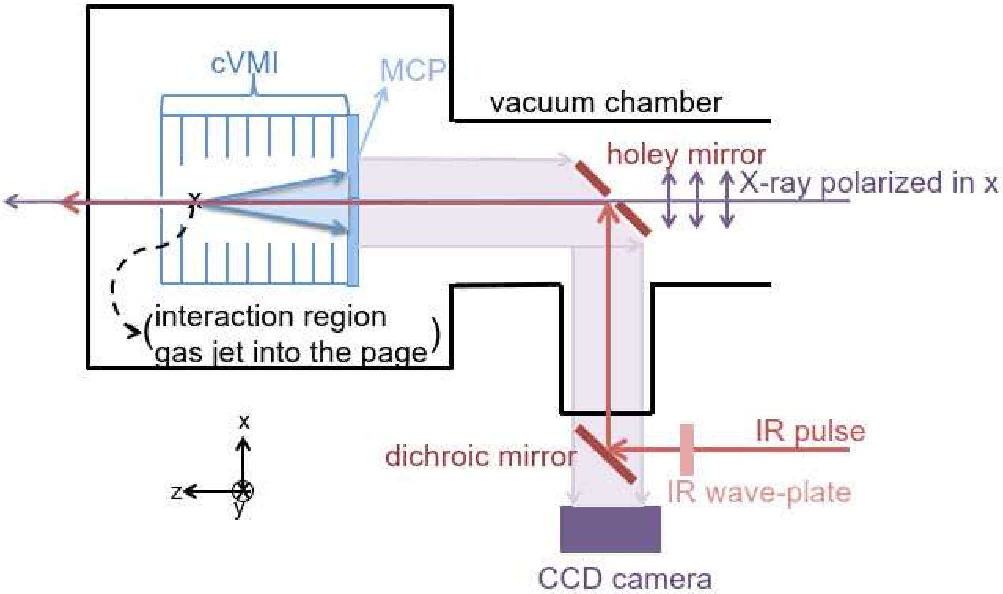


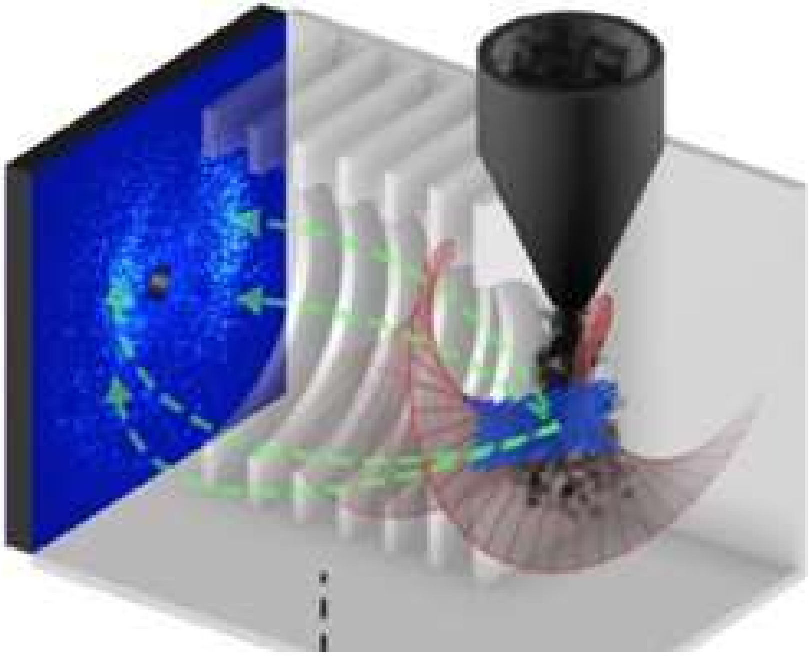


NAMASTE Option: Co-Ax-VMI

S. Li, J.P. Cryan et. al. (2018). AIP Advances, 8(11), 115308



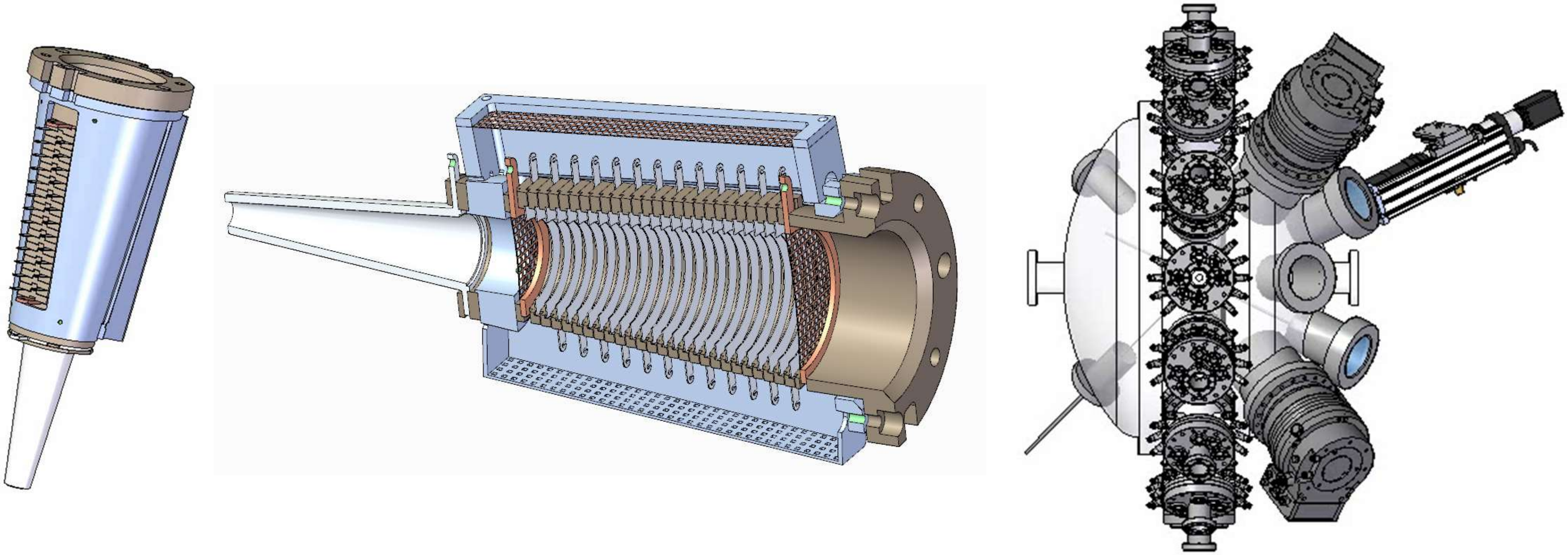




Science / Technique	Co-Ax-VMI
DAY ONE	**X**
Strong field	(x)
XAS	X
ARPES	X

NAMASTE Option: MRCOFFEE

Multi Resolution Cookiebox Optimized for Future Free Electron Laser Experiments



Science / Technique	MRCOFFEE
DAY ONE	---
High rep rate (1MHz)	X
High res PES	X
ARPES	X
Multiple edge ARPES	X

Specifications
0.25 eV / 70 eV
1.5 - 5° Accept. Angle / TOF
> 2000 V retardation
> 2 ret. settings

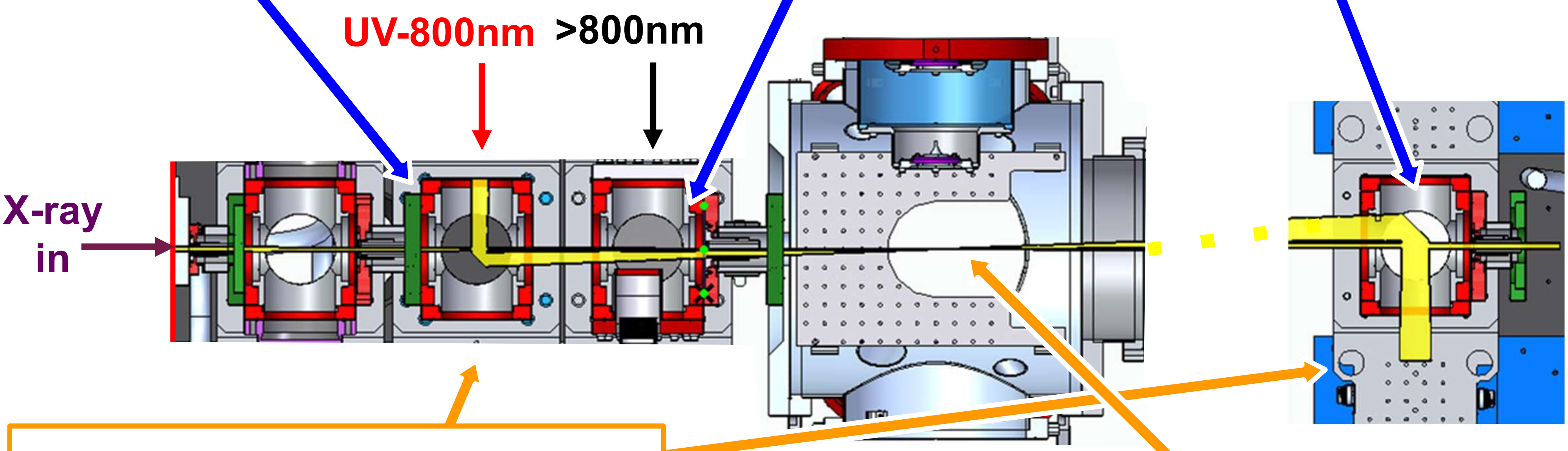
Diagnostic
Polarization
Pulse duration
SASE profile
Rel. Energy, Inensity
Beam position

Common Components in-coupling in non-collinear geometry and non-standard close in-coupling

Far in-coupling: common component, with multiple optics mounted for multiple wavelengths or redundancy

Close in-coupling: for NIR/MIR, to reduce focal length for these wavelengths (option for in-vacuum parabola in the future)

Out-coupling: to extract laser and enable measurement of transmitted light (e.g. timing, overlap, pulse duration etc.)



