

X-ray Diffraction and Spectroscopy Beamlines

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²Byeong-gwan Cho and ¹Ki-Jung Kim**

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²Research Center for Beamline, Korea Basic Science Institute

Nov. 06, 2025

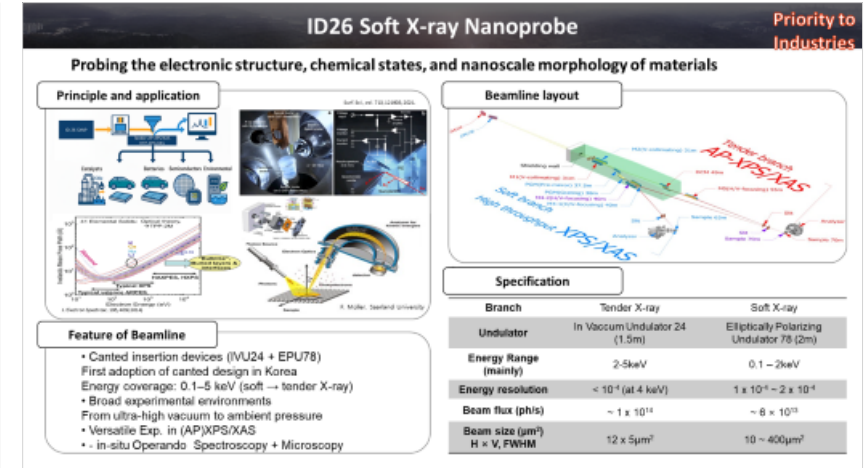
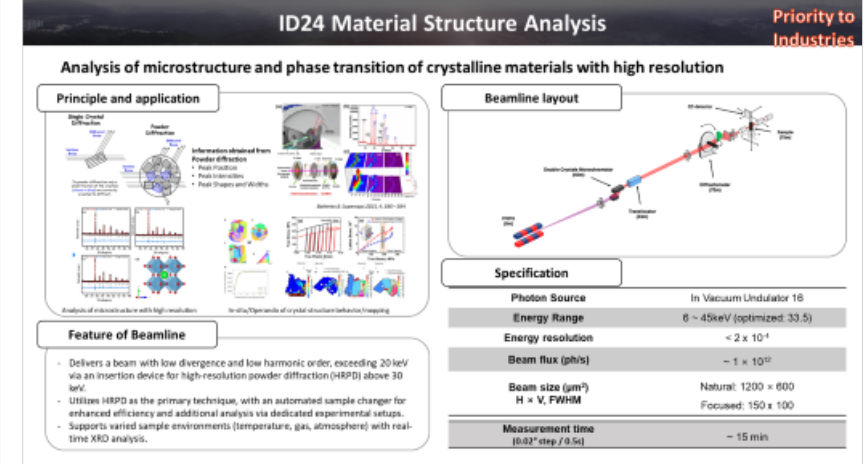
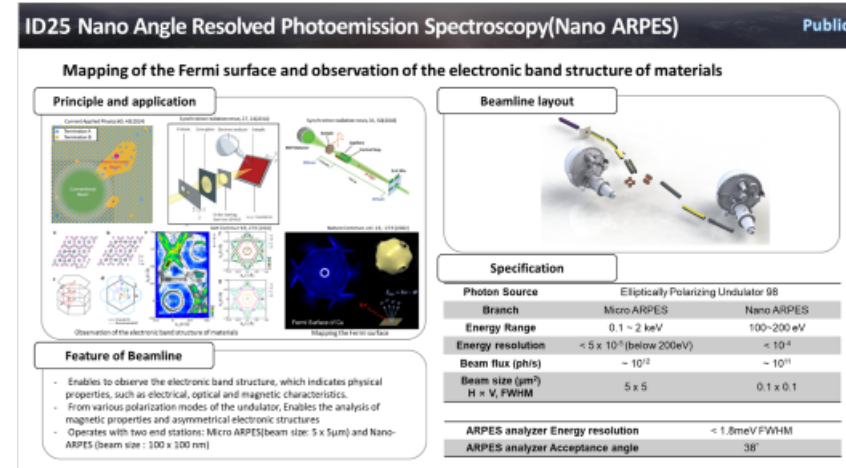
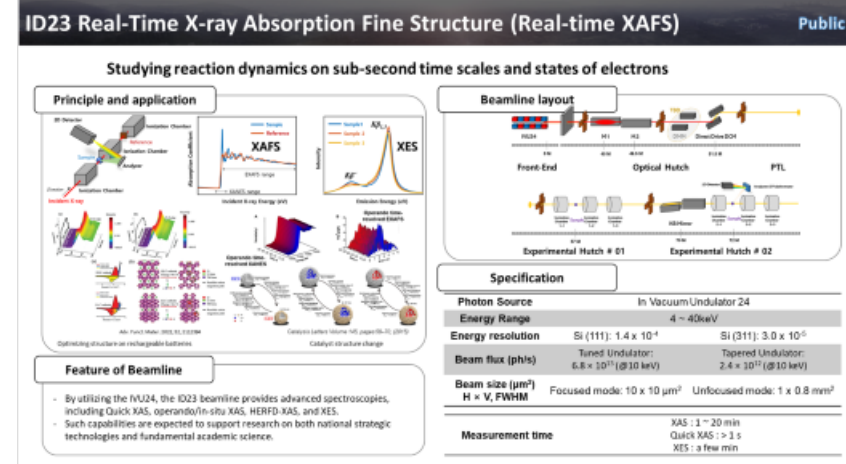
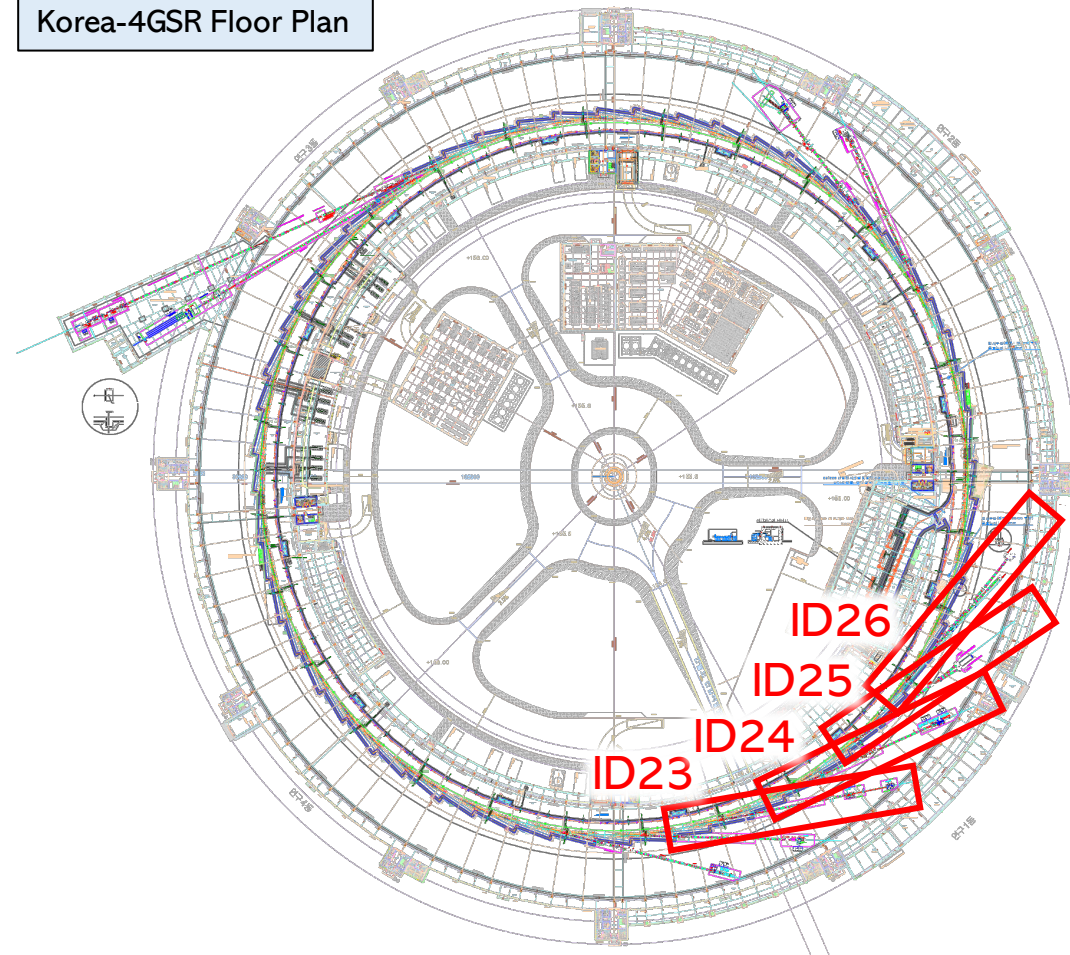


Outline

1. Overview
2. ID23 Real-Time XAFS
3. ID24 Material Structure Analysis
4. ID25 NanoARPES
5. ID26 Soft X-ray Nanoprobe
6. Others

1. Overview

Korea-4GSR Floor Plan



	Real-Time XAFS	MSA	Soft X-ray Nanoprobe	nanoARPES
Light source	IVU24	IVU16	IVU24+EPU78	EPU98
Energy range [keV]	4.0 ~ 40.0	6.0 ~ 45.0 (Optimized at 33 keV)	0.1 ~ 5.0	0.05 ~ 2.0
Supports	QXAFS, XAFS, XES, HERFD-XAS	HRPD, in-situ XRD, XAFS	XPS/XAS/SPEM	ARPES
Beam size (h x v, FWHM)	- Focused mode: $1 \times 1 \mu\text{m}^2$ - Unfocused mode: $1 \times 0.5 \text{ mm}^2$	$1 \times 0.5 \text{ mm}^2$	- Tender-B: $5 \times 12 \mu\text{m}^2$ - Soft-B: $36 \times 14 \mu\text{m}^2$	- micro-ARPES: $10 \times 10 \mu\text{m}^2$ - nano-ARPES: $0.1 \times 0.1 \sim 1 \times 1 \mu\text{m}^2$
Beam flux (ph/s)	- Tuned Undulator: $> 1.0 \times 10^{13}$ (@10 keV) - Tapered Undulator: $> 1.0 \times 10^{12}$ (@10 keV)	$> 1.0 \times 10^{12}$ (@33 keV)	- Tender-B: 1.5×10^{12} - Soft-B: 6.3×10^{11}	- micro-ARPES: $> 1.0 \times 10^{13}$ - nano-ARPES: $1.0 \times 10^{11} \sim 1.0 \times 10^{12}$

1. Overview

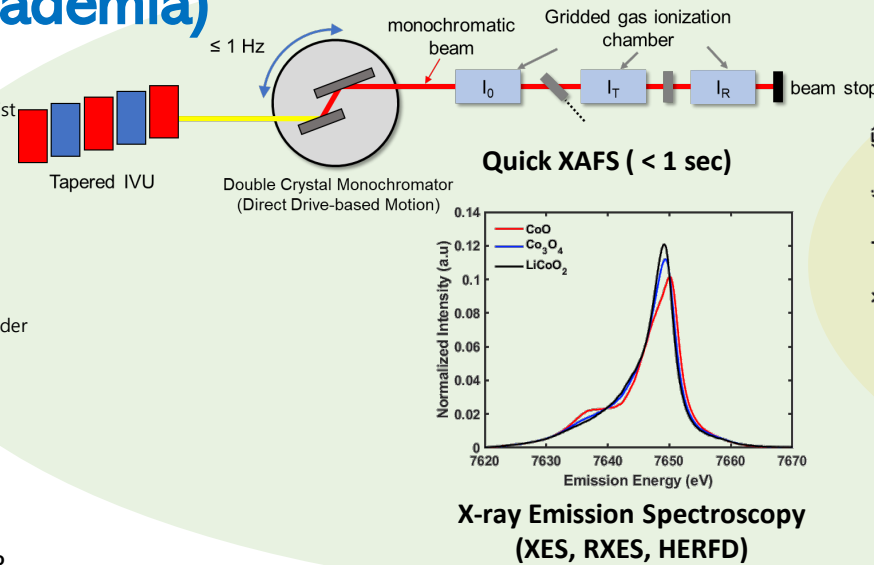
ID23 Real-Time XAFS

(Academia)

(PAL) Kug-Seung Lee
ID23 Beamline Advisor
PLS-II 8C Beamline Scientist

(PAL) In-Hui Hwang
ID23 Beamline Scientist
X-ray Science Group Leader

(KBSI) Byeng-Gwan Cho
ID23 Beamline Scientist



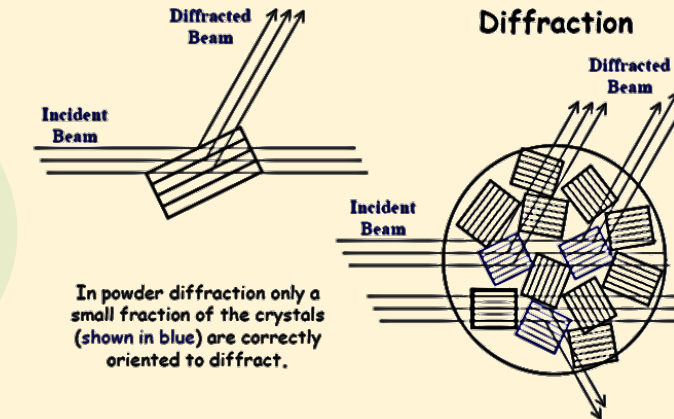
X-ray Absorption Spectroscopy (XAFS)

