



Technical Advisory Committee

HSS Endstation: Construction Progress and Experiment Planning

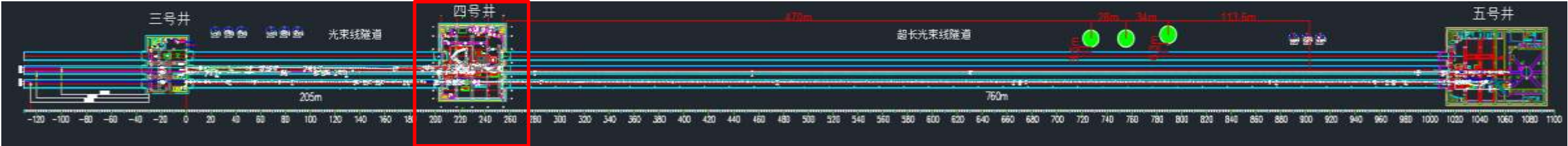
Kaiyu Zhang

Department of FEL-I, SHINE

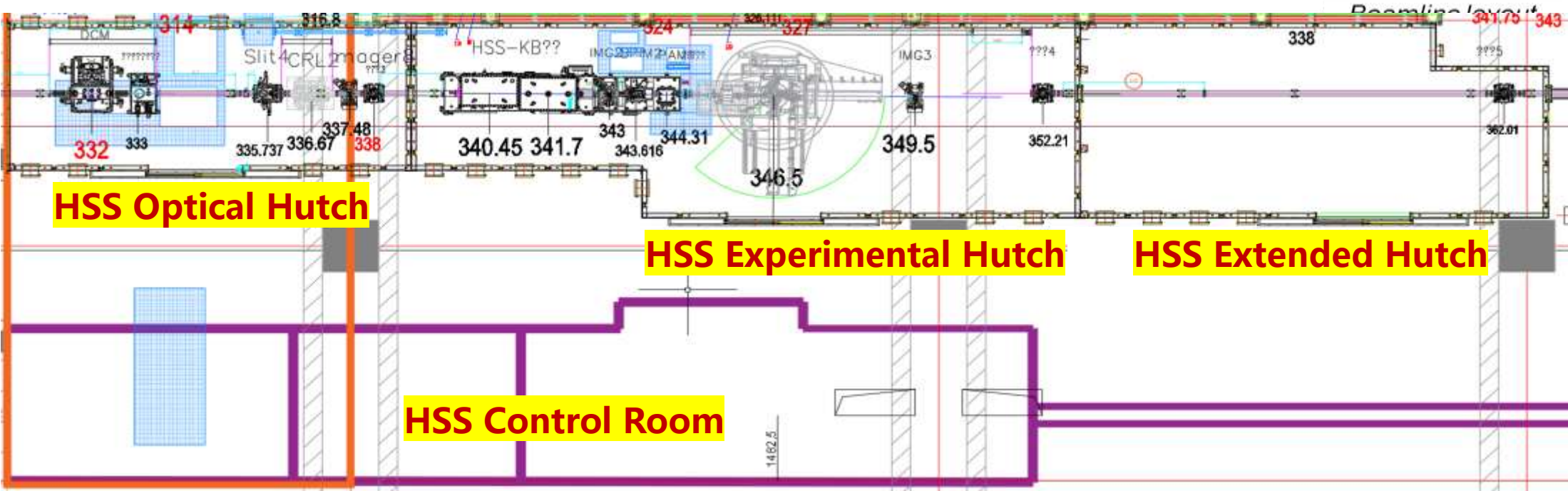
Center for Transformative Science, ShanghaiTech

October 19-21, 2026

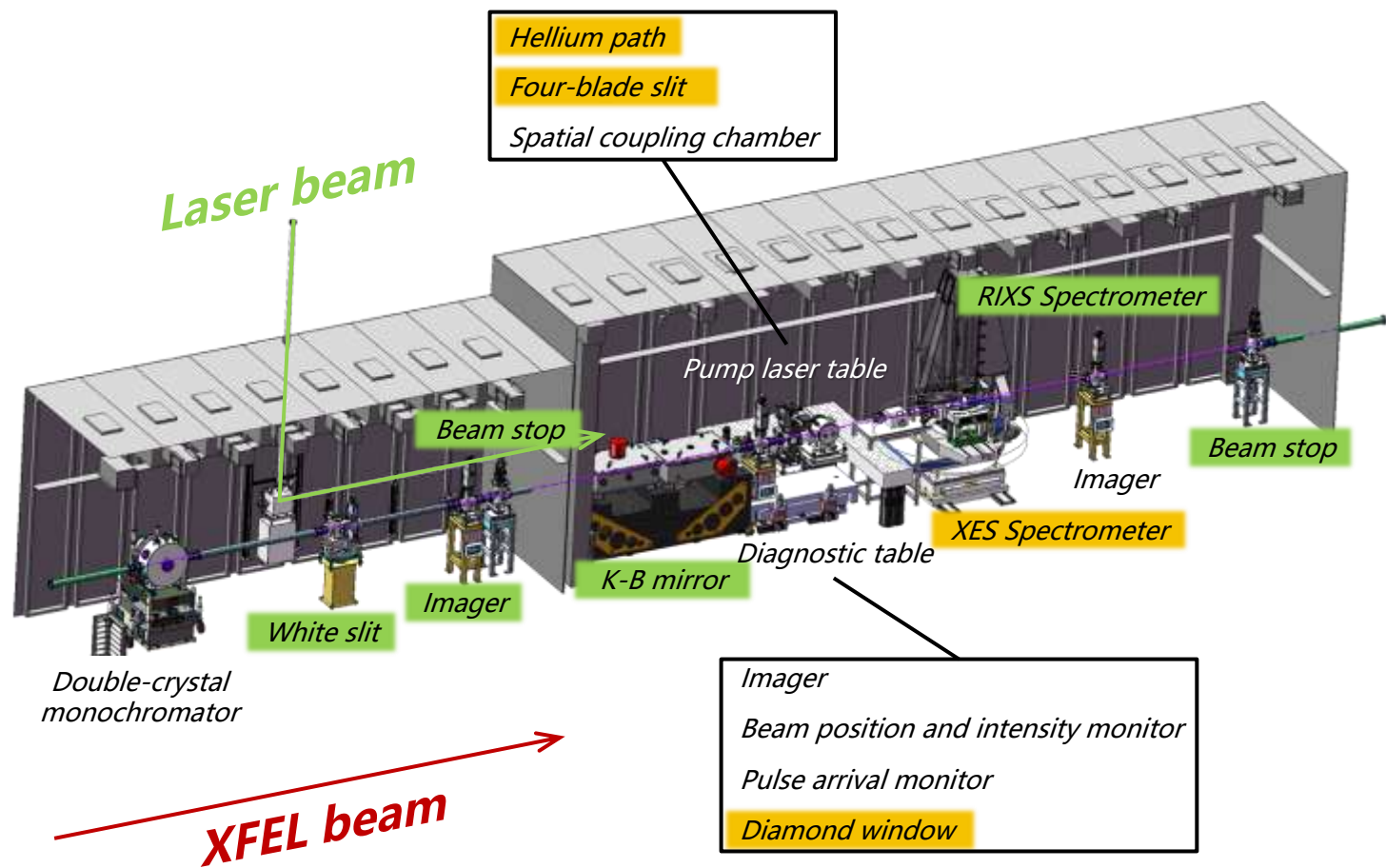
LOCATIONS AND LAYOUT



HSS locates near the experimental hall in FEL-I beamline (shaft # 4)