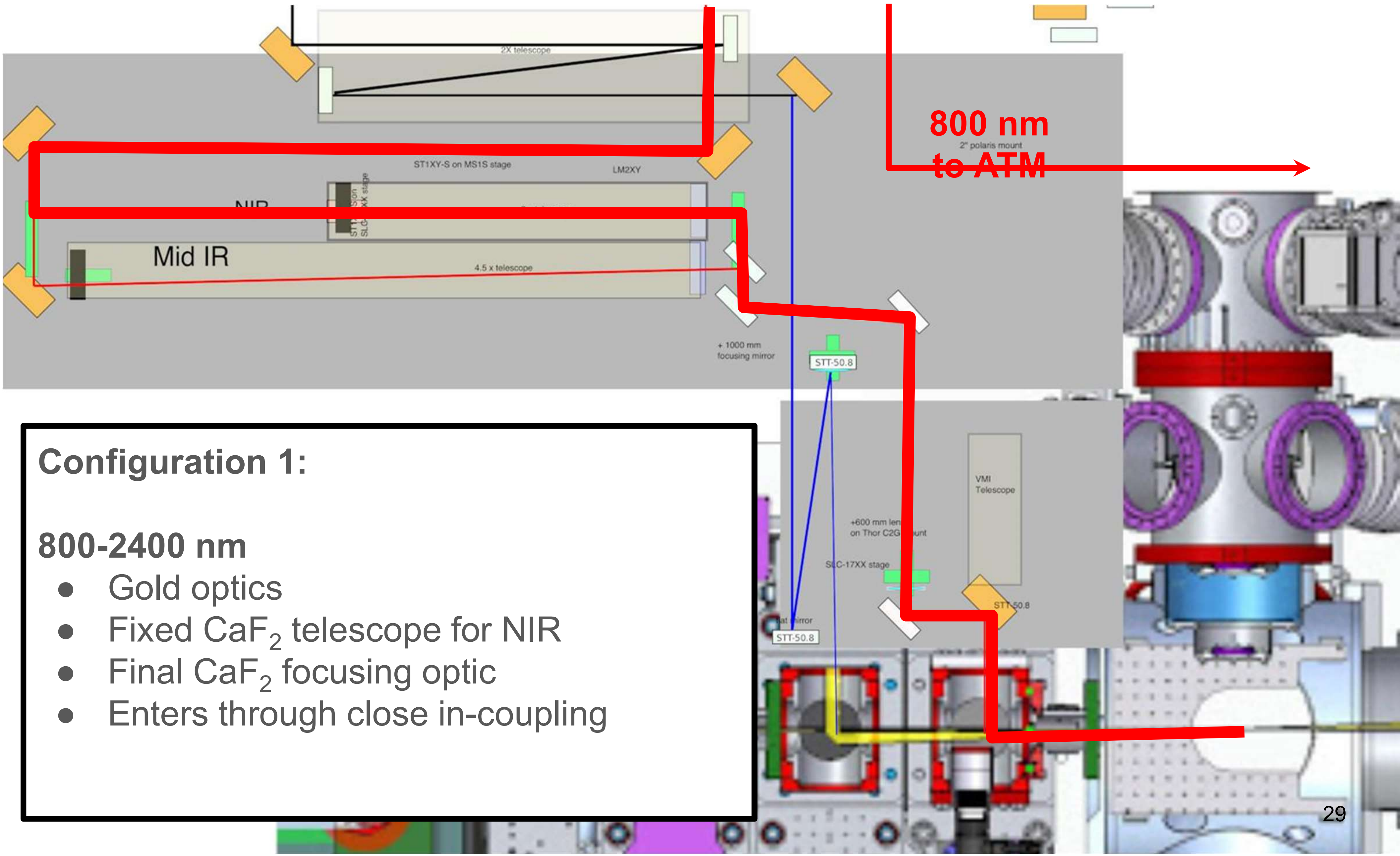
'On target' laser diagnostics:

- Energy, position, duration etc.
- Before in-coupling
- After out-coupling

Paddle at interaction point:

- YAG screen for spatial overlap
- Knife-edge/pinhole for beam size
- Diode/wire for coarse-timing

IP1: Optical layout incorporates separate paths for three wavelength ranges, to size beams appropriately

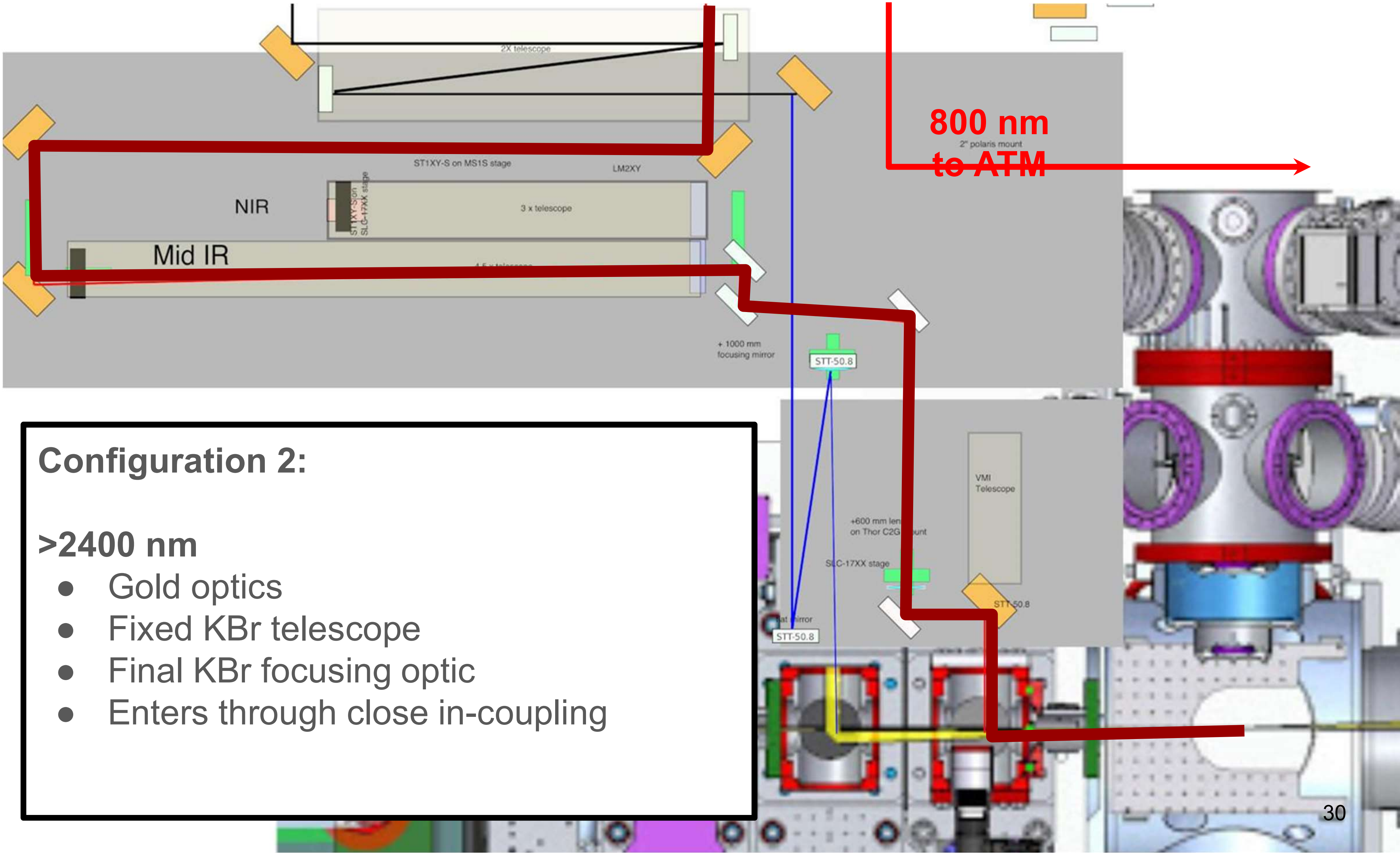


Configuration 1:

800-2400 nm

- Gold optics
- Fixed CaF_2 telescope for NIR
- Final CaF_2 focusing optic
- Enters through close in-coupling

IP1: Optical layout incorporates separate paths for three wavelength ranges, to size beams appropriately

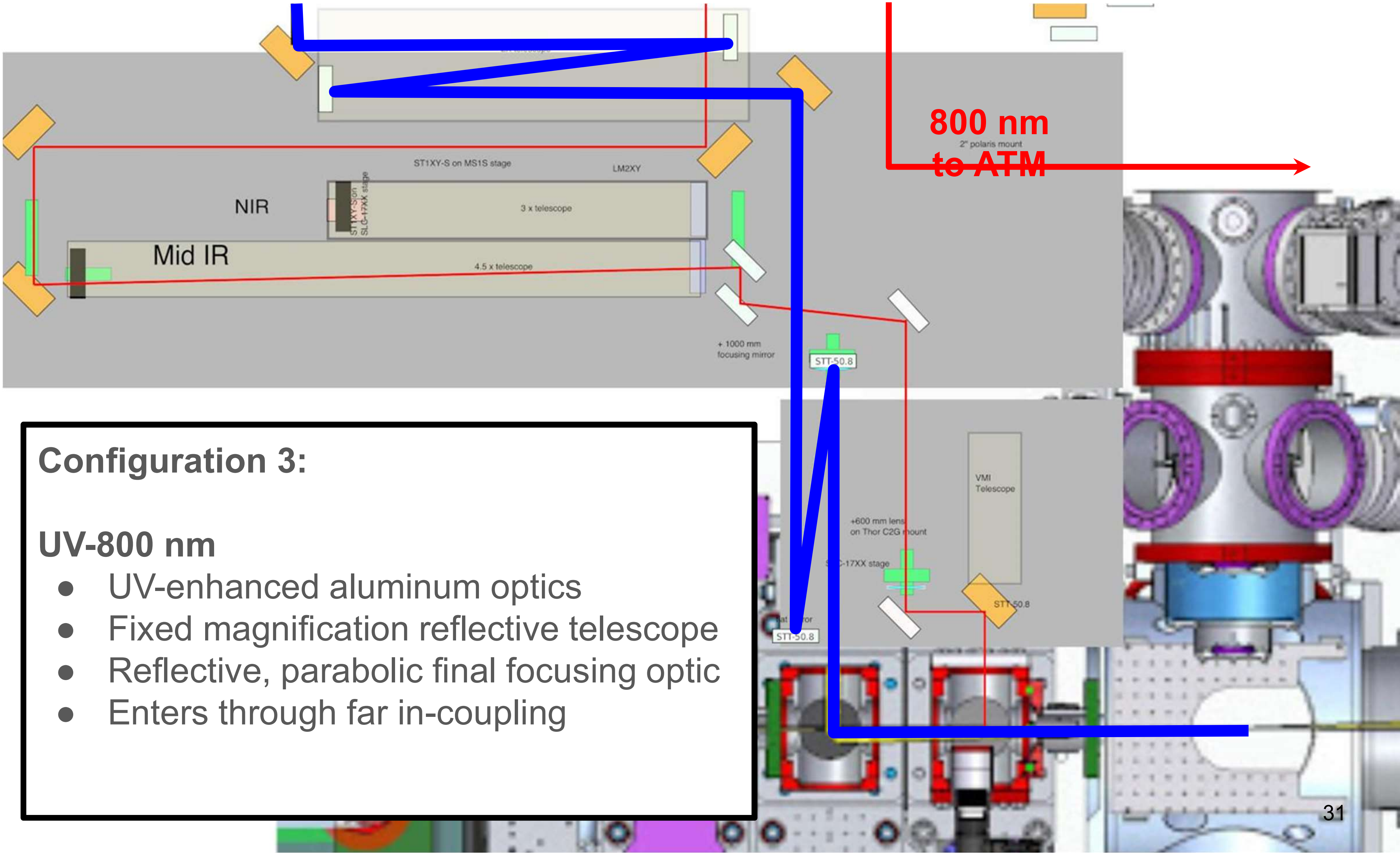


Configuration 2:

>2400 nm

- Gold optics
- Fixed KBr telescope
- Final KBr focusing optic
- Enters through close in-coupling

IP1: Optical layout incorporates separate paths for three wavelength ranges, to size beams appropriately

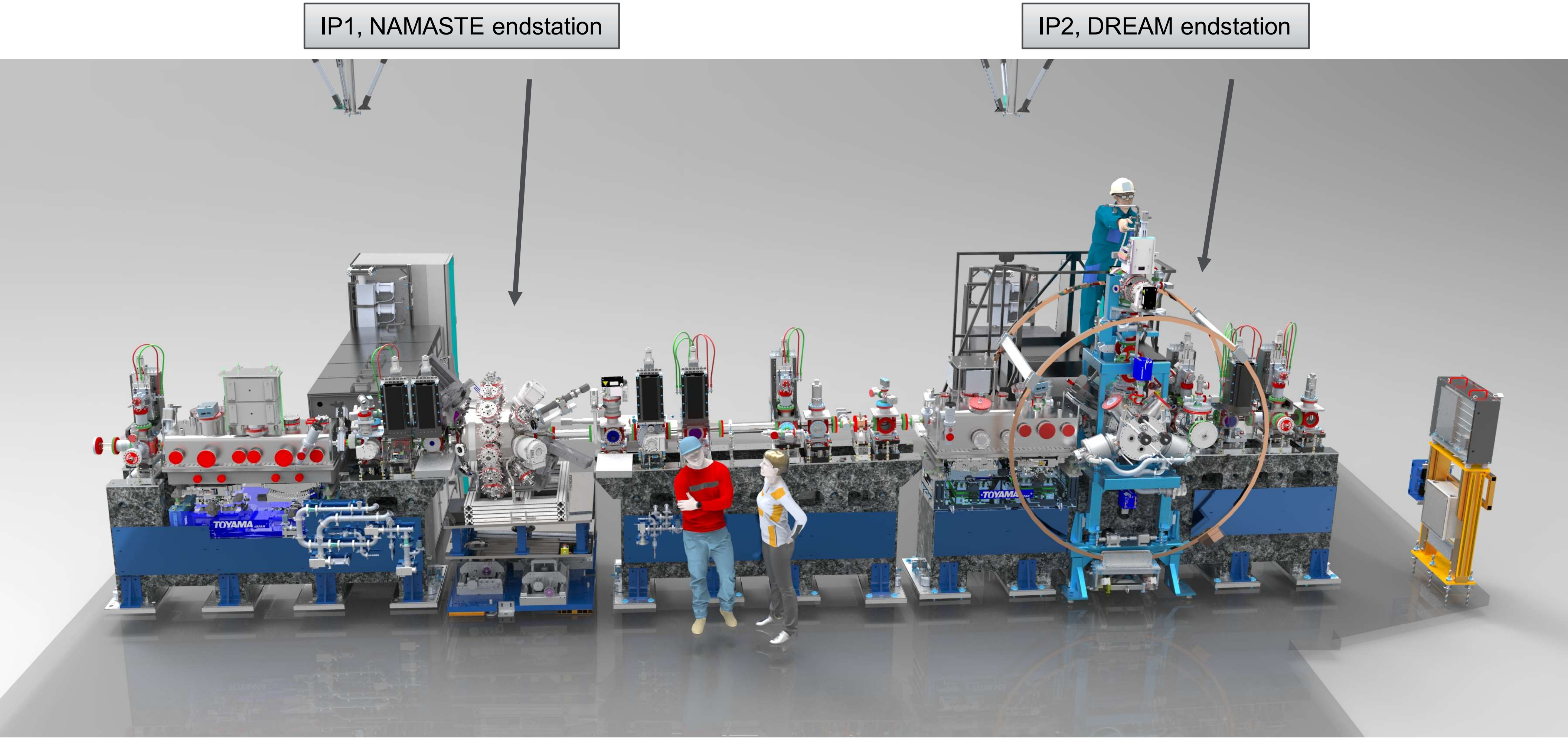


Configuration 3:

UV-800 nm

- UV-enhanced aluminum optics
- Fixed magnification reflective telescope
- Reflective, parabolic final focusing optic
- Enters through far in-coupling

TMO, DREAM Endstation (IP2)