ID24 Material Structure Analysis

(Industry)

Single Crystal Diffraction

Powder Diffraction



Powder Diffraction (HRPD, In-situ XRD)

(PAL) Tae-Yeong Koo
Korea-4GSR Beamlines Advisor

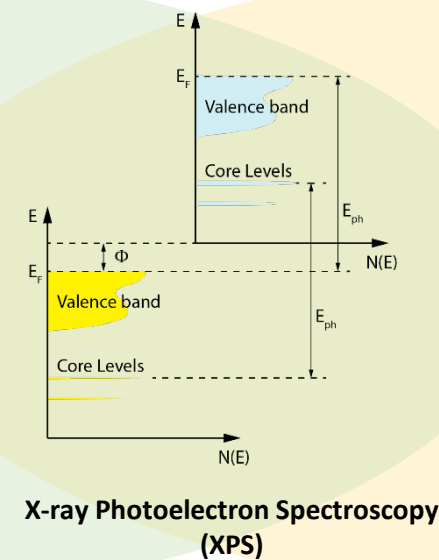
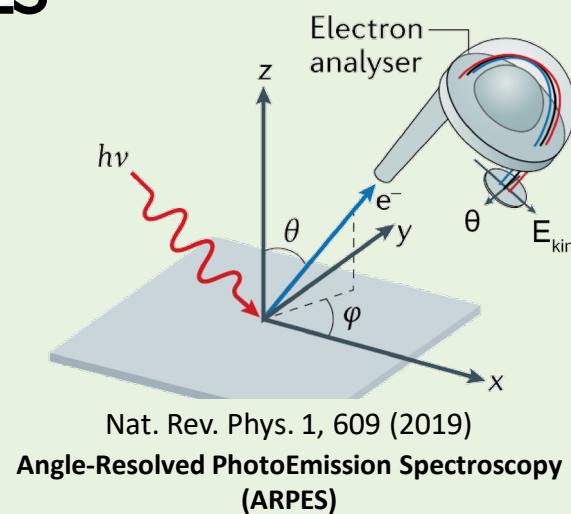
(PAL) Changwan Ha
ID24 Beamline Scientist

ID25 NanoARPES

(Academia)

(PAL) Byeong-Gyu Park
ID25 Beamline Advisor
PLS-II 4A1 Beamline Scientist

(KBSI) Sae Hee Ryu
ID25 Beamline Scientist



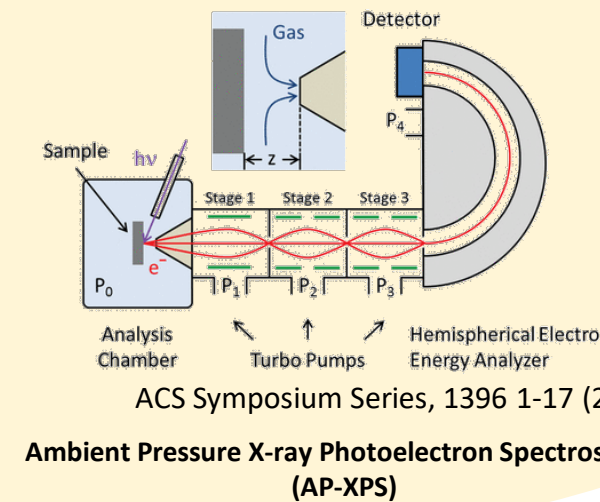
ID26 Soft X-ray Nanoprobe

(Industry)

(PAL) Ki-Jung Kim
ID26 Beamline Advisor
Deputy Director

(PAL) Jaeyoon Baik
ID26 Beamline Advisor
PLS-II 8A1 Beamline Scientist

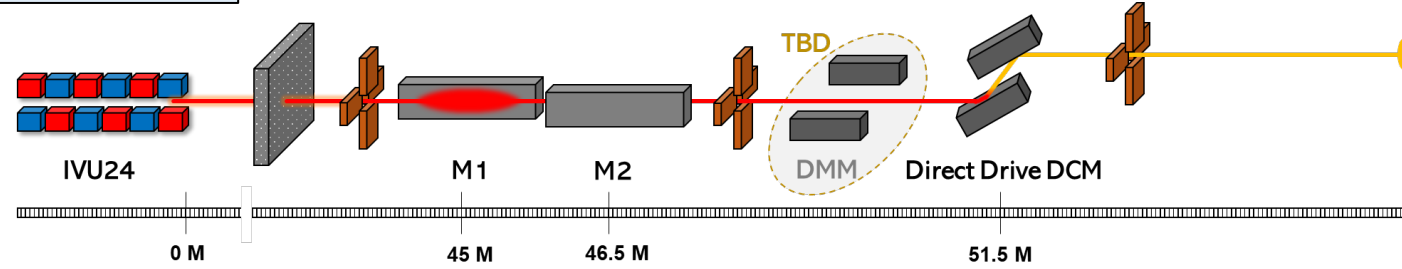
(PAL) Siwoo Noh
ID26 Beamline Scientist



ACS Symposium Series, 1396 1-17 (2021).

2. Real-Time XAFS

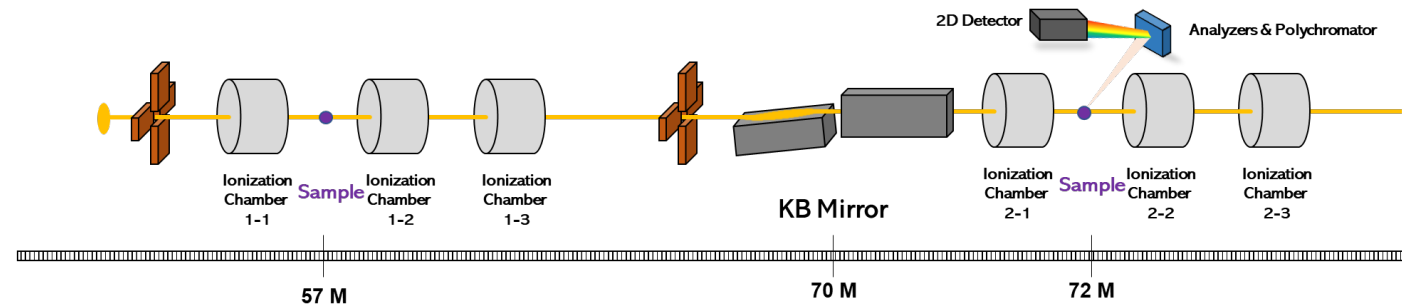
Beamline Layout



Front-End

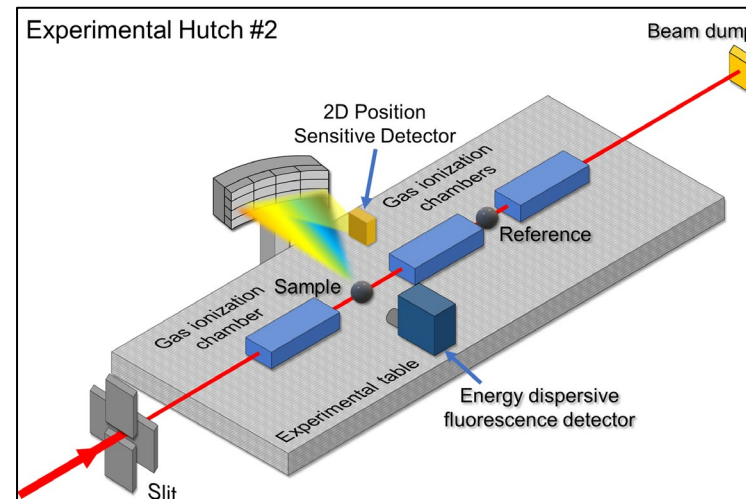
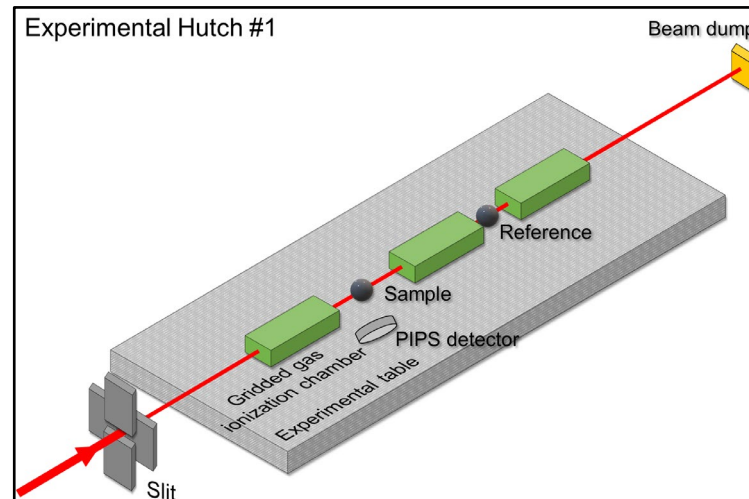
Optical Hutch

PTL



Experimental Hutch # 01

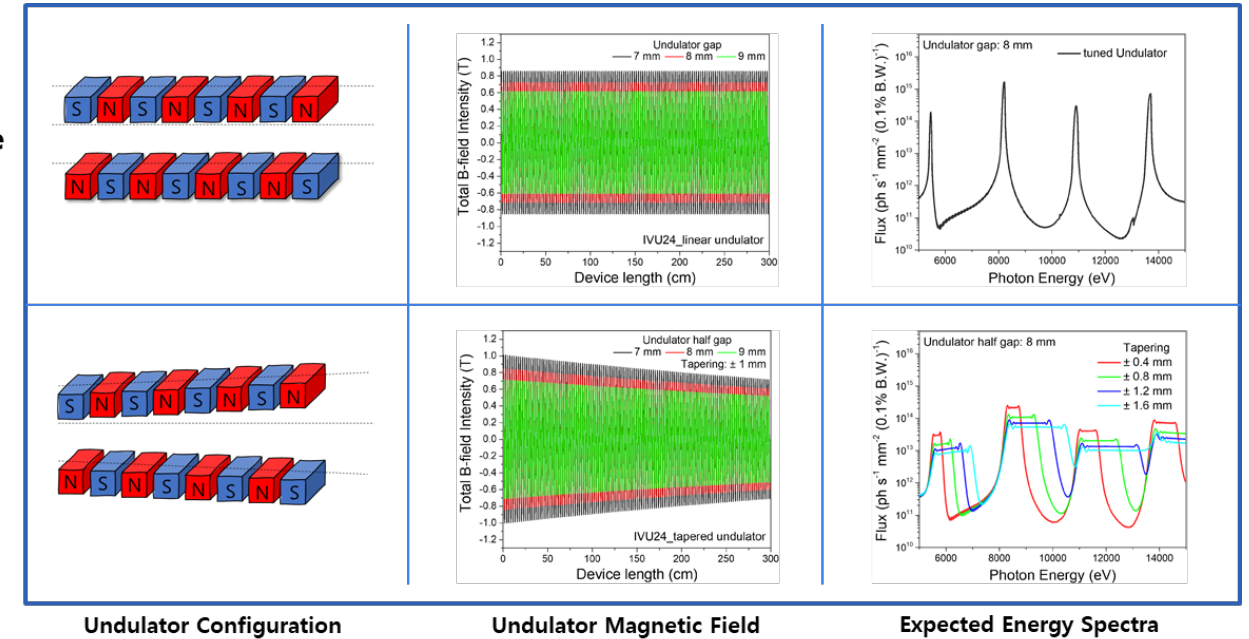
Experimental Hutch # 02



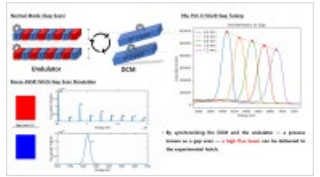
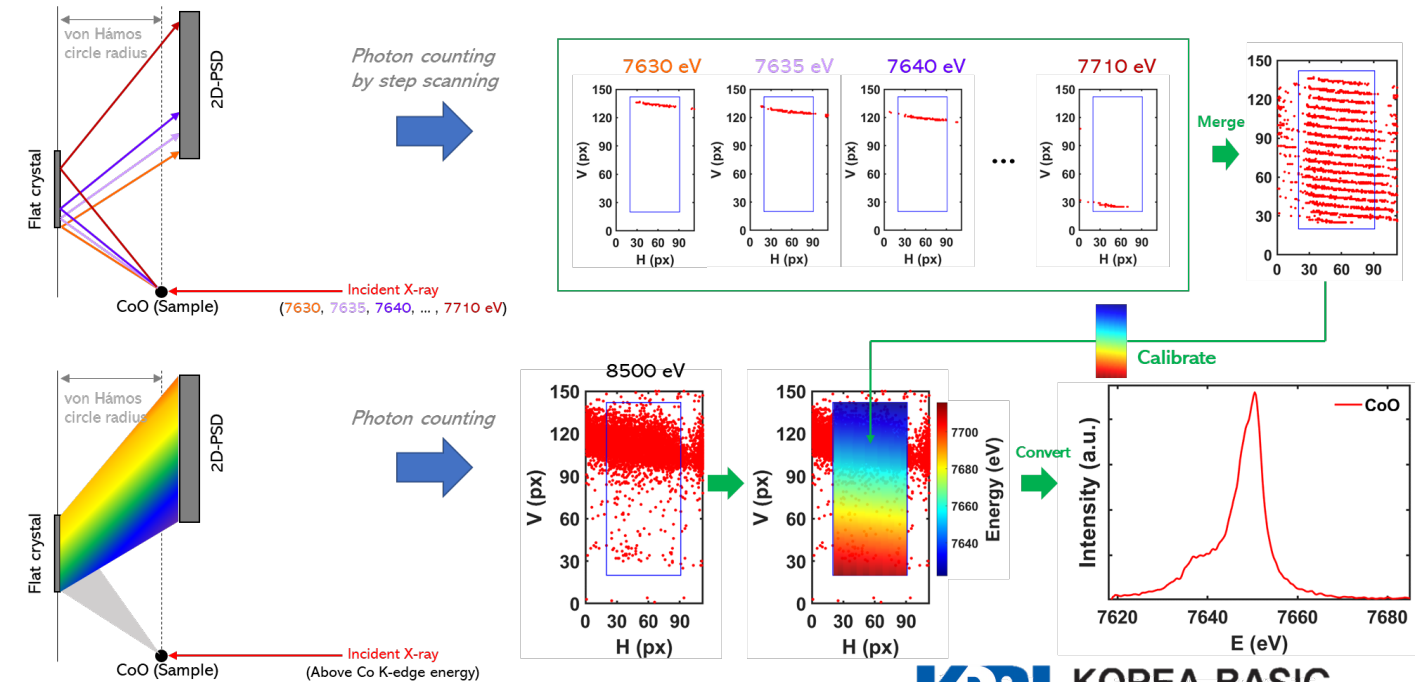
XAFS Scan