Hard X-ray Scattering and Spectroscopy endstation



Main Parameters	Values
Energy range	3~15 keV
Pulse energy @8GeV/100pC	170 μ J @ 7 keV 80 μ J @ 12.4 keV
Monochromator Energy resolution	Si(111): 2E-4 @ 3-15 keV Si(311): 5E-5 @ 5.6-15 keV
Type of focusing	K-B & (CRL in the future)
Focal spot size at sample (H×V, FWHM)	6 μ m~200 μ m
Detector	Jungfrau 0.5M Jungfrau 4M
Pump laser	1030 nm, FHG, THG, SHG 400-2500 nm, OPA 80 mJ/cm ² @ 420 nm & 100 μ m focal spot size
$\Delta E/E$	4E-5
ΔT	~ 100 fs

INSTALLATION PROGRESS OVERVIEW



2024.10.31



2025.6.20



Optical Hutch



K-B mirror



RIXS spectrometer



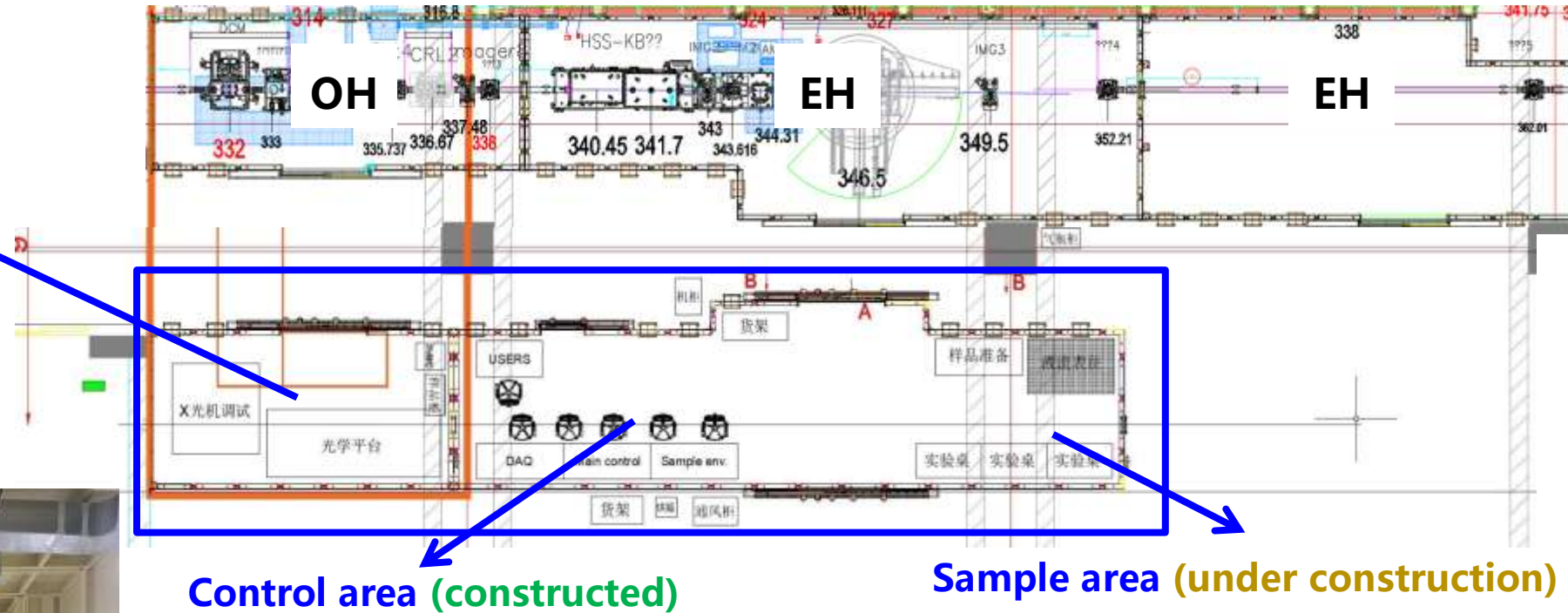
- 2020-2024 CDR & TDR
- 2025.10.22 TAC meeting, 90% Contract signing
- 2026.04.21 TAC meeting, Preparing for online installation
- 2026.07 Starting online installation
- 2026.08 White slit, Imager, Beam stop, K-B mirror installed
- 2026.09 RIXS spectrometer, Beam stop installed
- 2026.10.19 TAC meeting, Helium path, Sample system, XES spectrometer offline integrated and under testing
- 2027.03 Complete online installation and debugging
- 2027.04 All ready for XFEL
- 2027.10 Complete commissioning
- 2027.11 Achieving the acceptance criteria

7/16 equipments has been installed online

HUTCH ROOM PROGRESS

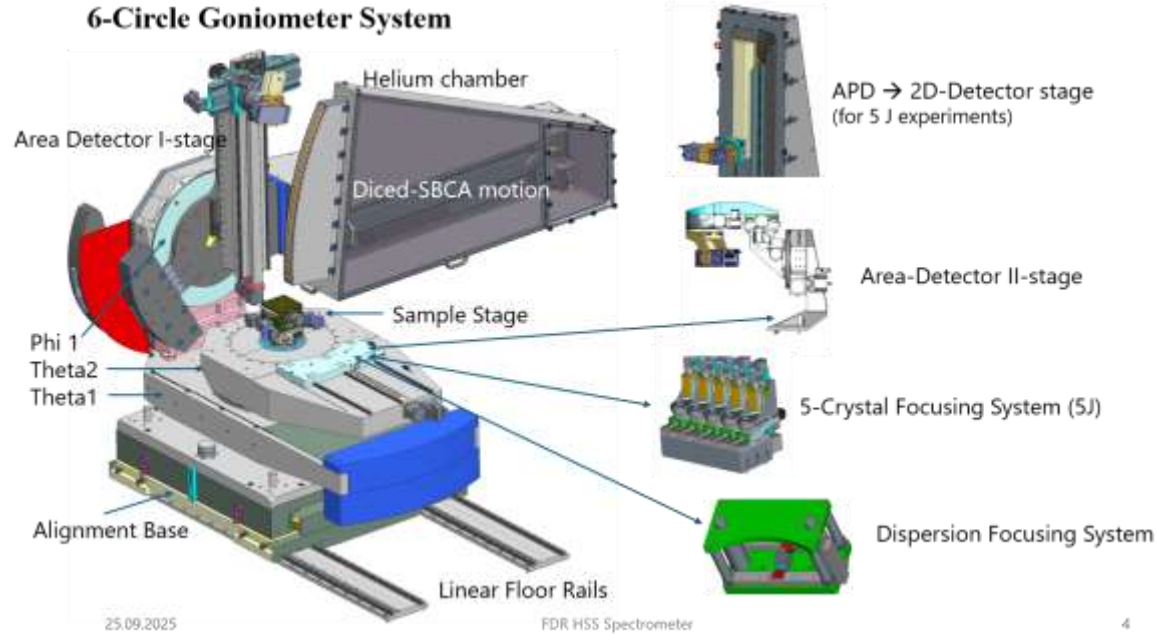


Offline Installing & Testing
for Bent Crystal,
Spectrometer Modules,
Coupling, ...
(under construction)