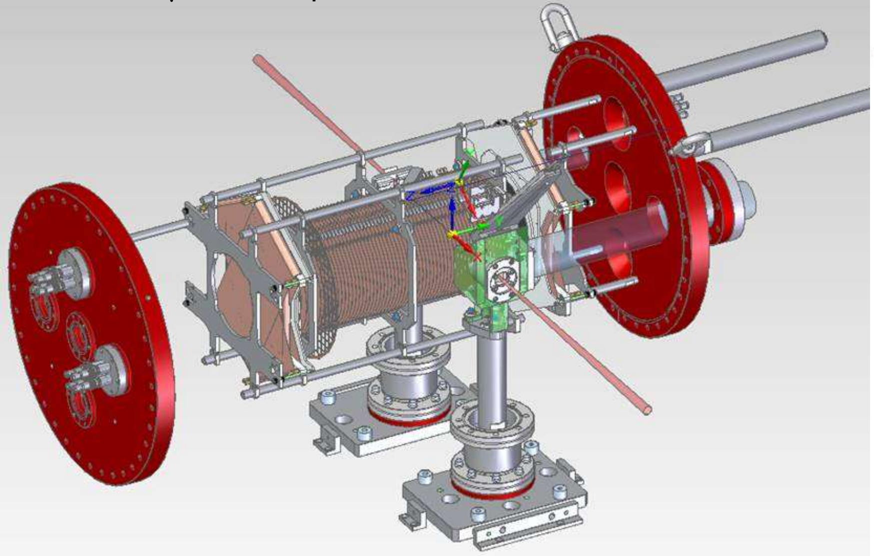


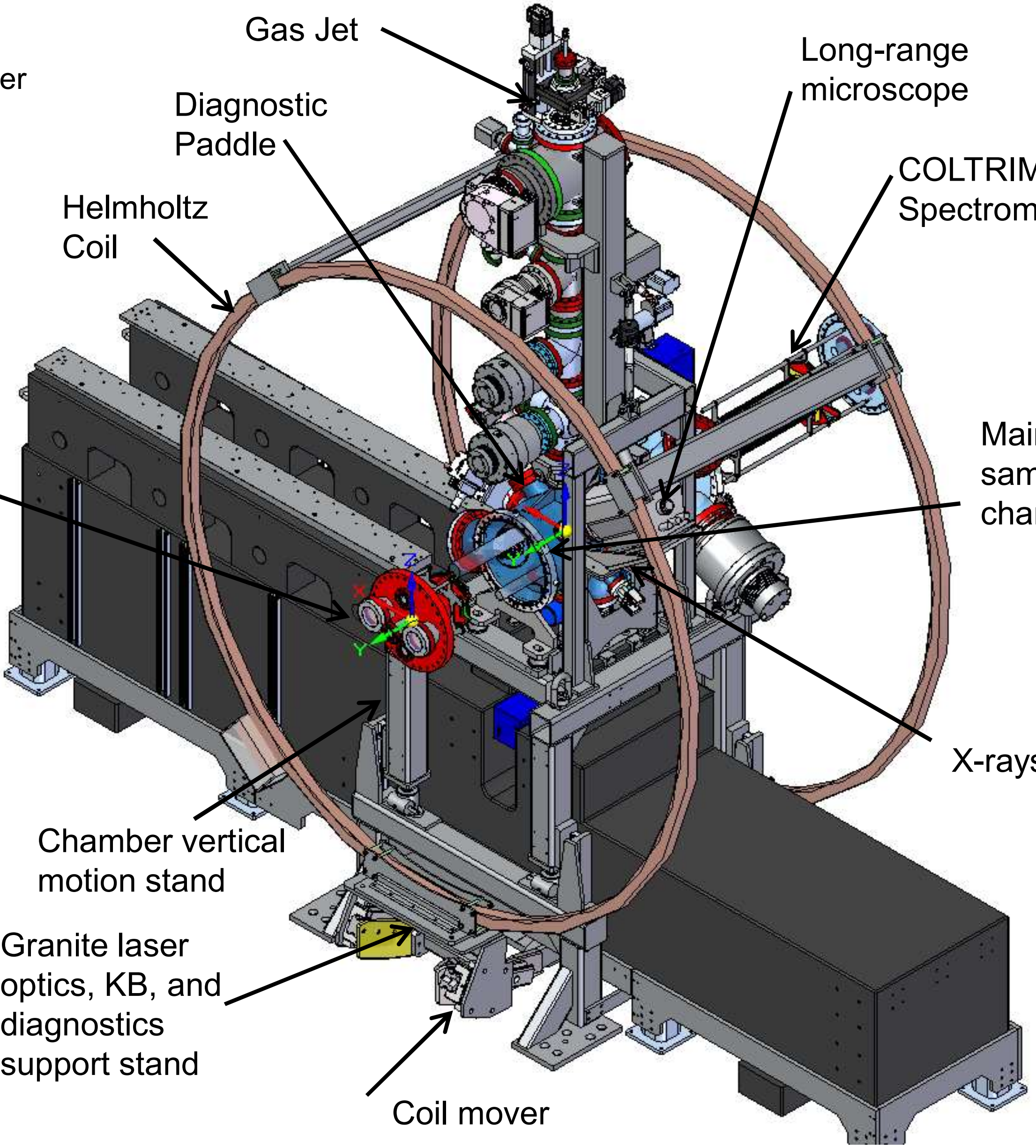
The new **D**ynamic **REA**ction **M**icroscope (DREAM) endstation will house a well-defined geometry and COLTRIMS type spectrometer as a standard configuration to accommodate extreme vacuum, sub-micron focus spot size, and target purity requirements dictated by the pump-probe class of coincidence experiments, 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 10^{21} photons/cm^2 with superconducting Linac X-rays

DREAM station

Main components and specs

- Experimental chamber
- Multistage differential pumping + gas jet and jet catcher
- 0.5 mm gas jet ϕ
- 1.5 m Jet source distance
- COLTRIM - eTOF, and iTOF spectrometers
- Laser in/out-coupling
- Earth magnetic field cancellation coils (yaw and roll)
- 6 DOF (manual) support with motorized Y
- Diagnostic paddle
- Long-range microscope
- ≤ 300 nm X-ray spot
- 5 μm Laser spot
- 0.5 μm overlap