Normal mode
(Gap Scan)

Taper mode
(Quick Scan)

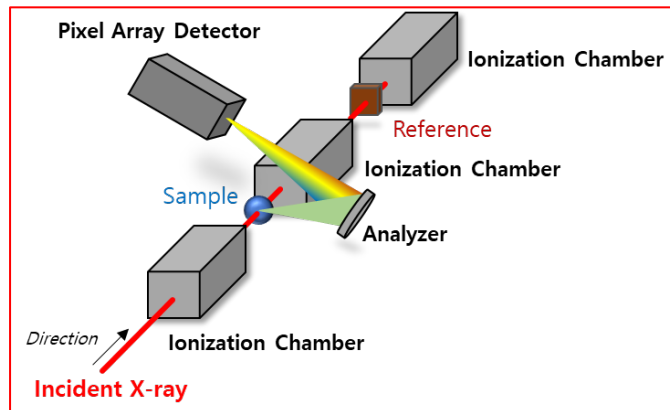


XES Scan



2-1. XAFS and XES

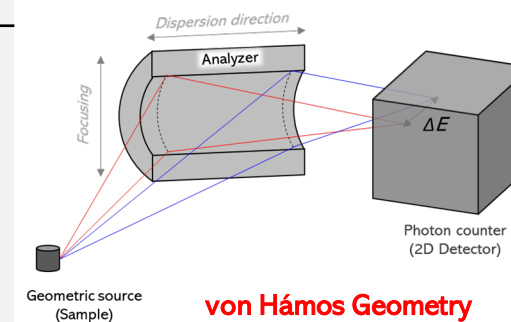
XAFS+ XES Measurement Setup



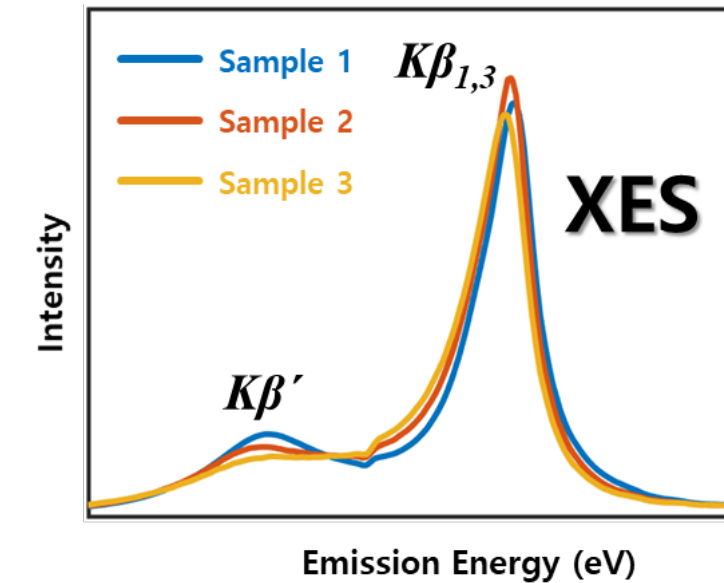
↓ XAFS Only

XES Data Acquisition

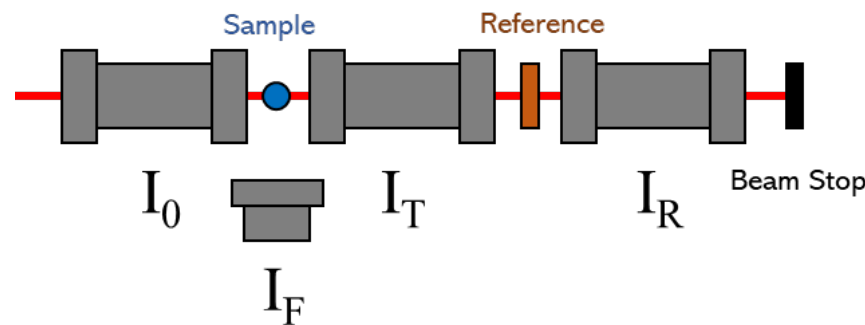
Feature	von Hámós Geometry
Crystal Shape	Cylindrically Bent
Focusing Geometry	Point-to-Line
Spectral Acquisition	Dispersive / Single-Shot (no movement needed for spectrum)
Energy Resolution	High
Measurement Speed	Very Fast (ideal for time-resolved studies)
Key Advantage	High efficiency, Single-shot capability



XES Spectra



XAFS Data Acquisition



Transmission Mode

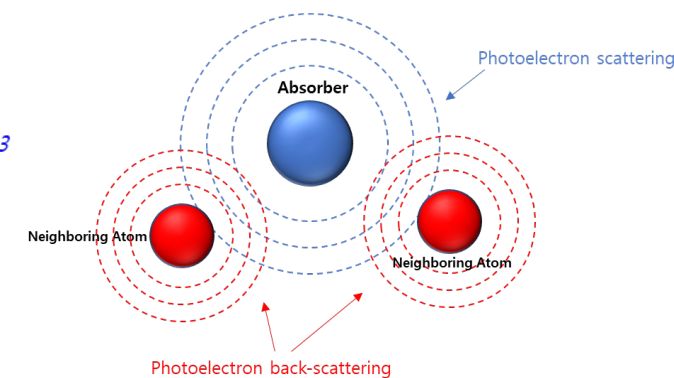
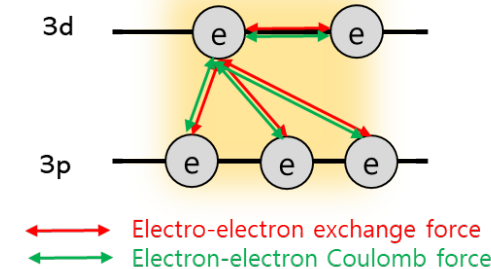
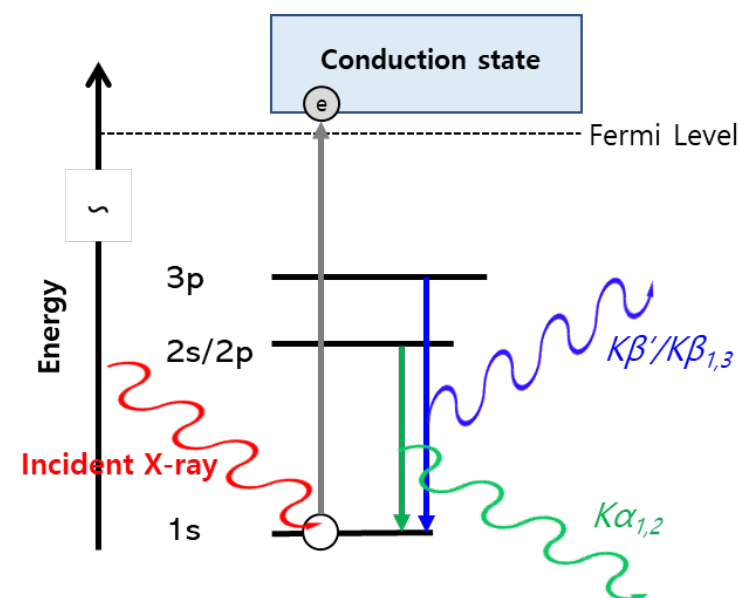
$$\mu_S(E) = \frac{1}{t} \ln \left(\frac{I_0}{I_T} \right)$$

$$\mu_R(E) = \frac{1}{t} \ln \left(\frac{I_T}{I_R} \right)$$

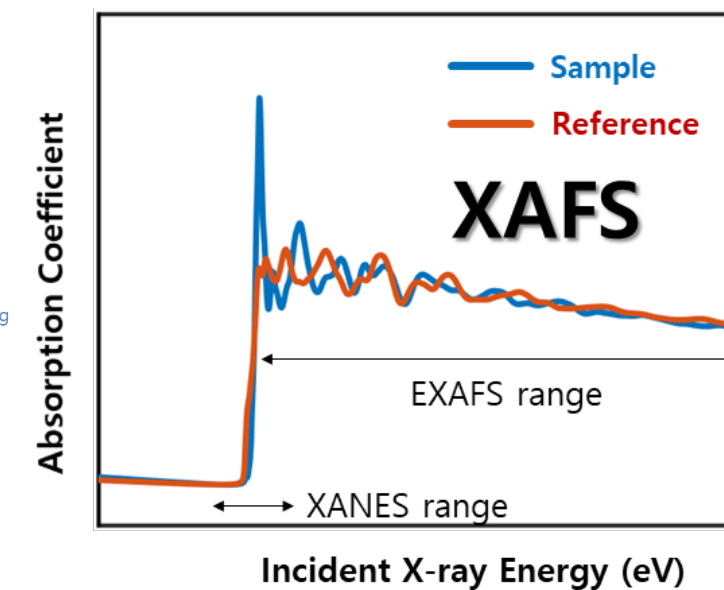
Fluorescence Mode

$$\mu_S(E) \sim \frac{I_F}{I_0}$$

Core Principles



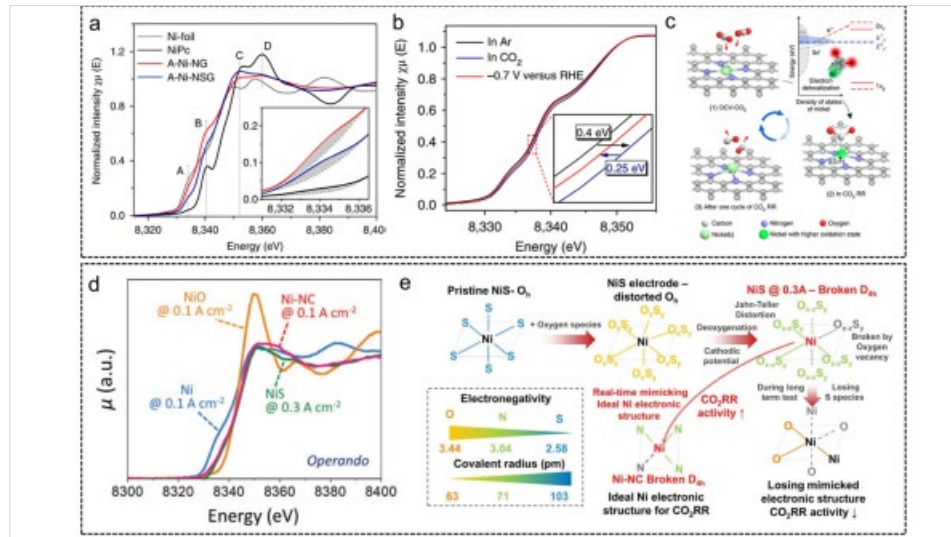
XAFS Spectra



2-2. XAFS Applications

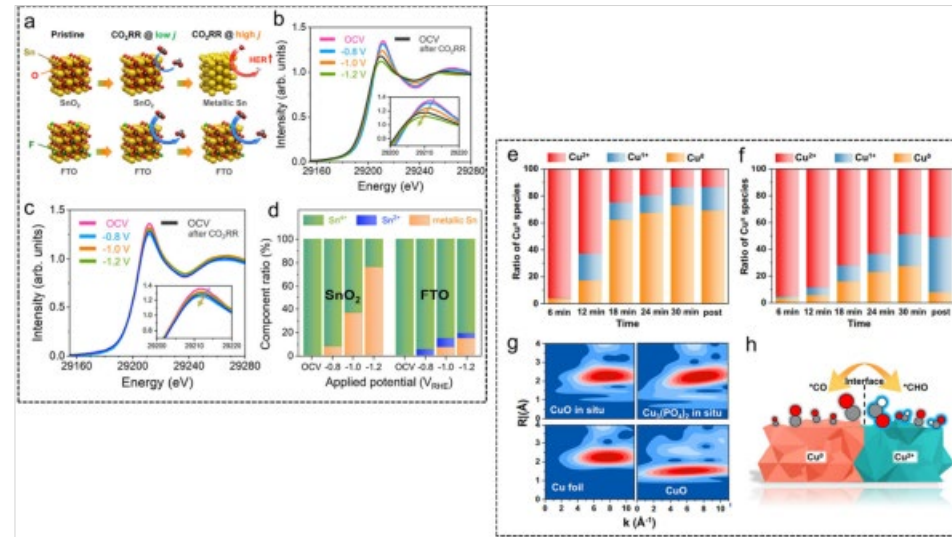
Main Article: Beibei Sheng et al., Communications Materials 6, 64 (2025).