INSTRUMENTS PROGRESS

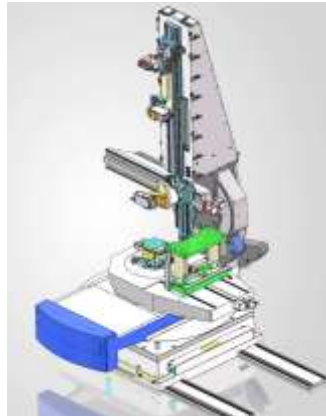
RIXS Spectrometer System



- The mechanical system has been installed, the JF detector, Crystals, and other parts will be integrated next month.
- Currently setting different configuration modes and developing control system by using SPEC and EPICS.

- **2021-2024** *CDR &TDR*
- **2024.12** *Contract signed*
- **2025.03** *PDR completed*
- **2025.09** *FDR completed*
- **2026.07** *FAT completed*
- **2026.09** *Delivery & install*

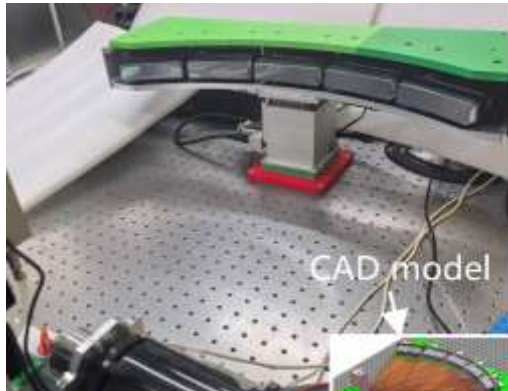
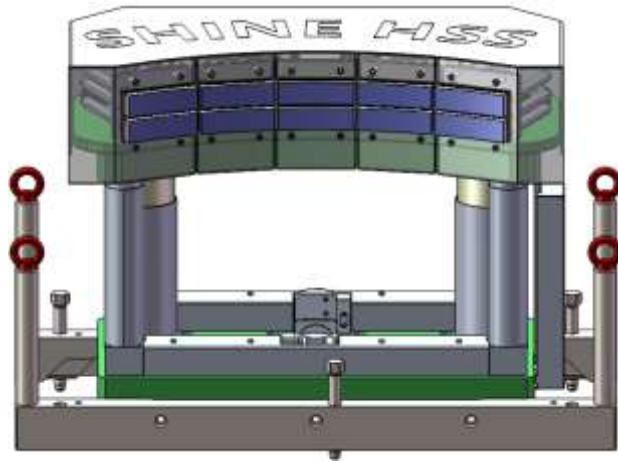
Acceptance criteria
 $\Delta E/E = 4 \times 10^{-5}$



INSTRUMENTS PROGRESS



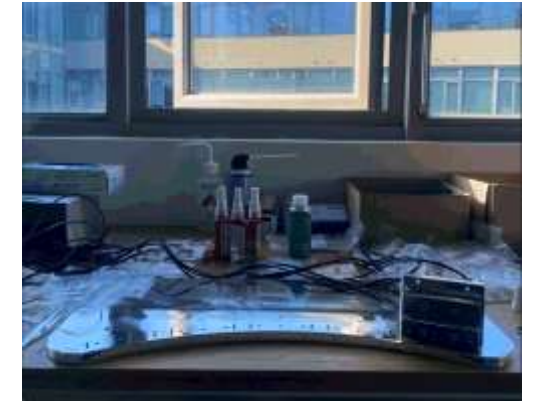
XES Spectrometer System



offline 1×5 module

- The XES spectrometer is developed and installed by ourself based on our offline technical identification of 1×5 analyzer array module.
- Currently performing the offline measurements, and updating the control system GUI, debugging with JF 0.5M DAQ.

- **2025.10** *CDR & TDR completed*
- **2025.12** *offline successfully identified*
- **2026.08** *All contracts signed*
- **2026.10** *Delivery & install*
- **2026.11** *Integration on RIXS spectrometer*