Gas Jet

Diagnostic Paddle

Helmholtz Coil

Long-range microscope

COLTRIMS Spectrometer

Laser in/out coupling

Main sample chamber

X-rays in

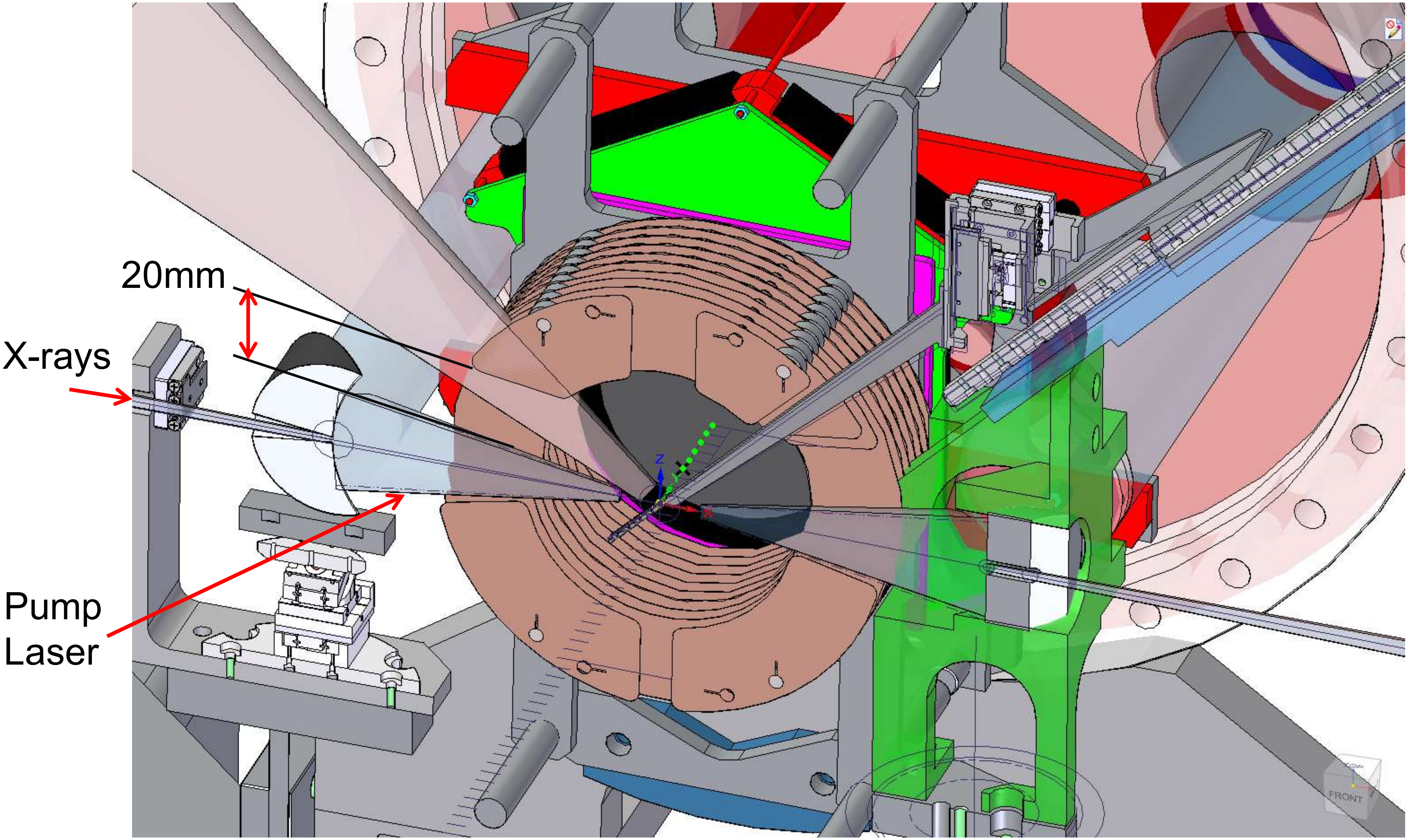
Chamber vertical motion stand

Granite laser optics, KB, and diagnostics support stand

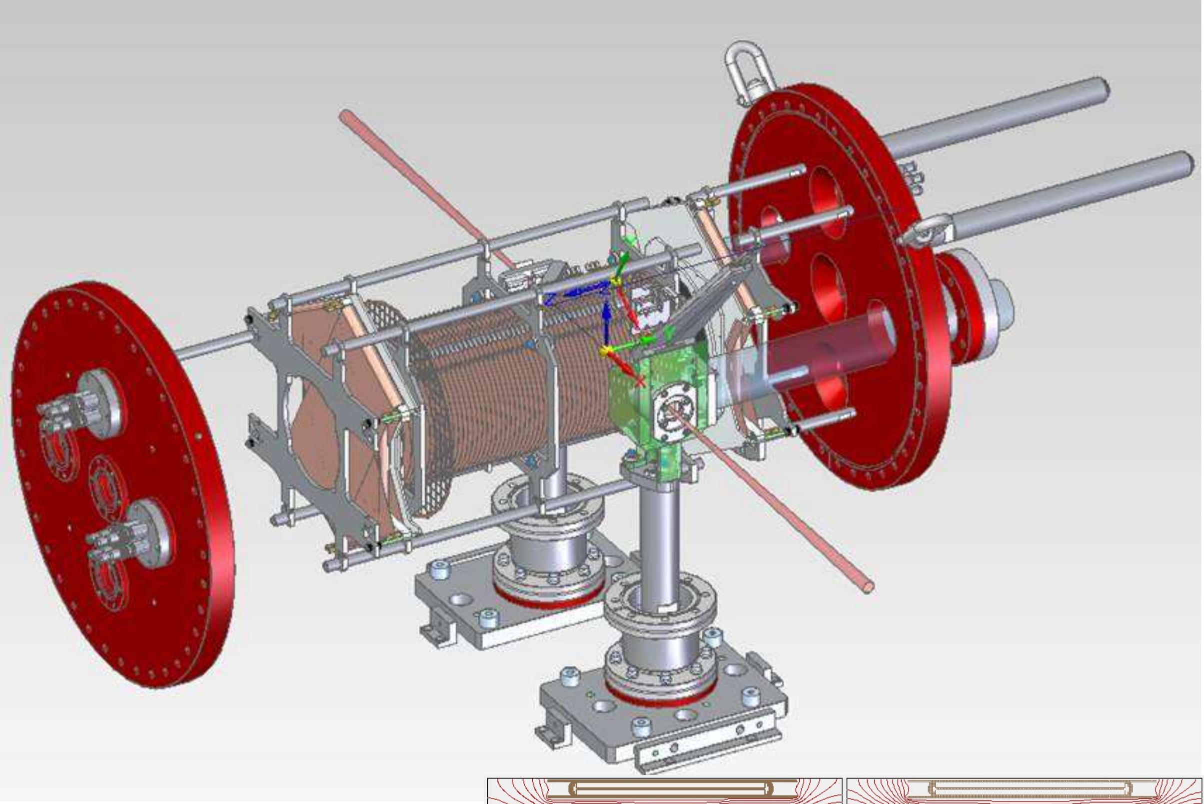
Coil mover

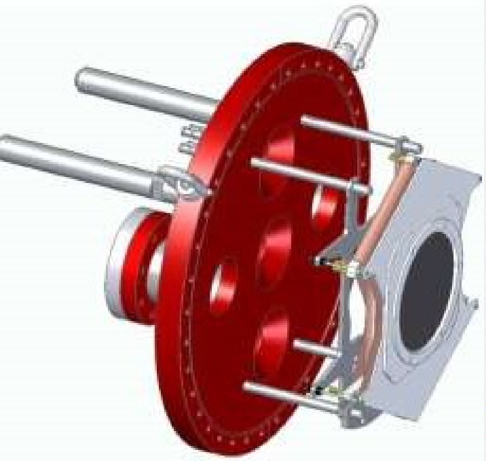
Spectrometer

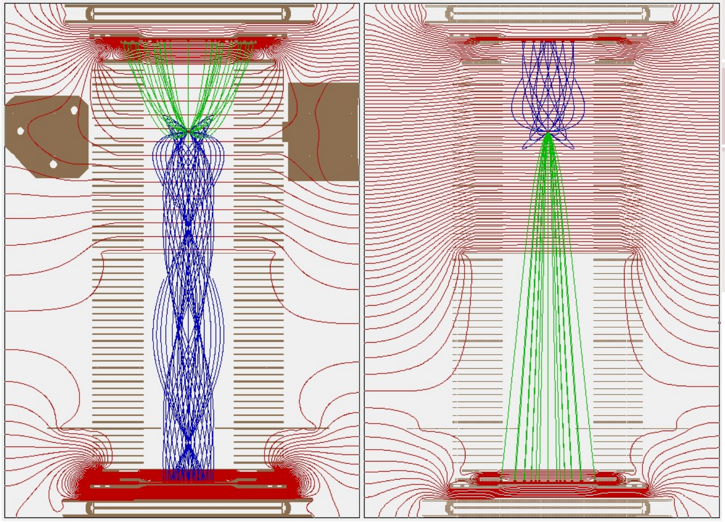
- Notches are included for laser path and diagnostic paddle



DREAM Spectrometer and Detector







DREAM
Hexanodes: 2x 120mm
Inner diameter: 125mm
Variable Spectrometer length
Max Voltage: 10 kV
Pt or dendritic Copper coated plates
e^- Resolution: dE/E ~1%
Collection efficiency: Ions> 50eV, e^- >200eV
Max B-Field: 35 Gauss
Detector time resolution: ~ 0.3 ns
Detector position resolution: ~ 250 µm

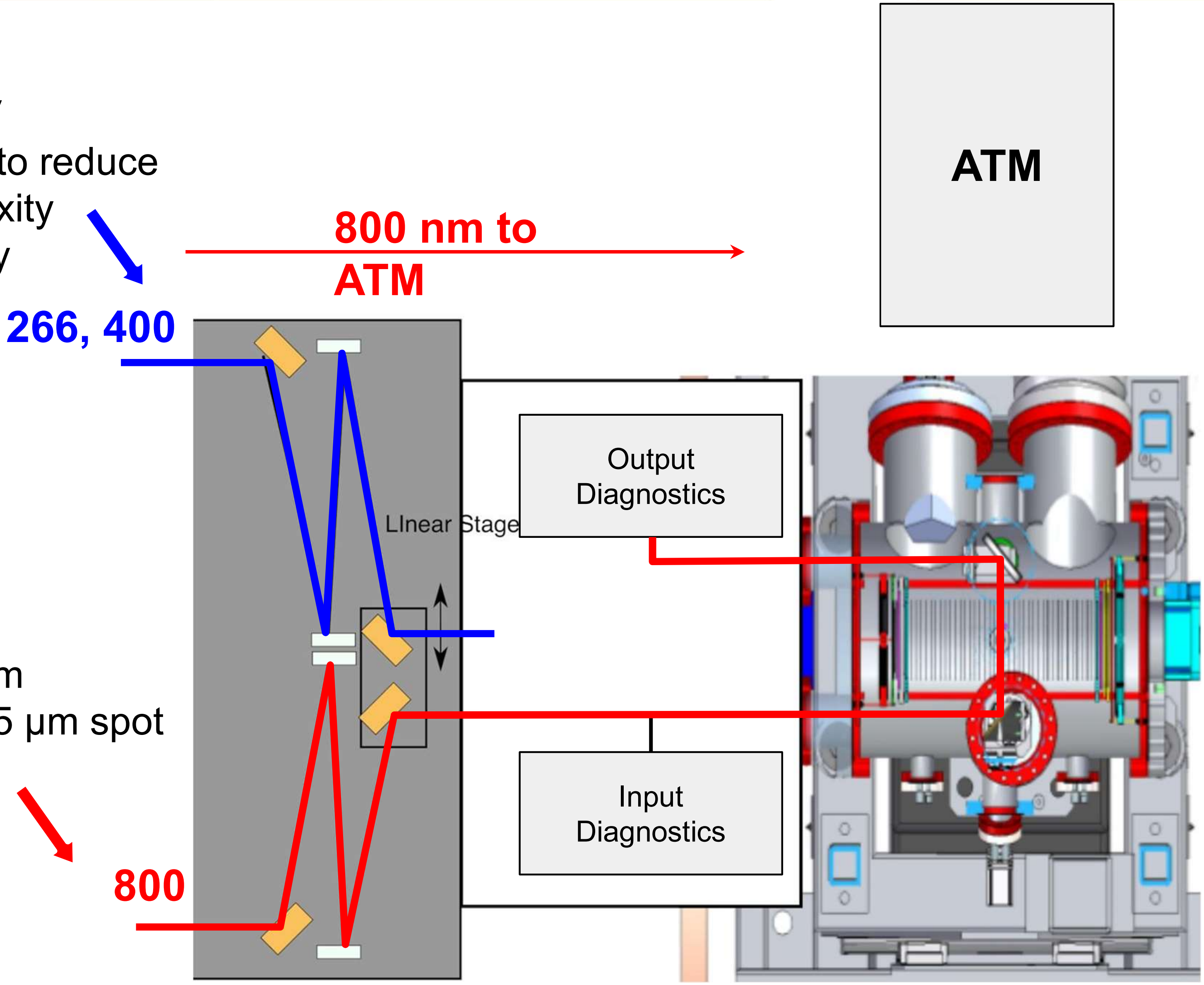
DREAM optical layout incorporates two configurations: one for 800nm, and one for harmonics