Electronic Structure and Charge Transfer



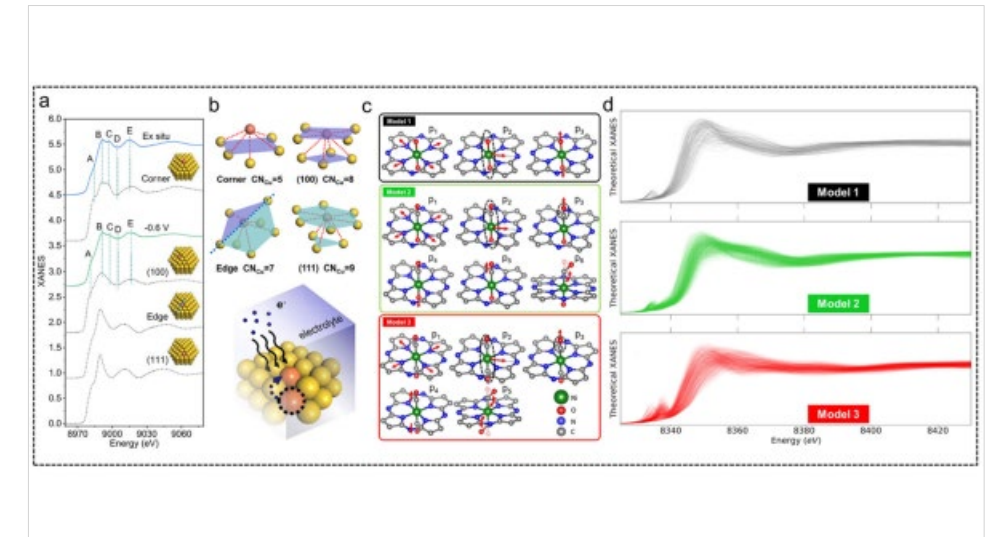
Yang, H. B. et al., Nat. Energy 3, 140–147 (2018).
Han, M. H. et al., Adv. Energy Mater. 12, 2201843 (2022).

Valence State Analysis



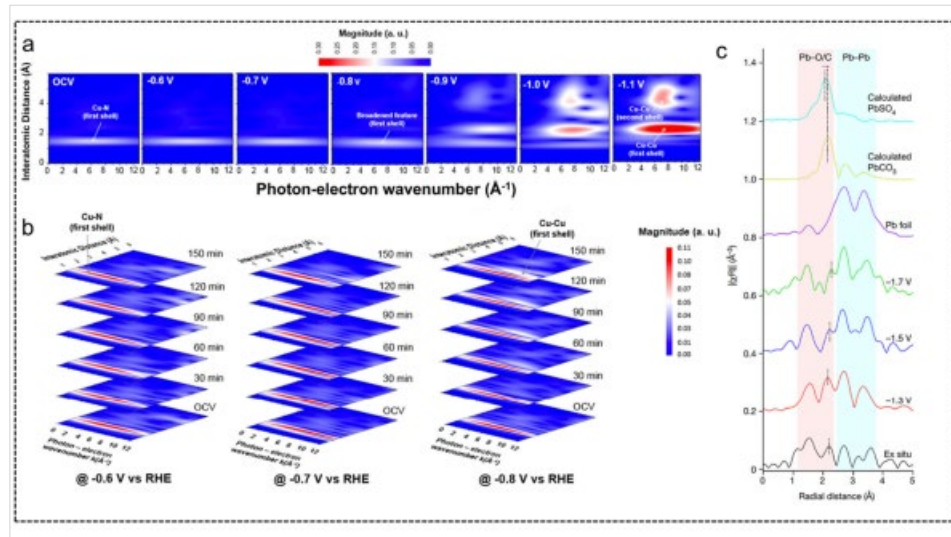
Ko, Y. J. et al., Nat. Commun. 13, 2205 (2022).
Zhang, X. Y. et al., Nat. Commun. 14, 7681 (2023).

Geometric Structure



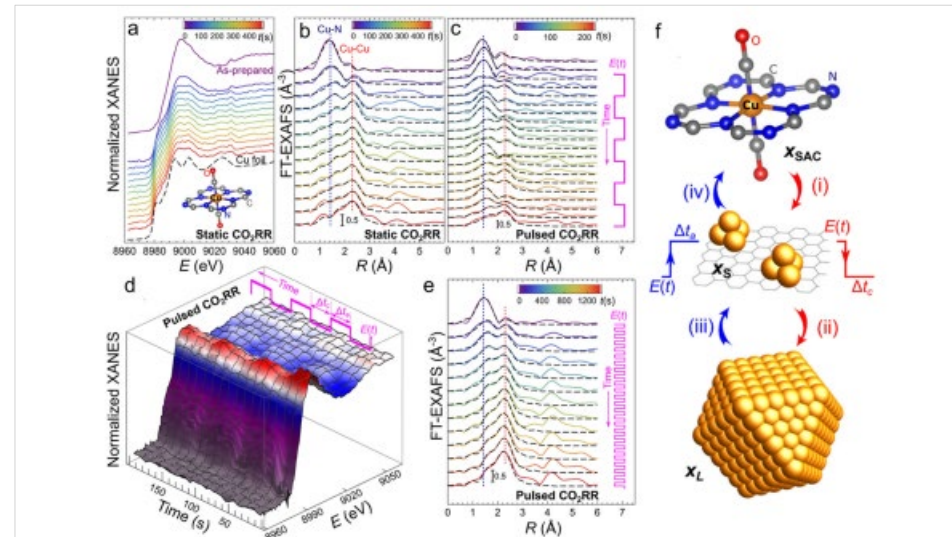
Liu, X. et al., Nano Lett. 20, 8319–8325 (2020).
Martini, A. et al., J. Am. Chem. Soc. 145, 17351–17366 (2023).

Coordination Structure/Number



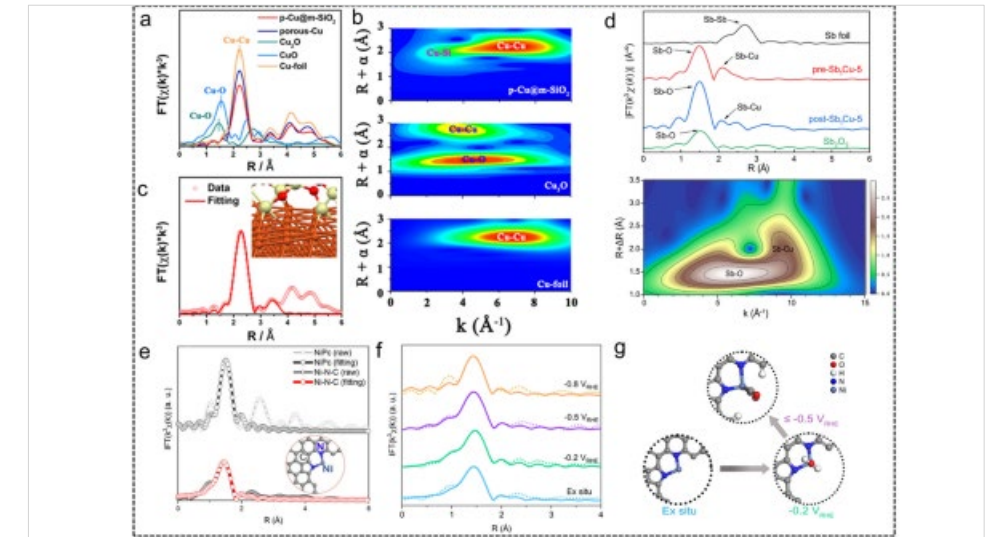
Xiong, W. F. et al., J. Am. Chem. Soc. 146, 289–297 (2024).
Li, J. et al., Nat. Commun. 14, 340 (2023).
Cao, D. et al., Opin. Electrochem 30, 100788 (2021).

Active Sites/ Structure Evolution



Cao, D., Shou, et al., Opin. Electrochem 30, 100788 (2021).
Fang, W. et al., Nature 626, 86–91 (2024).

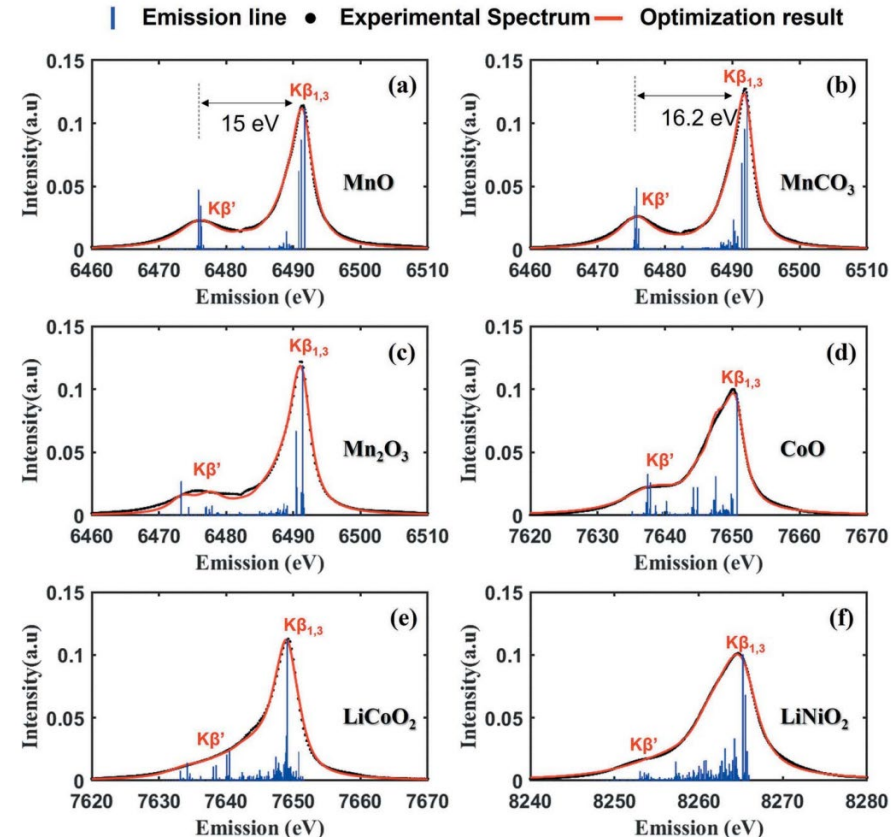
Real-Time Kinetic Processes



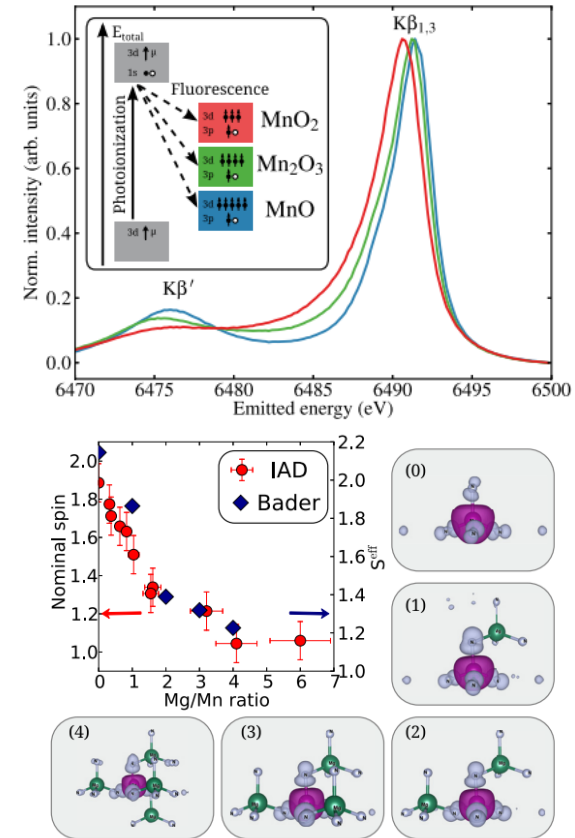
Timoshenko, J. et al., Nat. Commun. 15, 6111 (2024).

2-3. XES Applications

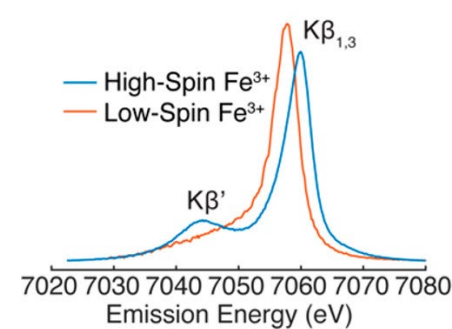
Ligand Field

J. Synchrotron Radiation **30** (5), 923-933 (2023).

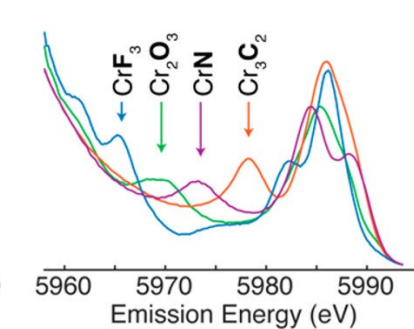
XES and RIXS: Spin State and Oxidation



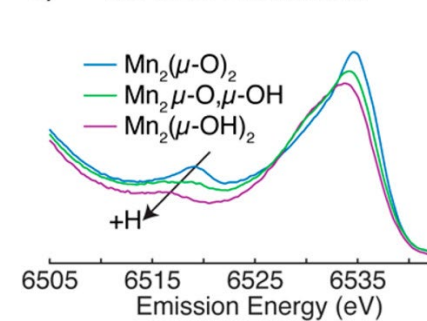
a) Kβ Mainline: Spin-State



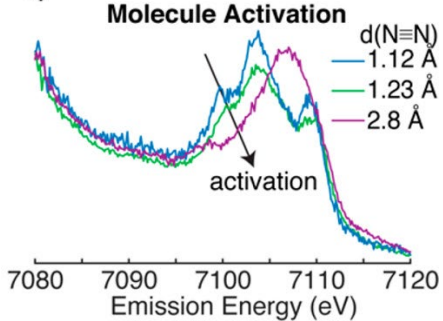
b) VtC XES: Atom Identity



c) VtC XES: Protonation



d) VtC XES: Small Molecule Activation

Sci. Technol. **29**, 023002 (2014).