30 Axis Motor controllers & rack

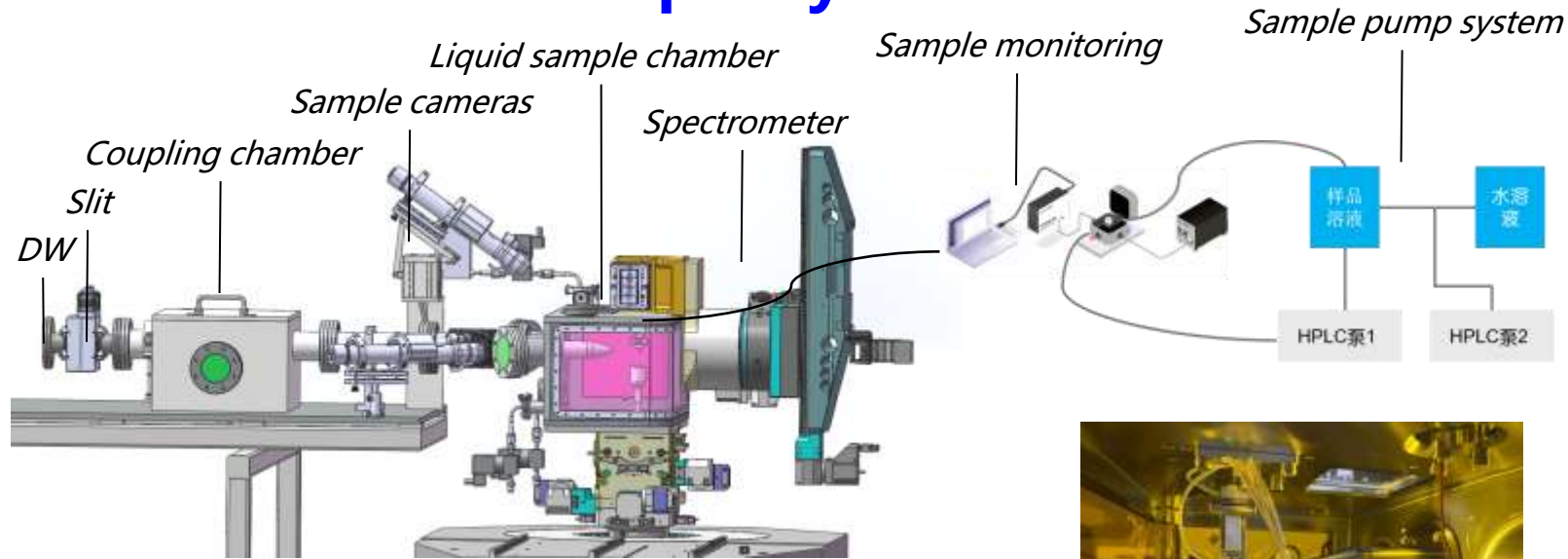


Assembled spectrometer

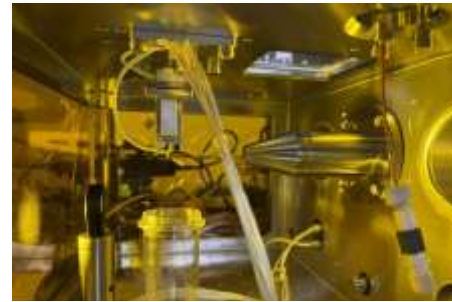
INSTRUMENTS PROGRESS



Helium Path and Sample System



Liquid sample pump



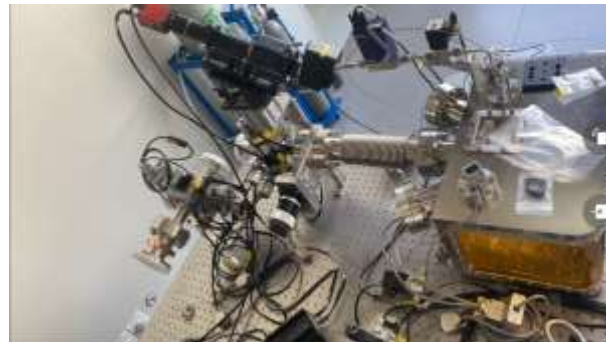
Liquid sample chamber



Liquid jet



Extended support laser table

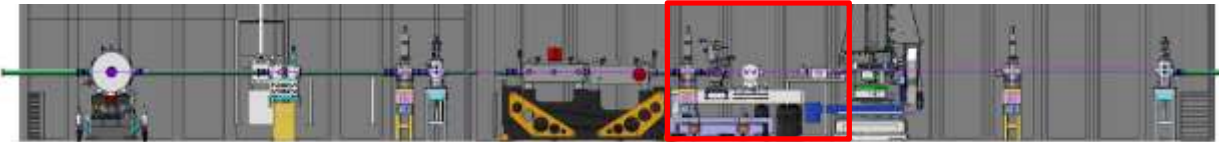


Helium path

SHINE

- 2025 CDR & TDR
- 2026.02 Contracted signed
- 2026.05 FDR completed
- 2026.09 Delivery & install
- 2027.01 Integration online