Configuration 1:

- x0.33 telescope for UV
- Generates larger spot to reduce spatial overlap complexity
- Non-collinear geometry

Configuration 2:

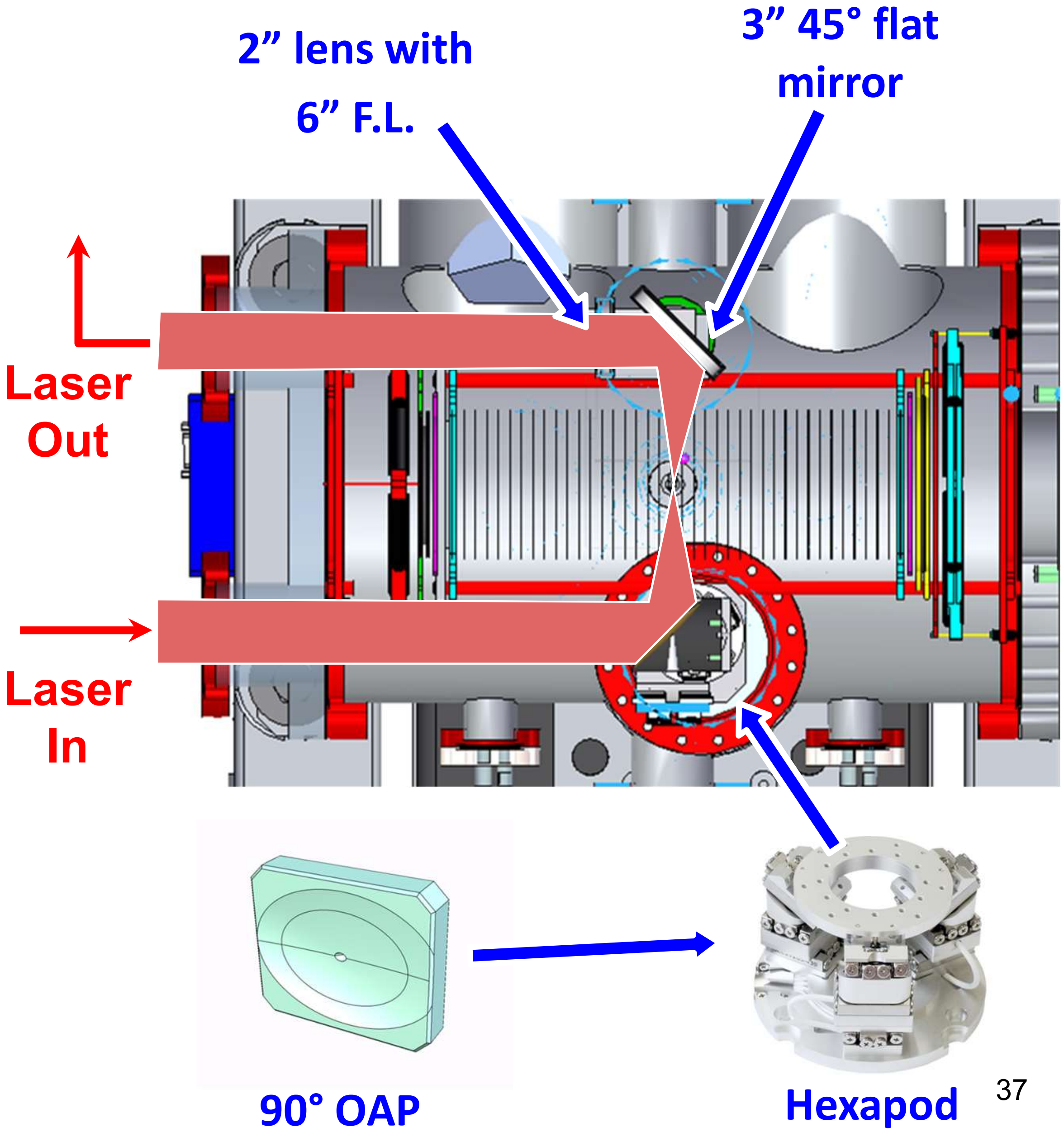
- x3 telescope for 800 nm
- Larger beam to reach 5 μm spot and high intensity
- Collinear geometry



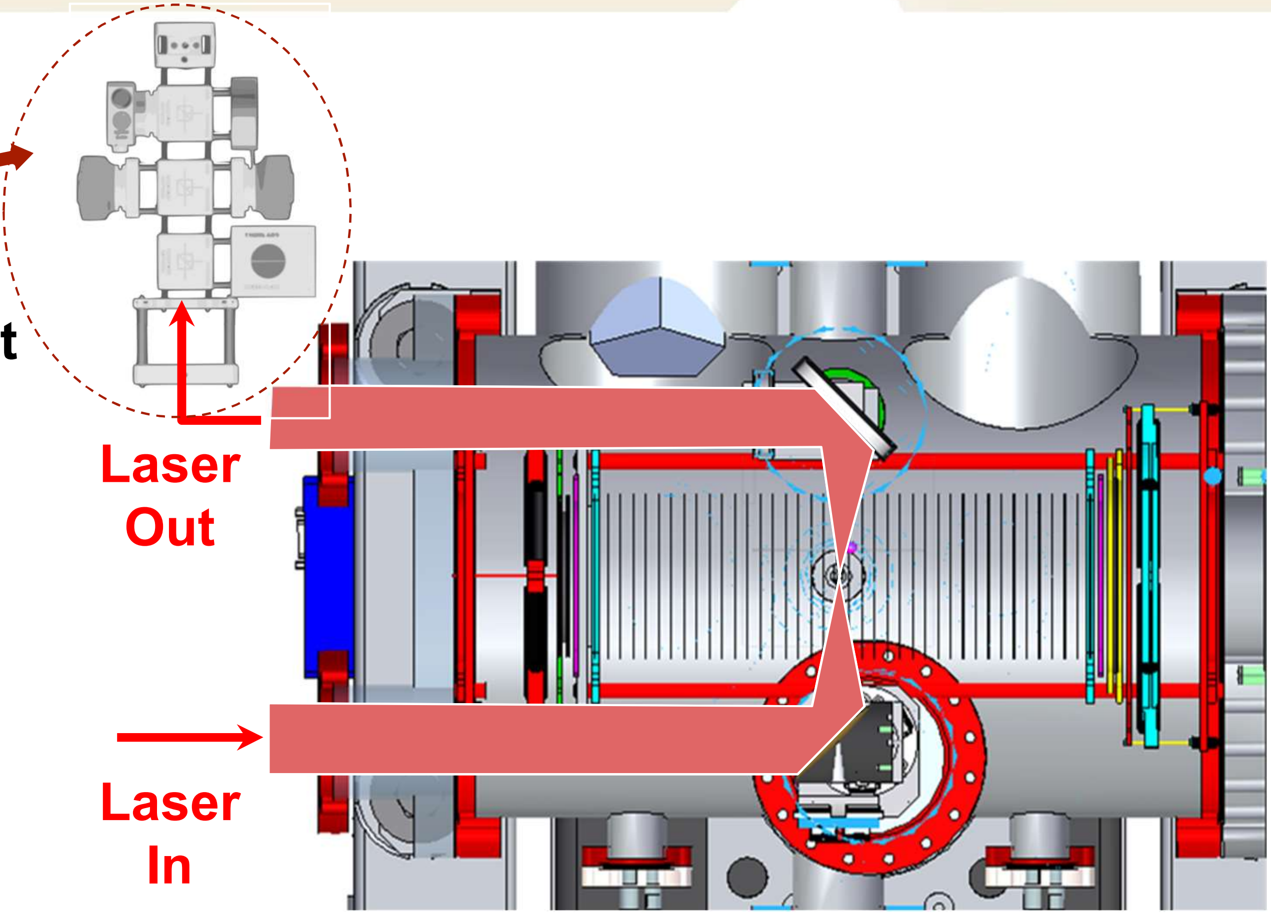
Non-standard in- and out- coupling to achieve small focal spot and provide online diagnostics of laser