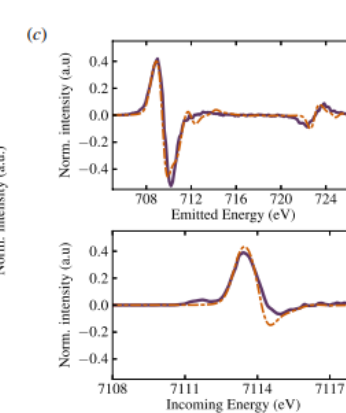
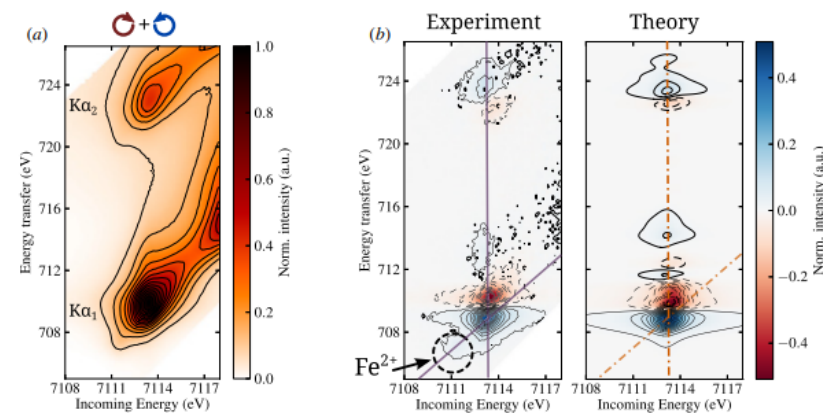
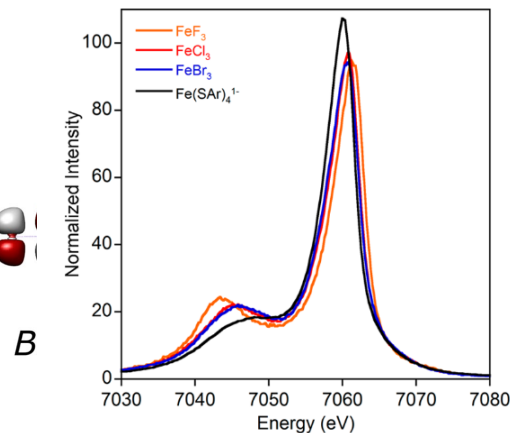
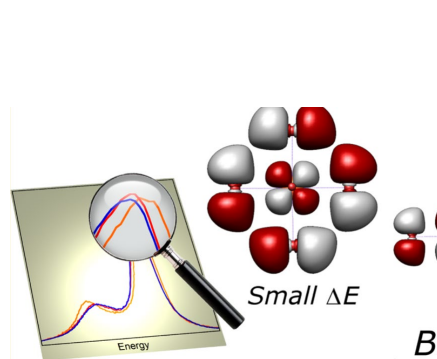
Scientific Information

- Spin state
- Ligand
- Local structure symmetry
- Local electrical information

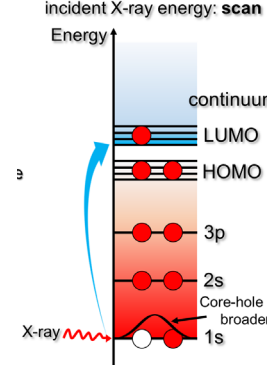
Disciplines

- Catalysis
- Material Science
- Earth Science
- Environmental Science
- Biology

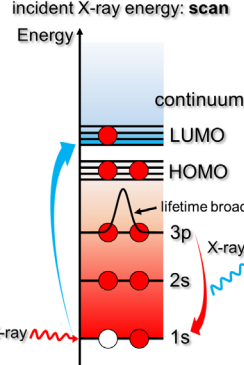
Fundamental Principles of XAS and XES



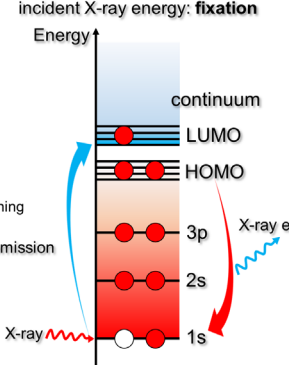
Conventional XANES



HERFD-XAS

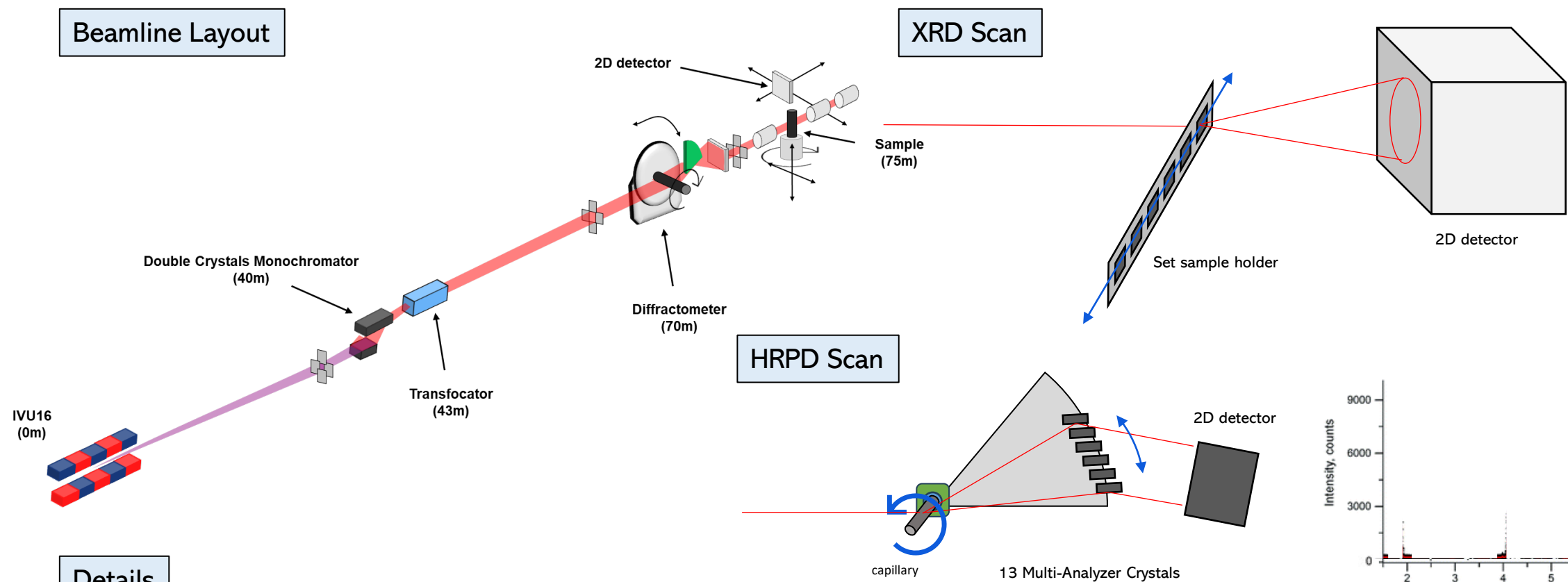


XES

ACS Catal. **12**, 5864–5886 (2022).

3. ID24 Material Structure Analysis

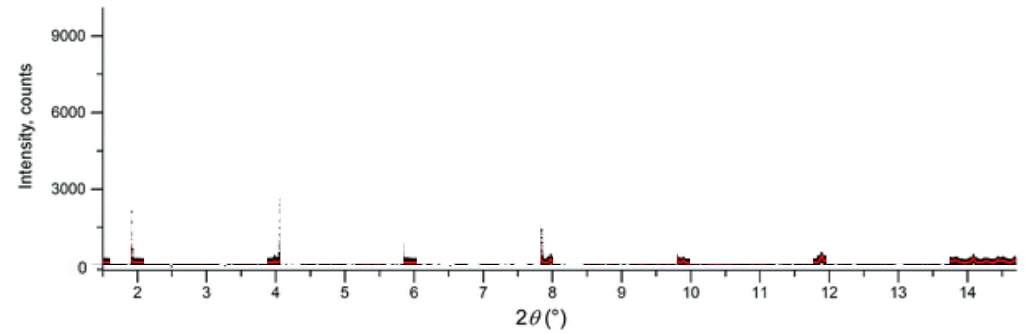
Beamline Layout



Data storage

- Data1
- Data2
- Data3
- Data4
- ...

Details



Estimated Beamline Performance for HRPD
Optimized energy: 33.5 keV (IVU16, Gap 6 mm)
Sample Capillary (1, 0.5, 0.3 mm capillaries)
Various Capillary holding mode (Spinning, In-situ, ...)
2θ Scanning range 3° ~ 40° (Optimized 5°~30°)
d-spacing ~1 ~ 8 Å
Angular resolution < 0.005°
Measuring time 15 min / sample
(0.02° step scan, expose time 0.5s)
TMAC crystals information
2° interval 13 crystals with single axis

Estimated Beamline Performance for 2D XRD
Optimized energy: > 20 keV (depending on detector)
2θ Max scanning range 10° ~ 40° (depending on SDD)
SDD range 500 ~ 2000 mm
Angular resolution range (0.006 ~ 0.08° in the range of 500-2000 mm SDD)
Measuring time < 1 min / sample

SDD	MAX 2θ	Angular Resolution	d-spacing range (d-spacing, half range)
500 mm	17.81°	0.010°	0.5 ~ 8.6 Å (2θ _{max} = 17°)
1000 mm	18.74°	0.007°	1.1 ~ 8.6 Å
2000 mm	9.37°	0.010°	2 ~ 16 Å

*TMAC crystals information
2° interval 13 crystals with single axis
150 μm pixel size, 0.5 mm sample thickness

HRPD + Multi-Sample Measurement
Optimized energy: 33.5 keV (IVU16, Gap 6 mm)
2θ Scanning range 3° ~ 40° (Optimized 5°~30°)
d-spacing ~1 ~ 8 Å
Angular resolution < 0.005°
Measuring time 15 min / sample

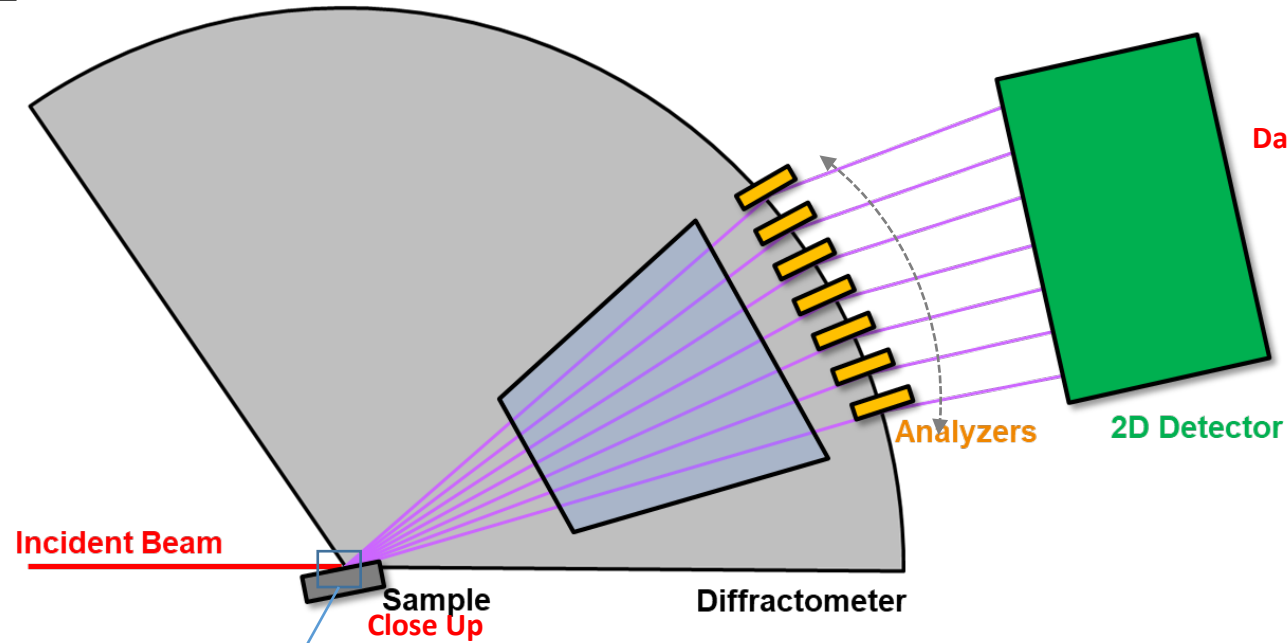
2D XRD + Multi-Sample Measurement
Optimized energy: > 20 keV (depending on detector)
2θ Max scanning range 10° ~ 40° (depending on SDD)
SDD range 500 ~ 2000 mm
Angular resolution range (0.006 ~ 0.08° in the range of 500-2000 mm SDD)
Measuring time < 1 min / sample