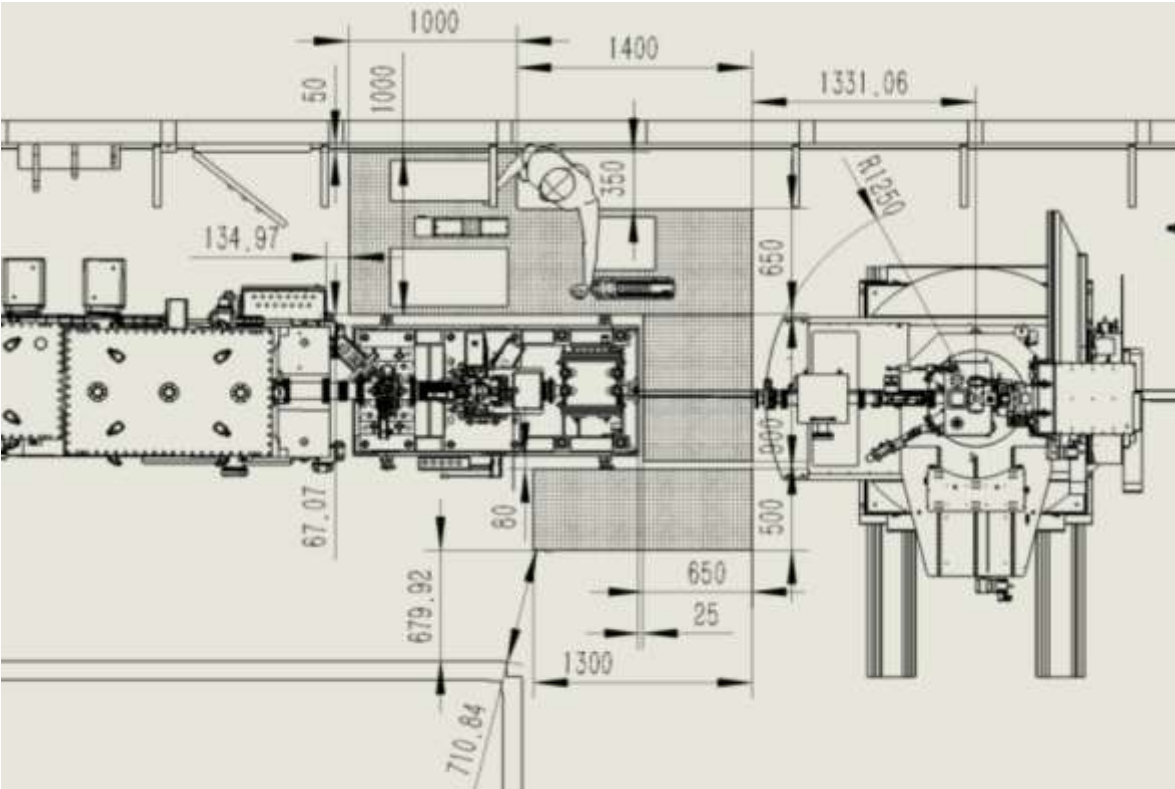
INSTRUMENTS PROGRESS



Pump Laser System

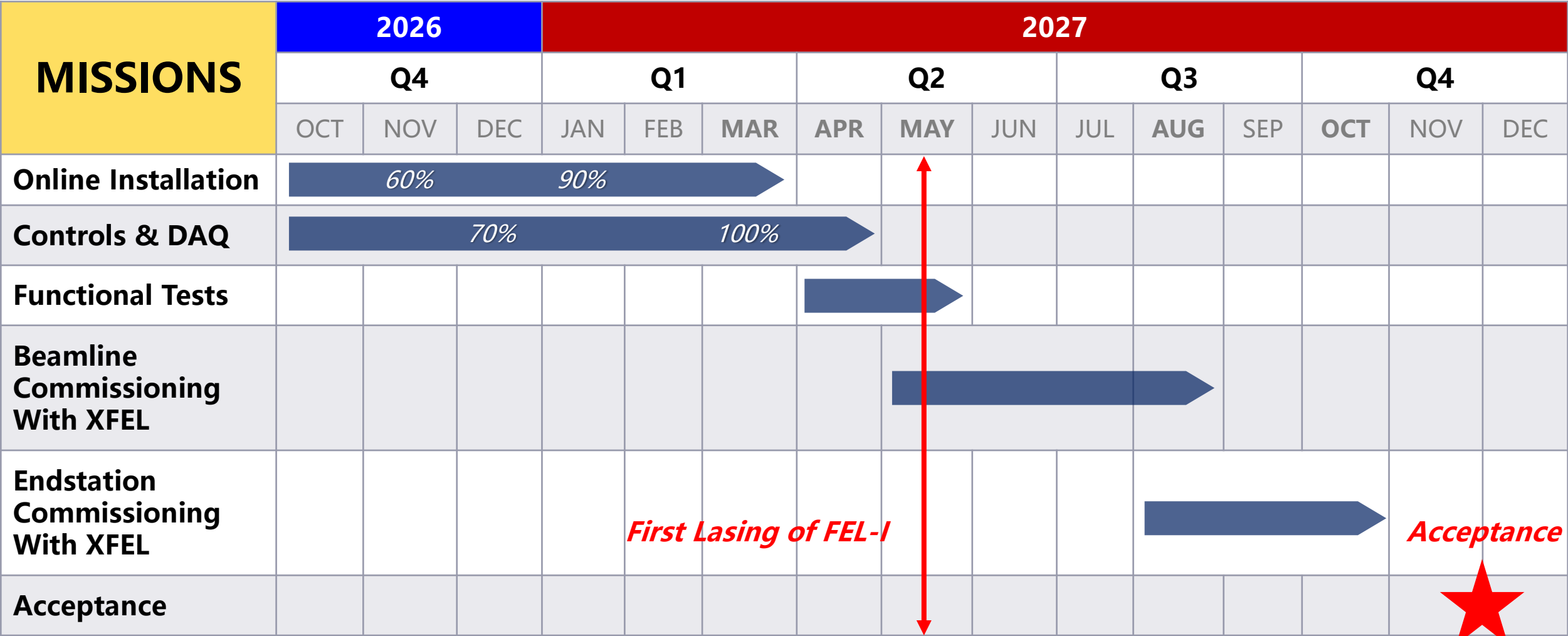
Current Status: Under design
Proposed Installation: Mar. 2027

- The table size has been decided and is under manufacturing
- The laser layout, spatial coupling, pulse arrival monitor are under designing.



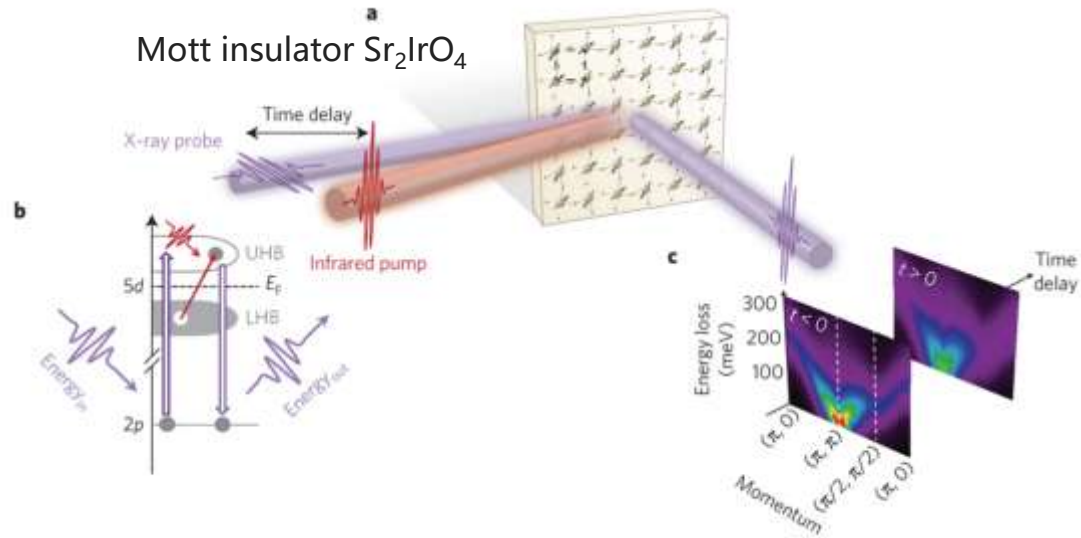
Pump laser parameters	
• Central wavelength	1030 nm
• Wavelength conversion	FHG (257 nm), THG (343 nm), SHG (515 nm) OPA (400~2500 nm)
• Repetition rate	≤100 kHz
• Pulse duration (FWHM)	≤50 fs @ 1030 nm
• Laser spot size at sample • (1/e ² diameter)	50~500 μm
• Fluence at sample (mJ/cm ²)	80mJ/cm ² @ 100 um spot size, 420 nm
• Time delay resolution	5 fs
• Time delay range	-10~1000 ps

INSTALLATION AND COMMISSIONING PLAN



SCIENCE CASES — Magneton or dd transition

- Time-resolved Ir L₃ (11.215 keV) edge magnetic RIXS at *XPP, LCLS*



Pump Laser:

2 μm , ~ 100 fs, 0.5~13.8 mJ/cm^2 ,

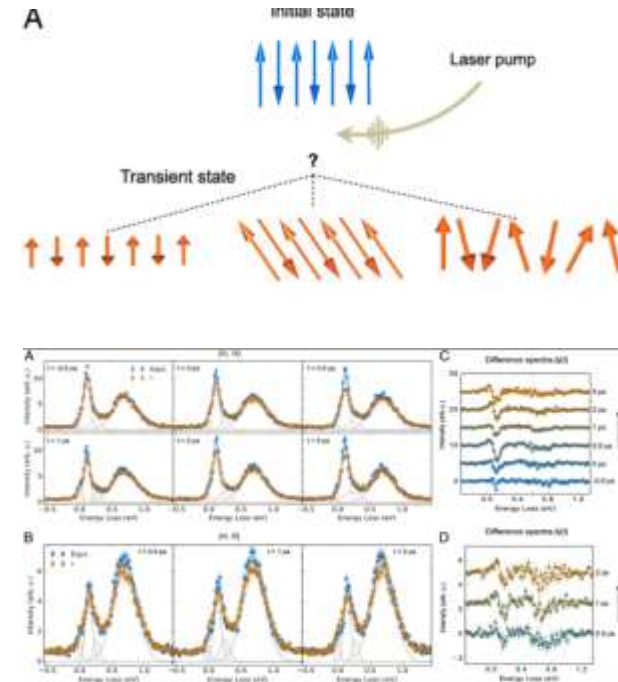
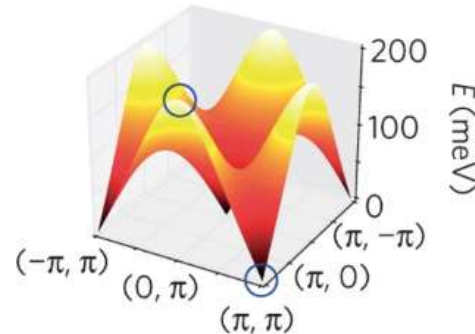
XFEL:

11.215 keV, ~ 10 fs, 120 Hz,

total E resolution ~ 70 meV

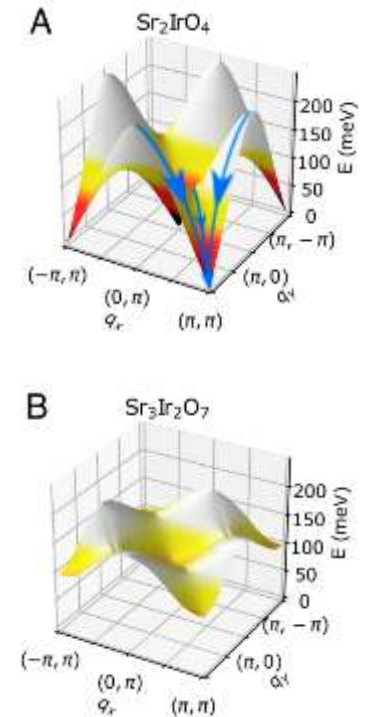
momentum resolution $\pm 0.5 \text{ \AA}^{-1}$

time resolution 500 fs



Pump Laser: 2 μm , 20 mJ/cm^2 845- μm focus;

XFEL: 11.215 keV, ~ 10 fs, 50- μm focus

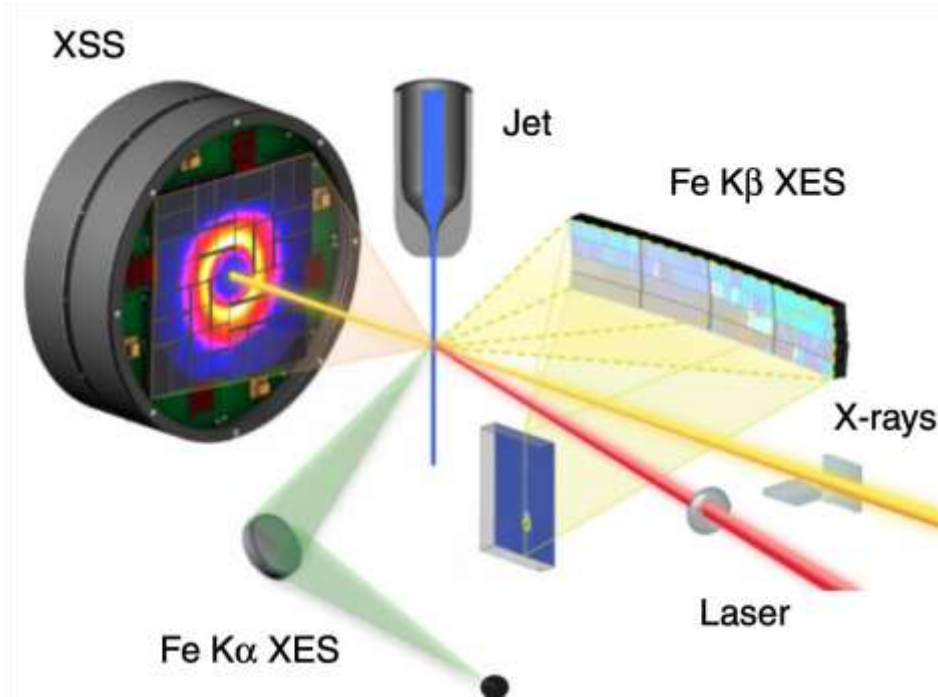


Nat. Mater. 2016, 15, 601.

Proc. Natl. Acad. Sci. 2021, 118(22), e2103696118.

SCIENCE CASES — Electronic and structural dynamics

- Time-resolved Fe K α & K β XES and XSS at *LCLS and SACLA*



Nat. Chem. (2021)
Nat. Commun. (2021)
Nat. Commun. (2020)

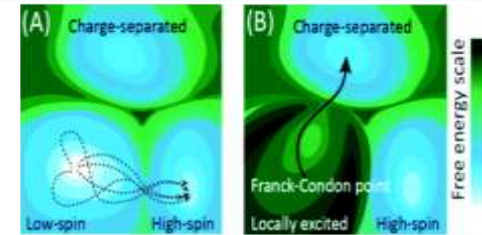
Chem. Sci. (2019)
J. Phys. Chem. B (2016)
ACS Nano (2024)

Nat. Commun. (2023)
Chem. Sci. (2023)
Nature Commun. (2015)



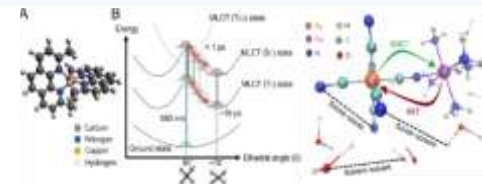
Physics

- Spin crossover
- Nuclear wavepacket motion
- Electron-phonon coupling
- Liquid-liquid phase transition



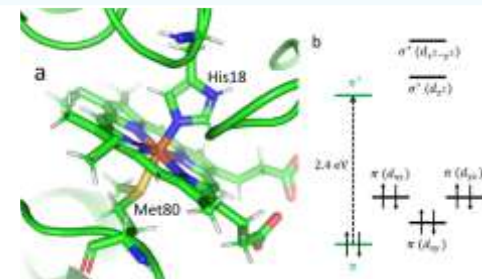
Chemistry

- Molecular dissociation and rearrangement
- Ultrafast solvation
- Multi-channel relaxation



Biology

- Photodissociation mechanism of cytochrome c
- Axial structural distortion
- Energy transfer and biological functions