Laser optics in the chamber

- **110mm focal length, holey, glass, 90° parabola with 33mm clear aperture**
- **Mounted on 6 D.o.F. nonmagnetic, UHV-compatible ‘hexapod’**
- **Additional holey mirror to send laser out of chamber through lens to re-image to diagnostics**



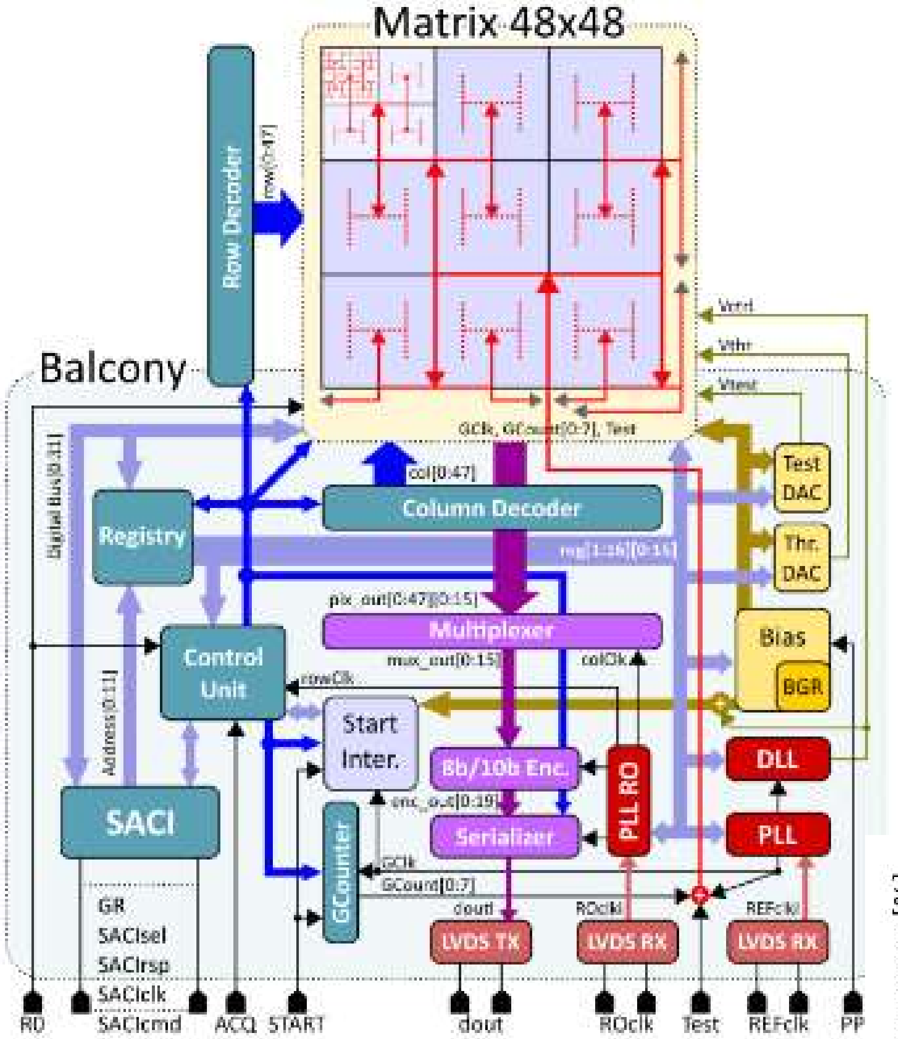
Diagnostics at output to provide information on laser parameters at the interaction point



- **Focus imaged to equivalent plane**
- **Provides an alignment reference**
- **Online beam monitoring**
    - ○ **Energy**
    - ○ **Position**
- **Feedback to beam delivery module to correct pointing**
- **Wavefront measurement**

Risk: Maintaining spatial overlap of 800nm with X-rays will be very challenging. Potential need for veto on spatial overlap. Diagnostics key to managing this.

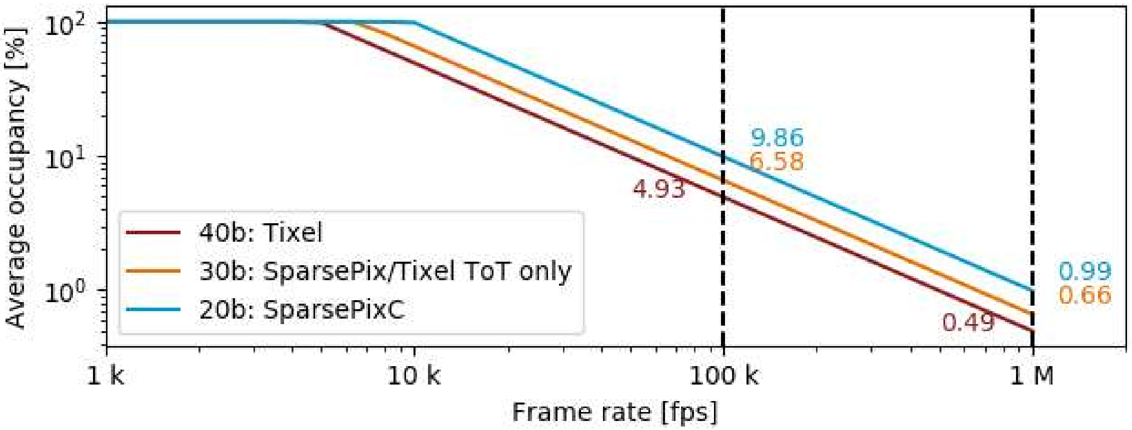
TIXEL: Time Resolving Imaging Detector for LCLS II



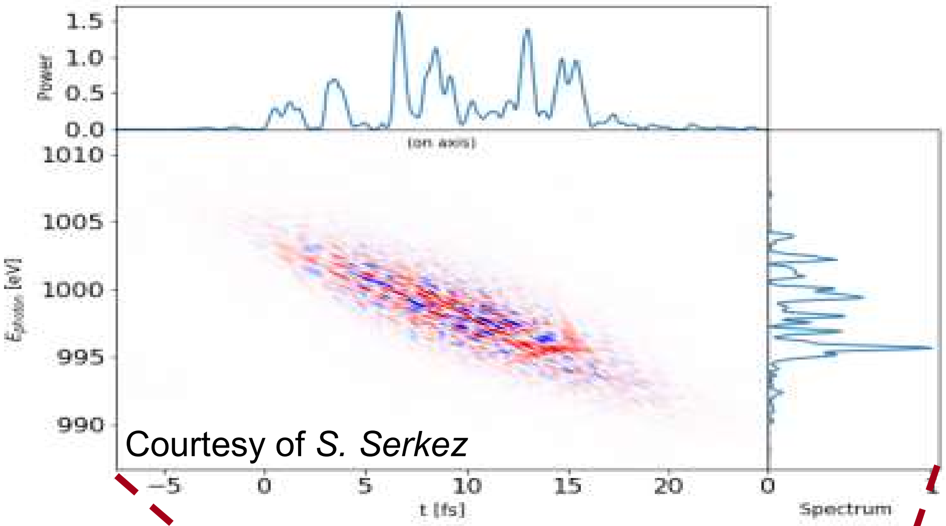
- Scalable architecture
- 48x48 prototype
- 176x192 targeted full ASIC size

- Serial encoded LVDS output
- 0.13 µm CMOS technolog
- Back end compatible wit ePix family interface

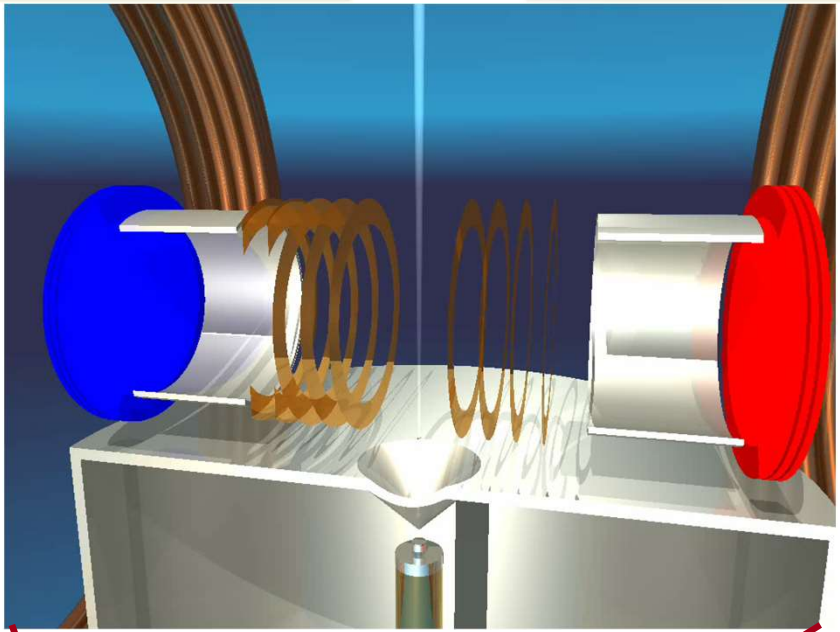
	Tixel
Matrix size	192 x 176
Readout BW	8 Gbps
Links	x8 LVDS
Encoding	10/12b
Bits / event	40
Readout full-frame	202 µs
Max chip hit rate	165 Mhits/s
Max hit rate area	49 Mhit/s/cm^2
Camera x16 ICs	2640 Mhits/s