3-1. HRPD (High Resolution Powder Diffraction)

HRPD Measurement Setup

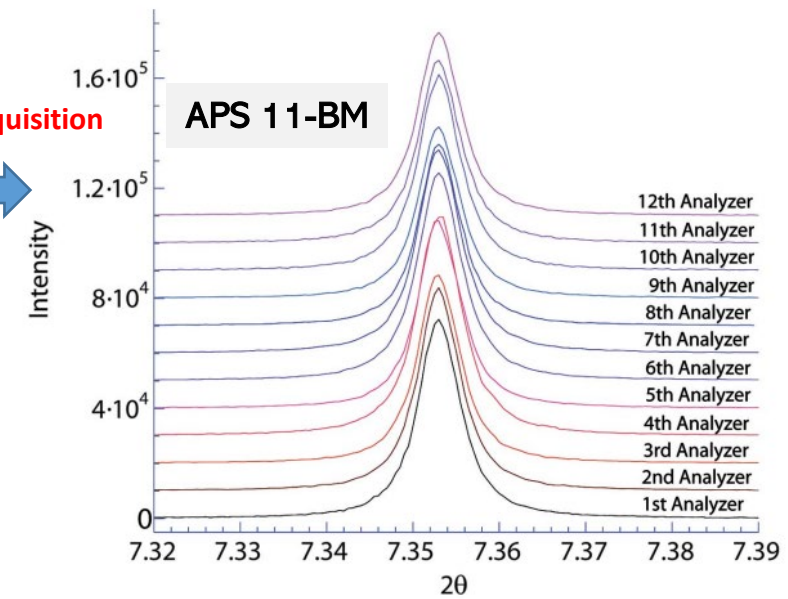


ESRF-EBS ID22



Data Acquisition

Multi-analyzers



J. Synchrotron Rad. 15, 427–432 (2008).

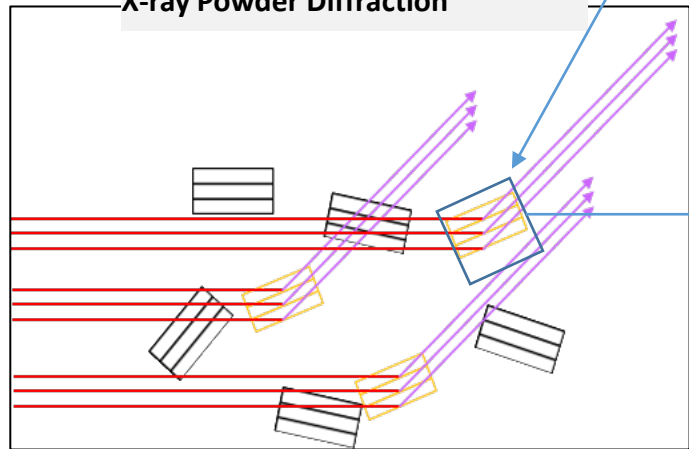
Features

- High q-range coverage
- High peak resolution
- Sensitivity

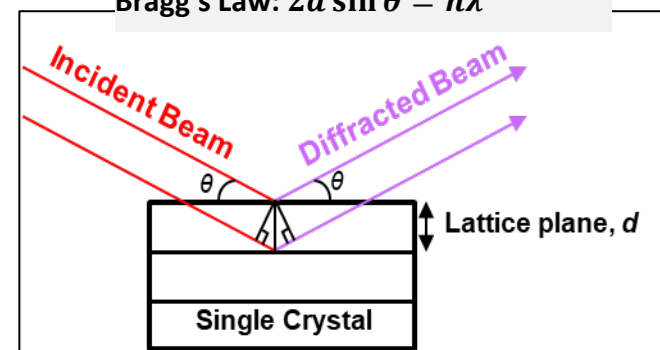
Application

- Energy Materials
- Chemistry & Nano Science
- Life Science / Pharmaceuticals
- In-situ / Operando Studies

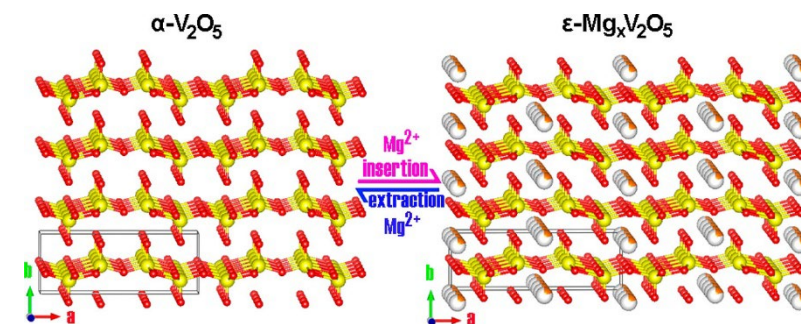
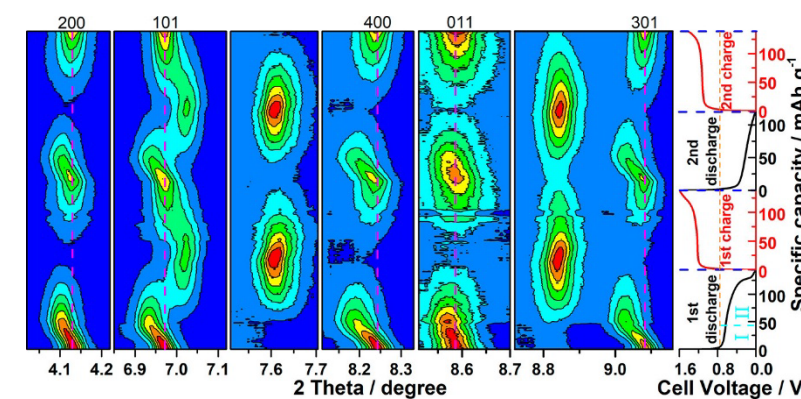
X-ray Powder Diffraction



Working Principle of XRD

Bragg's Law: $2d \sin \theta = n\lambda$ 

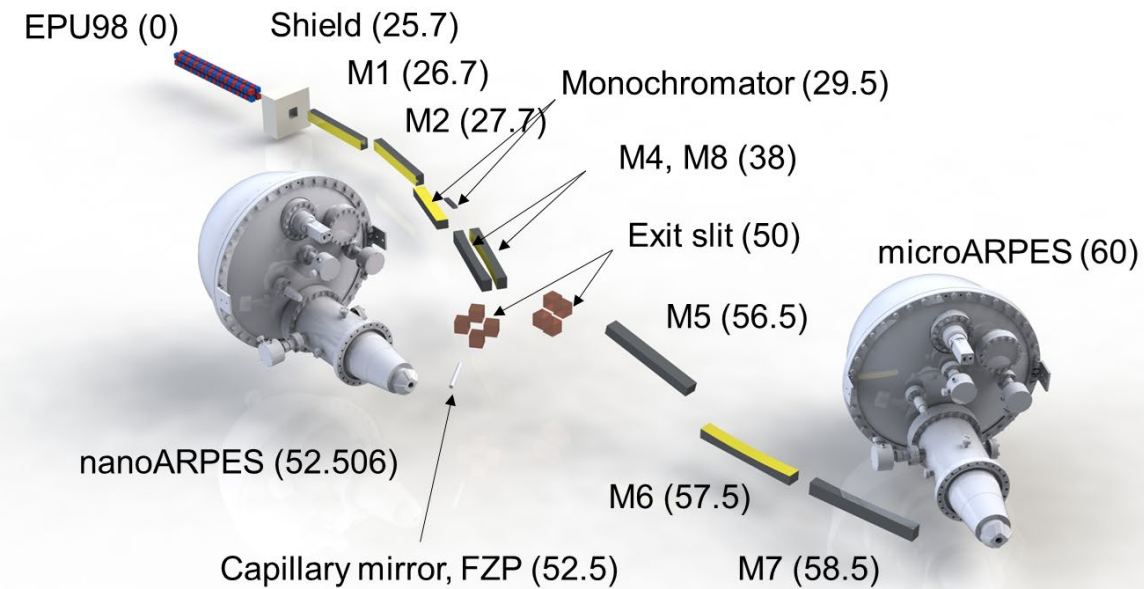
Applications



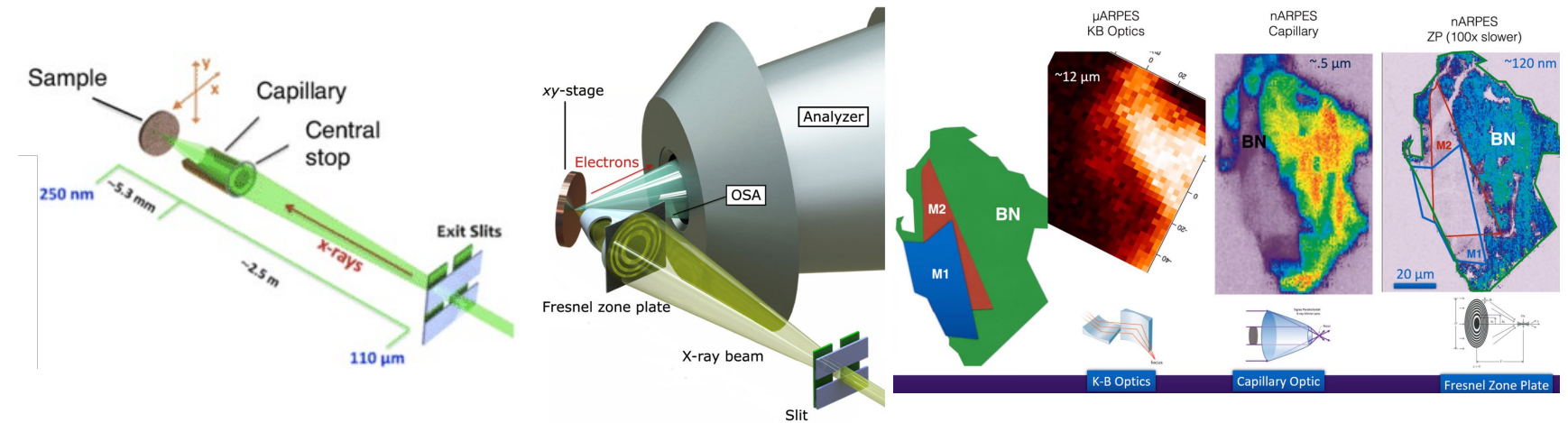
J. Am. Chem. Soc. 141, 2305 (2019)

4. ID25 NanoARPES

Beamline Layout



NanoARPES



Specifications

nanoARPES Branch

Spot size: 1 μm (100 nm)

Targets: small single crystals

Exfoliated few layers

Moire superlattices and heterostructures

In-operando devices (gating, strain)

**Spatial resolution, stability and repeatability,
fine control over beam alignment and
scanning**

microARPES Branch

Spot size: 10 μm

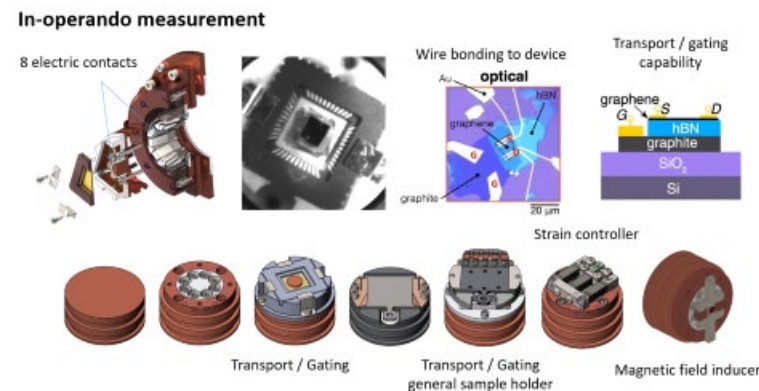
Targets: Large-domain crystals

Standard thin films

Bulk crystals

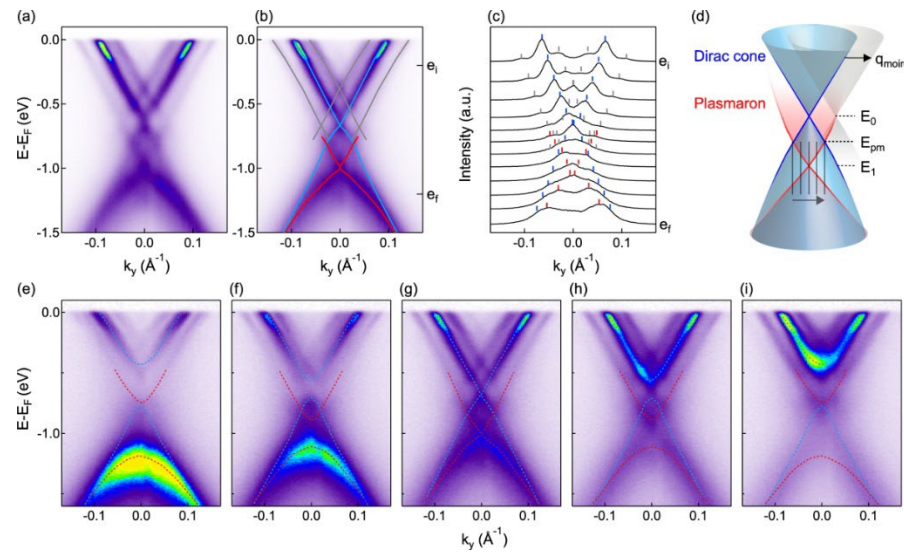
In-operando devices (magnetic field, dosing)