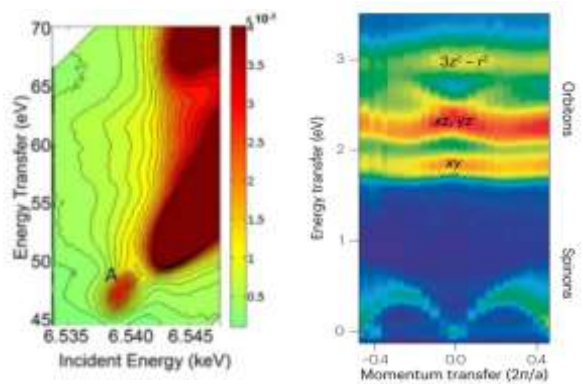
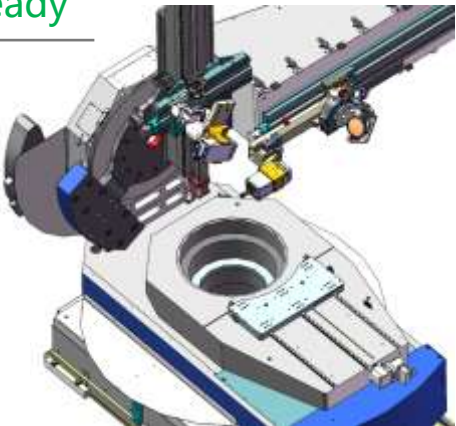
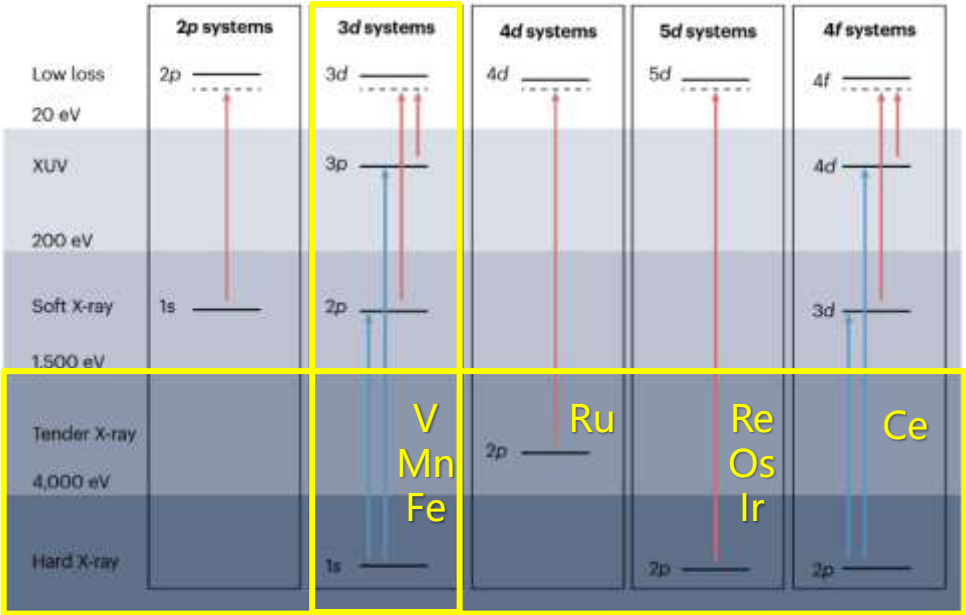
PILOT EXPERIMENTS and READINESS — RIXS



- The pilot experiments are mainly designed based on Accelerator (Energy, Element) and Beamline ($\Delta E/E$) parameters at present.

Experimental parameters

Sample	MnO (Mn^{2+}), Mn_2O_3 (Mn^{3+}), and MnO_2 (Mn^{4+}) Standard solid sample	ready
XFEL photon	Mn @ 6539 eV, Fe @ 7112 eV	
Monochromator	DCM Si(311) for dd or CT <i>try Si(333) harmonic for magnons</i>	
Spot size on sample	10 μm (V) x 30 μm (H)	
Spectrometer	RIXS spectrometer	ready
Detectors	Jungfrau 0.5M, accumulation mode	ready



RIXS is more for acceptance $\Delta E/E$ during comissioning

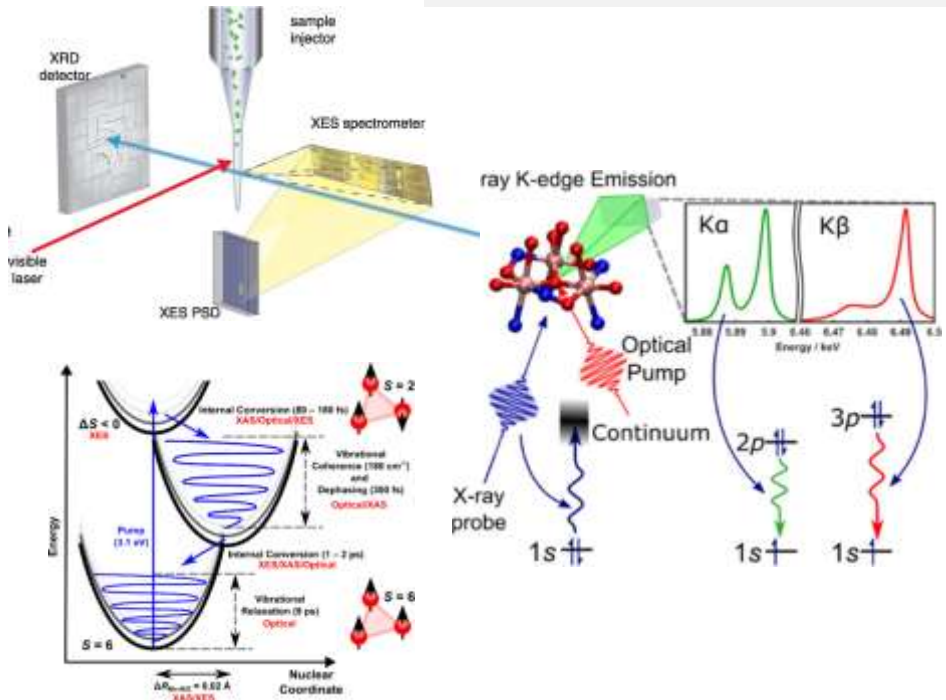
PILOT EXPERIMENTS and READINESS — tr-RXES+XSS

- Photochemical Dynamics of Photoinduced Spin Crossover in $[\text{Fe}(\text{bpy})_3]^{2+}$
- Photoinduced Jahn–Teller Distortion in $\text{Mn}(\text{acac})_3$
- Oxidation Dynamics of the Kok Cycle in Photosystem II (PSII) Mn_4CaO_5

Experimental parameters based on the current situation

Sample	20~50 mM $[\text{Fe}(\text{bpy})_3]^{2+}$ 50-300 μm Liquid jet, Helium flow	ready
XFEL photon	$\text{Fe} \geq 7112 \text{ eV}$, 100 μJ , 30 fs	
Monochromator	DCM Si(311) or Si(111)	
Spot size on sample	10-50 μm (V) x 200 μm (H)	
Repetition rate	10 Hz - 1 kHz	
Pump laser	400-600 nm, 10-15 $\mu\text{J}/\text{pulse}$, 0.5 kHz	
Time window	-1~5 ps fine scan, 5~20 ps medium scan	
Spectrometer	XES spectrometer	ready
Detectors	Jungfrau 0.5M and 4M, 1 kHz	ready
Total time resolution	$\leq 100 \text{ fs}$	

Collaborations:
Wenkai Zhang (BNU),
Yifeng Jiang (ECNU),
Qingyu Kong (SOILEI),
Tetsuo KATAYAMA (JASRI),
Yohei Uemura (EuXFEL), *etc.*