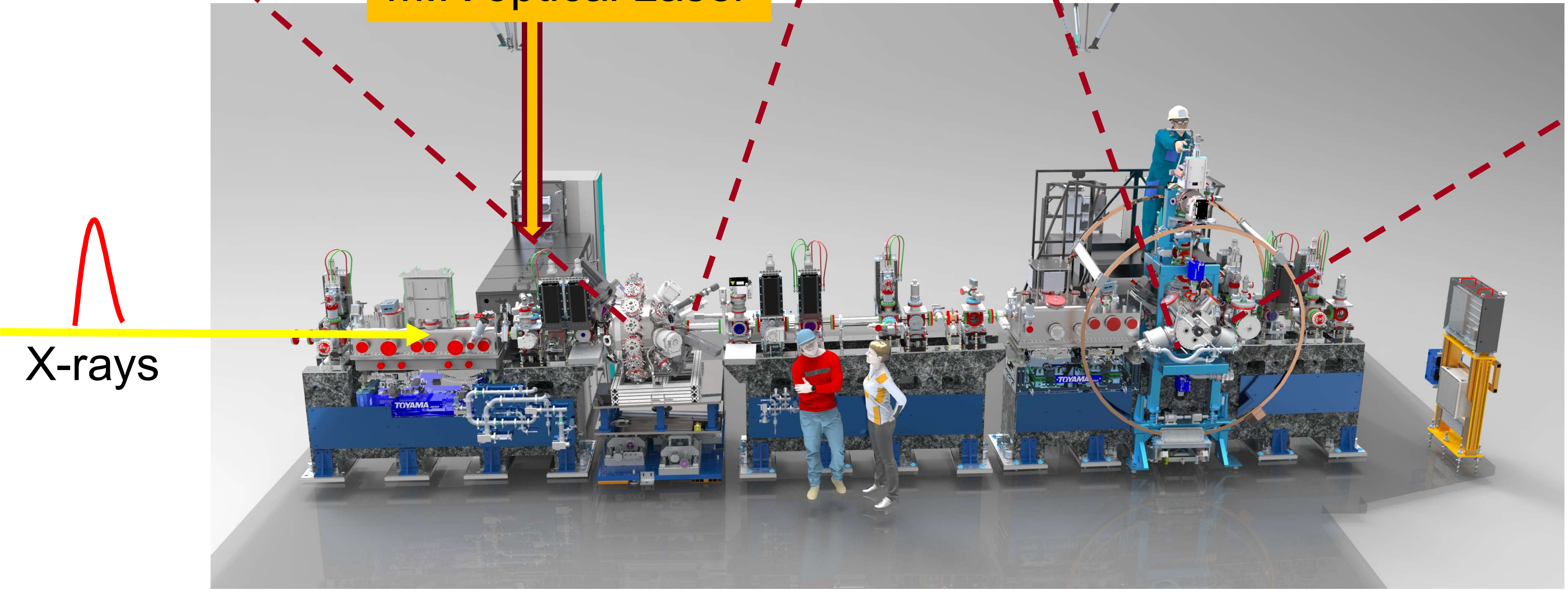
TMO – the new standard of charged particle spectroscopy



Courtesy of *S. Serkez*



MIR optical Laser

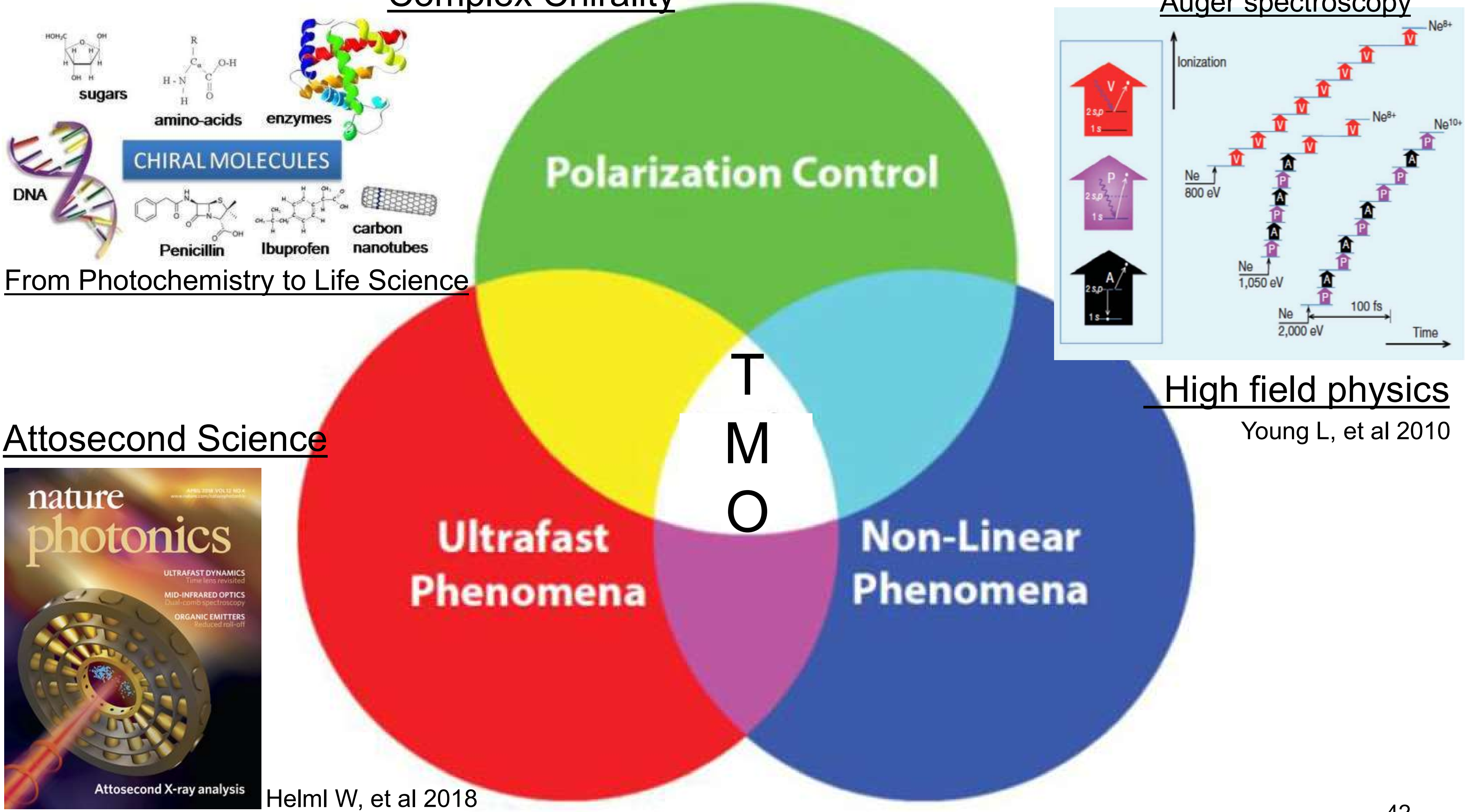


X-rays

L2SI – Schedule (Instruments ready for X-rays)

	Task	Date
CuRF	**TMO: IP1 (LAMP, cVMI, MPES)**	**10/2020**
CuRF	RIX (ChemRIX)	12/2020
CuRF	RIX (SurfSpec)	08/2021
CuRF	RIX (qRIX)	01/2022
CuRF	RIX (k-microscope)	01/2022
CuRF	**TMO: IP1 (MRCOFFEE)**	**02/2022**
CuRF	**TMO: IP2 (DREAM)**	**03/2022**
SCRF	RIX (qRIX)	07/2022
SCRF	**TMO: IP2 (DREAM)**	**07/2022**
SCRF	**TMO: IP1 (MRCOFFEE)**	**07/2022**
SCRF	RIX (k-microscope)	09/2022
SCRF	RIX (SurfSpec)	12/2022
SCRF	TXI	01/2023

Future Scientific Impact of TMO



Complex Chirality

From Photochemistry to Life Science

From non-linear photo-processes to resonant Auger spectroscopy

High field physics

Young L, et al 2010

Attosecond Science

Helml W, et al 2018

From charge migration, EWP and correlation to fs charge transfer involving nuclear rearrangement