**High photon flux, excellent energy resolution,
simplified, user friendly operation.**



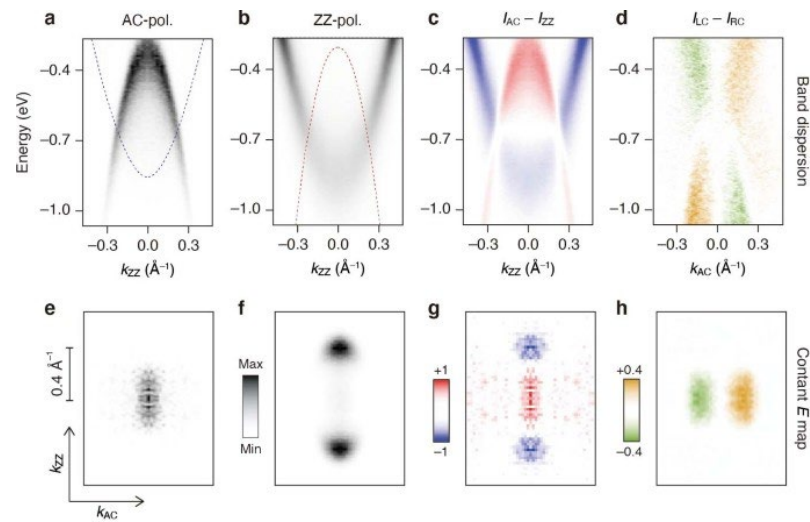
4-1. ARPES

Plasmaron



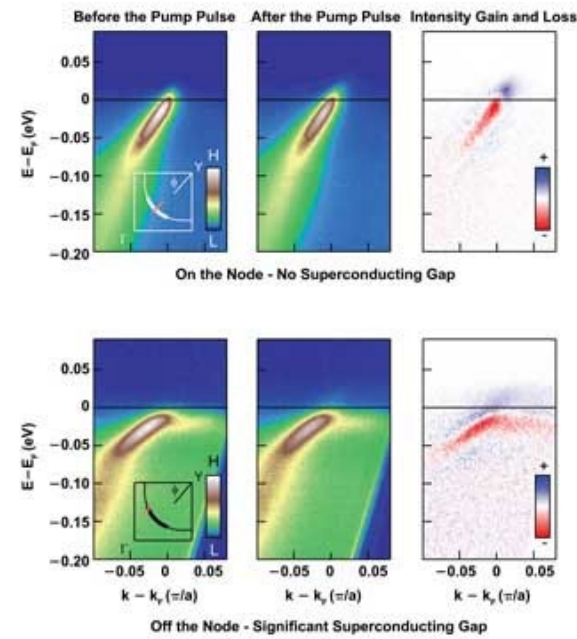
Science 328, 5981 (2010)

Pseudospin Order



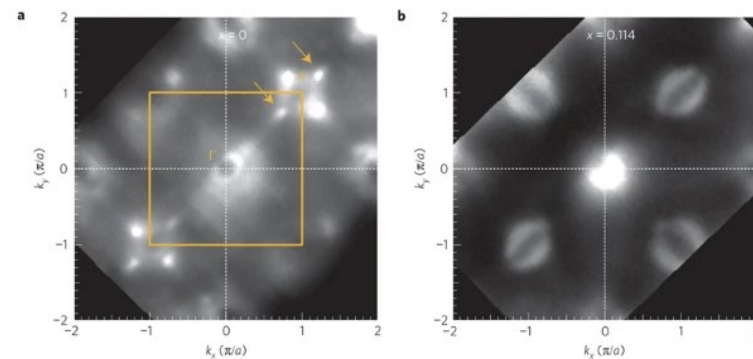
Nat. Mater. 19, 277 (2020)

SC Gap Formation



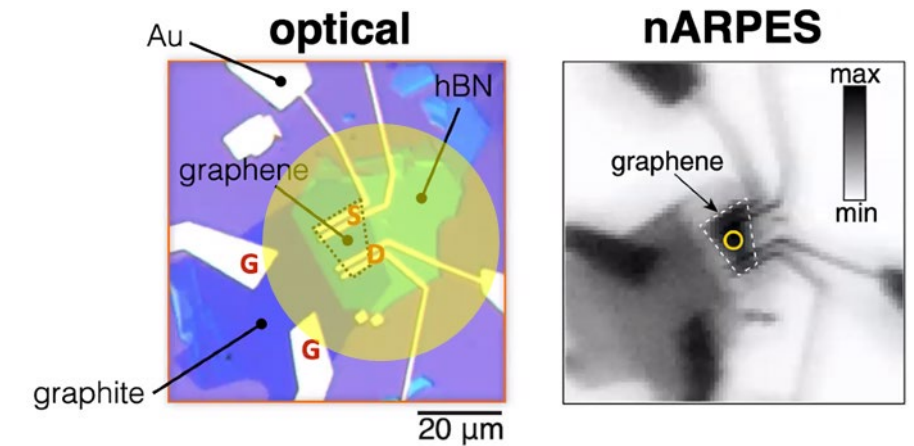
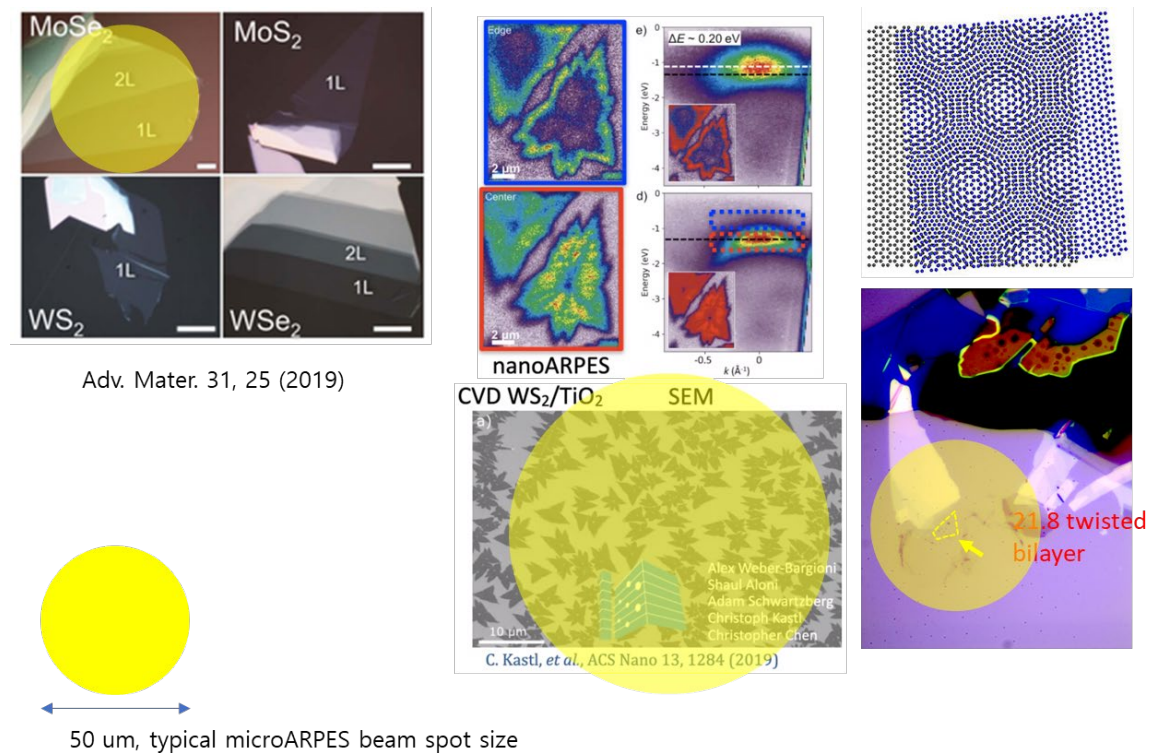
Science 336, 6085 (2012)

Spin Order



Nat. Phys. 6, 419 (2010)

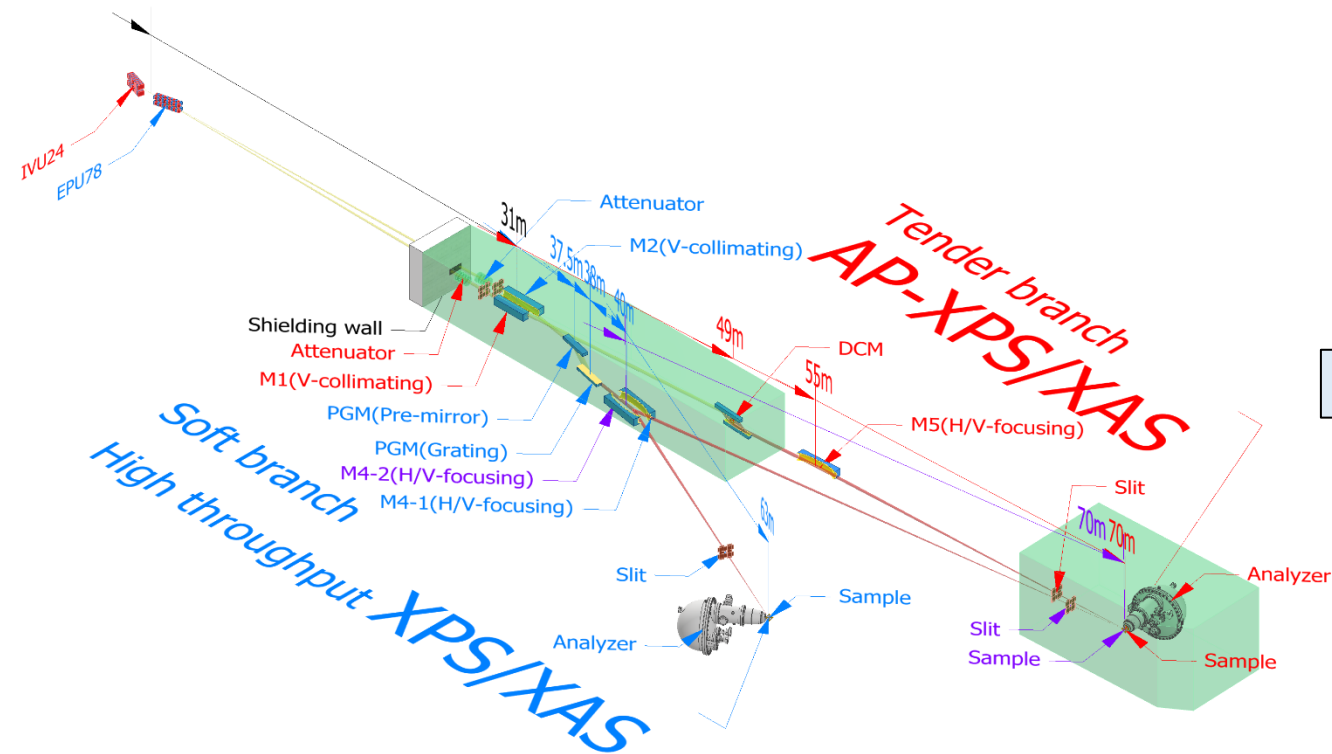
Space-resolved Probing



Phys. Rev. B 101, 201409 (2020)