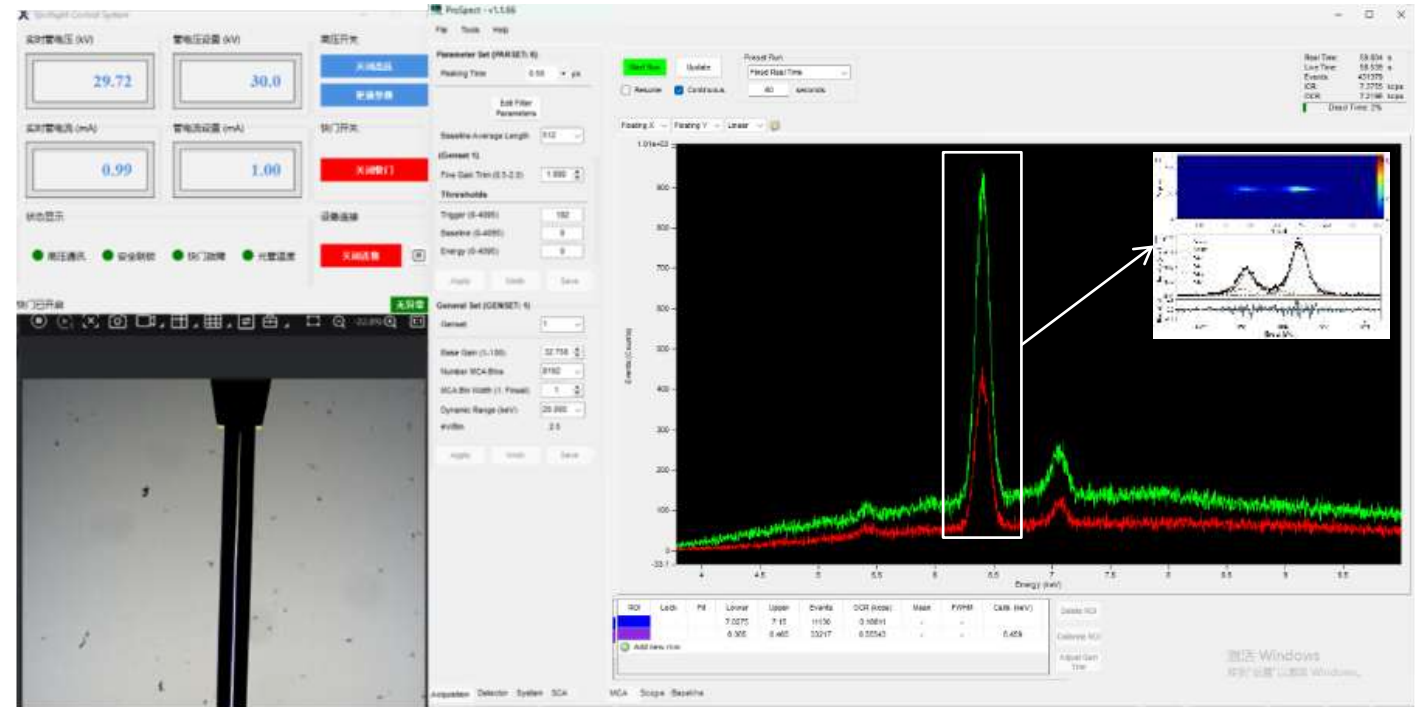
PILOT EXPERIMENTS and READINESS — LAB.



- Pre-experiments for Fe emission spectroscopy, especially for **sample system testing**.
- **Fe K_{α} and K_{β} has been collected successfully**, and will be detected with spectrometer in high energy resolution mode by the end of this year (Fe and Mn $K_{\alpha_{1,2}}$ and $K_{\beta_{1,3}}$ and $K_{\beta_{2,5}}$).
- DAQ and control system has been developed for the offline testing.

X-ray focal spot: 170 μm

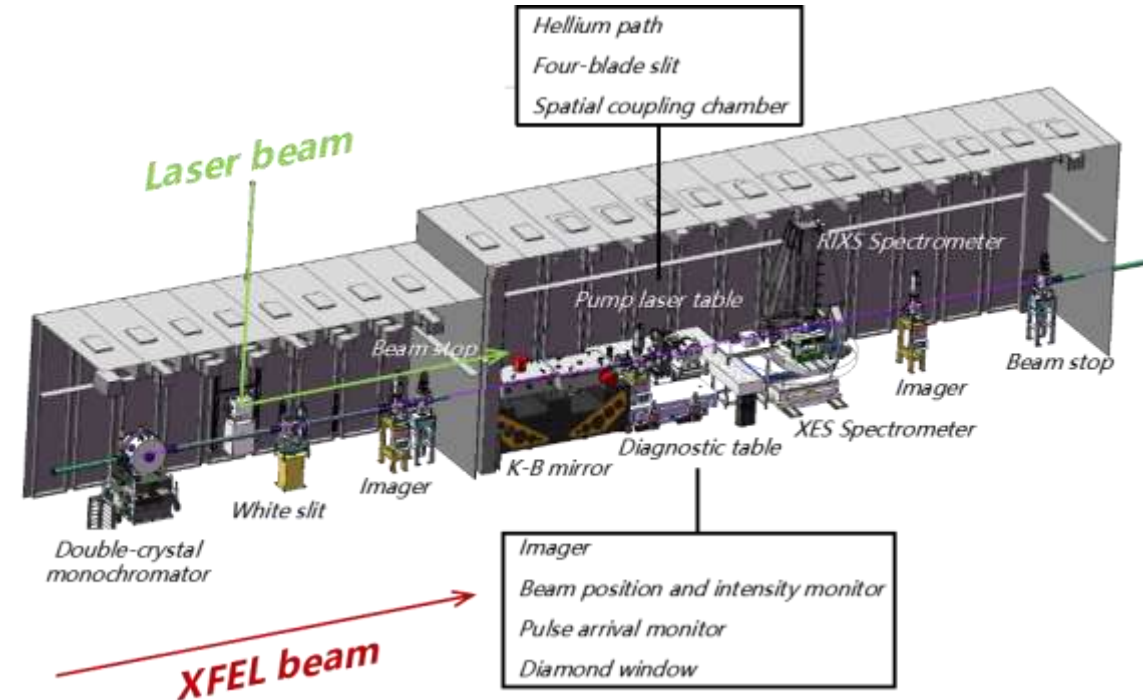
Sample: 30 mM $[\text{Fe}(\text{bpy})_3]\text{Cl}_2$ aqueous
200 μm liquid jet



OBSTACLE AND CHALLENGES

The very tight installation and commissioning period.

Beamline	1. K-B mirror performance verification
	2. Double-crystal monochromator delivery time (Mar. 2027) needs to be guaranteed
Diagnosis	1. Alignment laser system, Pulse arrival monitor, Spatial coupling chamber contracts have not been signed
Pump laser	1. Laser table delivery time (Jan. 2027) needs to be guaranteed
	2. Optical layout design and setup should be done as early as possible
Endstation	1. The very constrained space of EH
	2. The remaining contracts for acceptance and pilot experiments



It is more important for us to find out the unique features and difference between us and the LCLS-II HE, and other XFELs.

** XAS and XES is quite commonly and widely usefull.
But what is the real important and those community needs to be identified.*

1. Hard RIXS spectrometer
2. Tender X-ray region
3. Methodological combination

ACKNOWLEDGEMENTS

We are deeply thankful to TAC meeting members, our collaborators, and many experts whose insightful suggestions were pivotal to the successful establishment of our endstation!

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-



Kaiyu Zhang



Niandu Wu



Bing Li



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