5. ID26 Soft X-ray Nanoprobe

Beamline Layout



Specifications

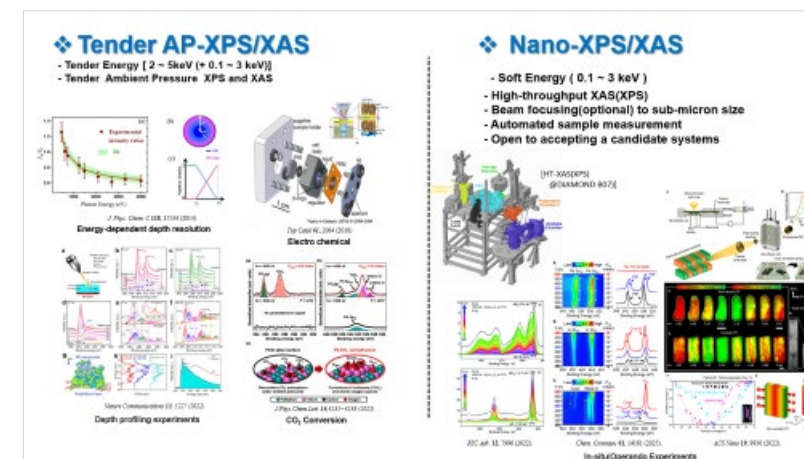
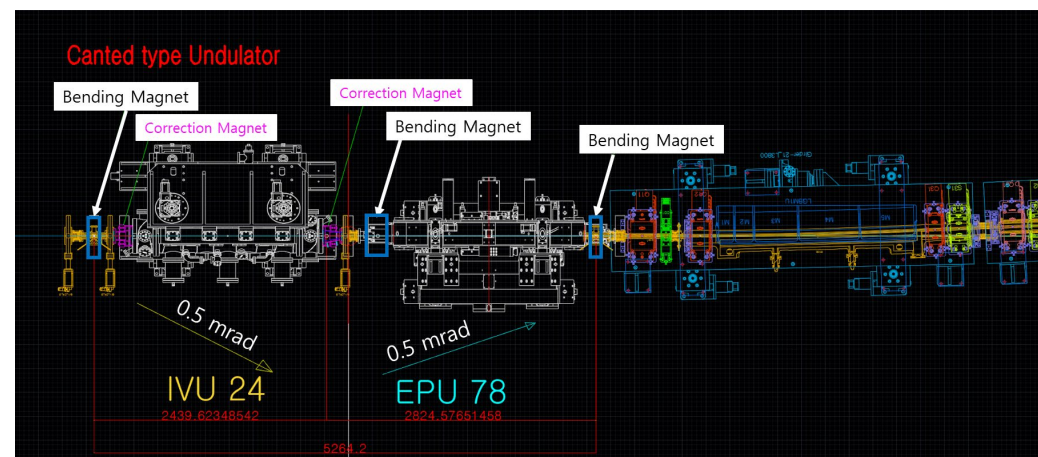
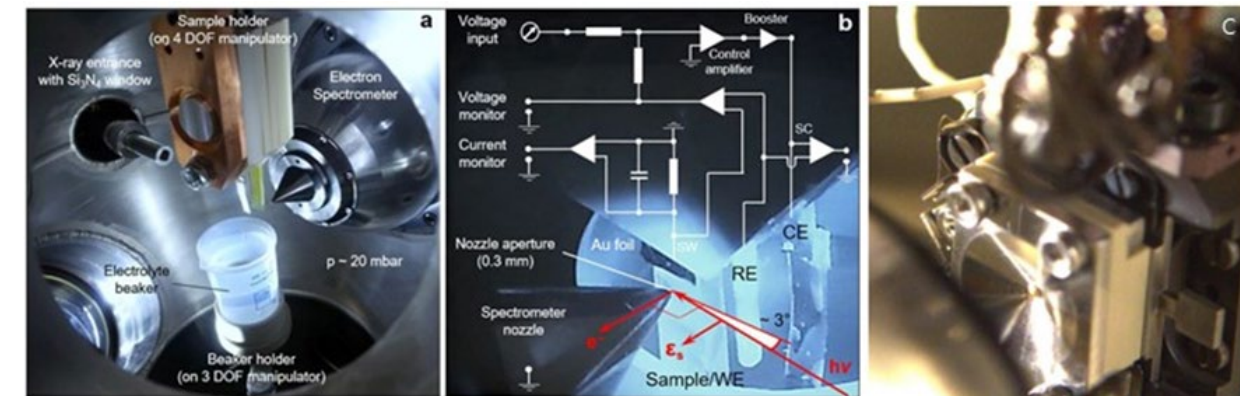
Tender XPS/XAS branch

- Beam size : $\sim 10 \text{ um} \times 5 \text{ um}$
- Energy range (2 – 5 keV) + (0.1 – 3 keV)
- Real-time analysis of electrode interiors and interfaces
- **Bulk- and surface-sensitive** characterization
- In-situ analysis under **ambient conditions**

Nano XPS/XAS branch

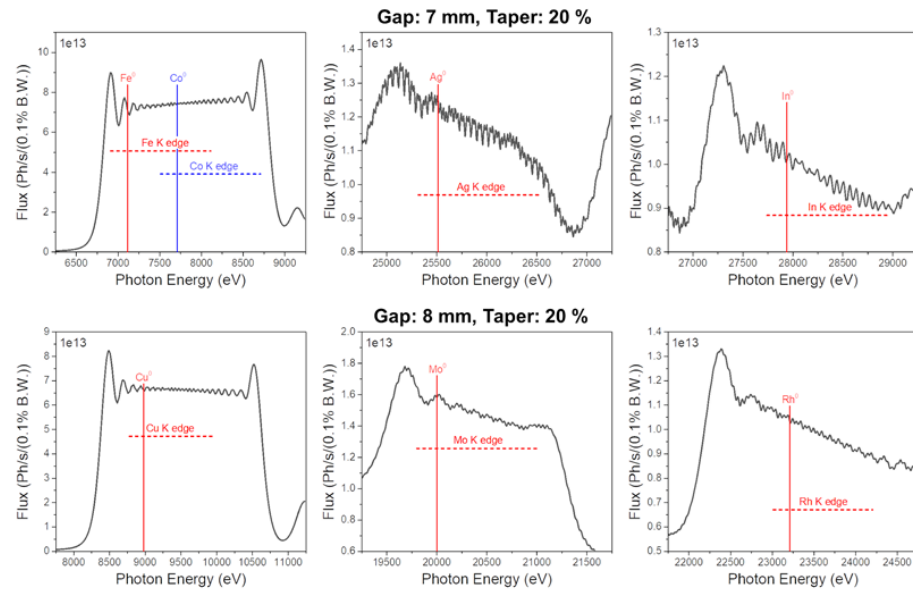
- Beam size: $\sim 20 \text{ um} \times 30 \text{ um}$
- Energy range 0.1 – 3 keV
- Standard XPS/XAS under UHV
- Optimized for **rapid, repetitive measurements**
- **High-throughput screening** capability

Features

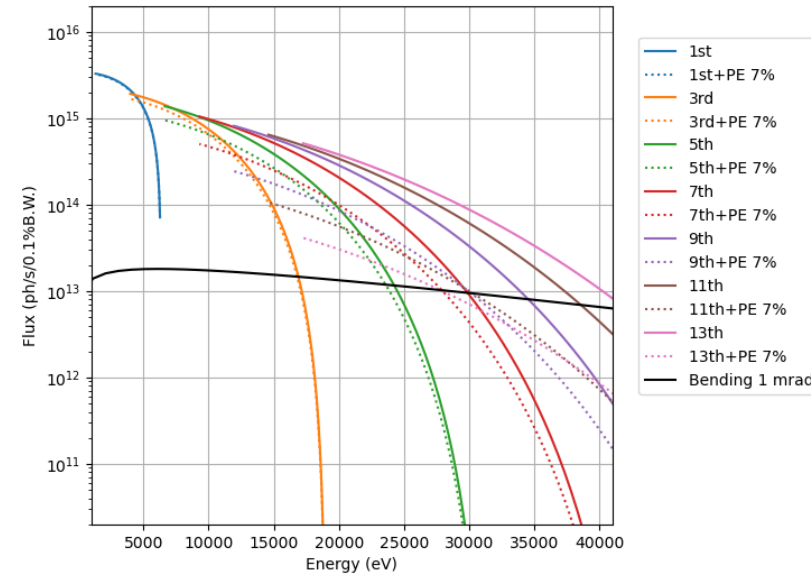


6. Others

Light Source



Phase Error Effect



ID23 Real-Time XAFS

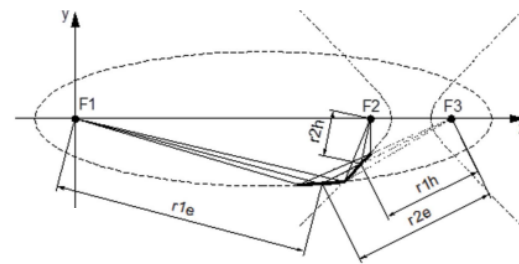
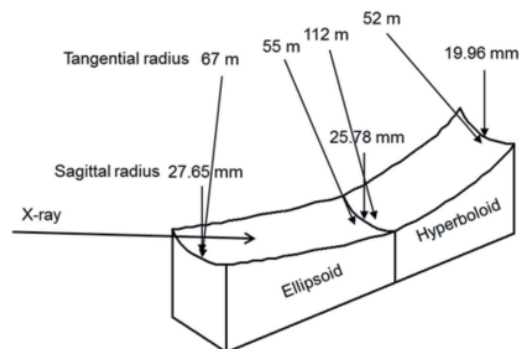
- Updated Layout without Channel-cut DCM

ID24 Material Structure Analysis

- Modification of Undulator
IVU24 -> IVU16
- Updated Layout with New Optics

Focusing Optics

Wolter Mirror

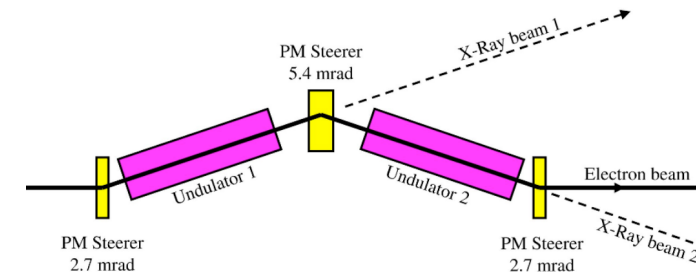


J. Synchrotron Rad. 27, 1103 (2020)

ID25 NanoARPES

- Replacement of Focusing Mirror
Wolter Mirror-> KB Mirror

Front-end Configuration



Upgrade of the insertion devices at the ESRF, IPAC10, Kyoto

ID26 Soft X-ray Nanoprobe

- Change of FE Configuration
Tandem-> Canted

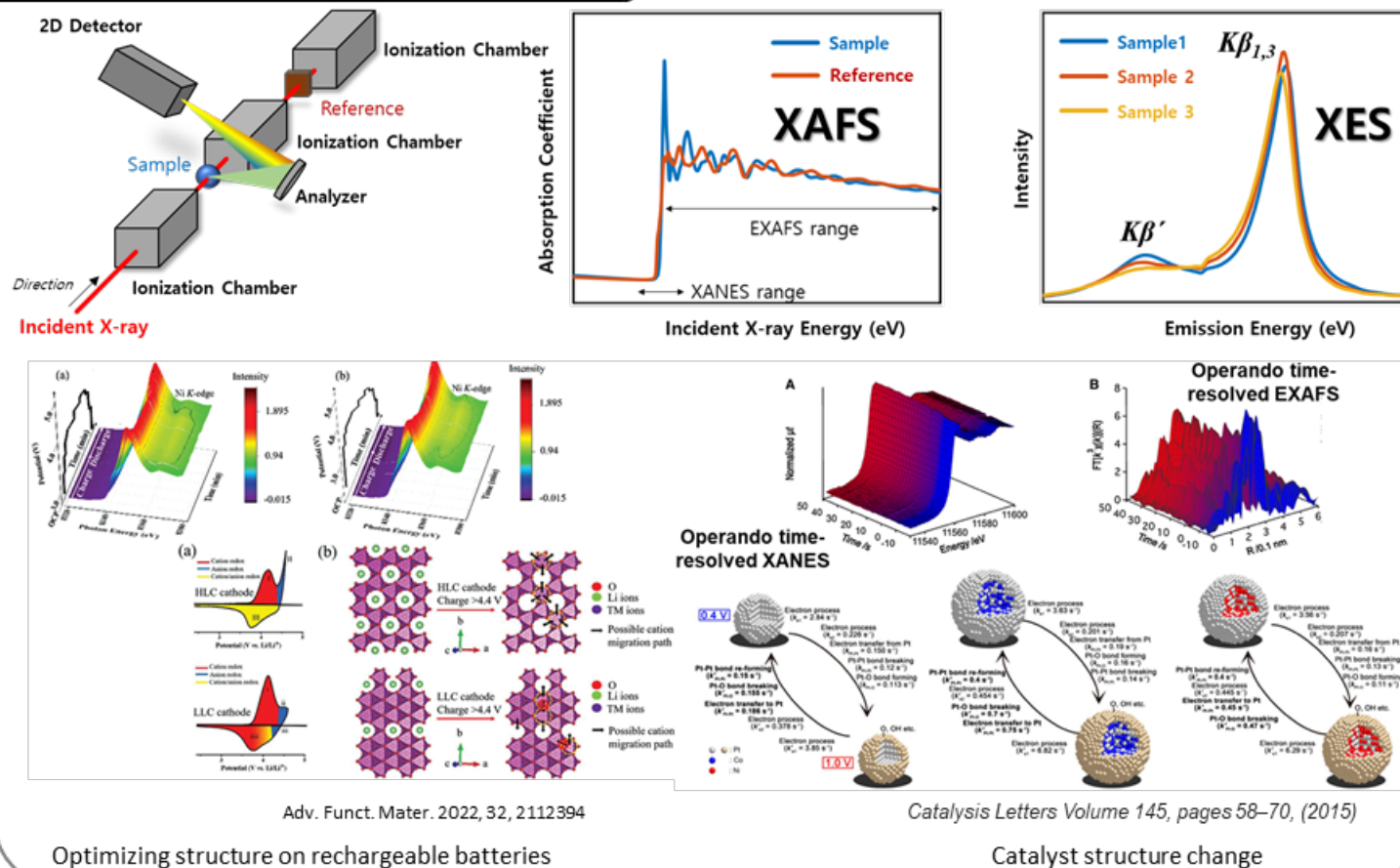
Summary

	Real-Time XAFS	MSA	Soft X-ray Nanoprobe	nanoARPES
Light source	IVU24	IVU16	IVU24+EPU78	EPU98
Energy range [keV]	4.0 ~ 40.0	6.0 ~ 45.0 (Optimized at 33 keV)	0.1 ~ 5.0	0.05 ~ 2.0
Supports	QXAFS, XAFS, XES, HERFD-XAS	HRPD, in-situ XRD, XAFS	XPS/XAS/SPEM	ARPES
Beam size (h × v, FWHM)	- Focused mode: $1 \times 1 \mu\text{m}^2$ - Unfocused mode: $1 \times 0.5 \text{ mm}^2$	$1 \times 0.5 \text{ mm}^2$	- Tender-B: $5 \times 12 \mu\text{m}^2$ - Soft-B: $36 \times 14 \mu\text{m}^2$	- micro-ARPES: $10 \times 10 \mu\text{m}^2$ - nano-ARPES: $0.1 \times 0.1 \sim 1 \times 1 \mu\text{m}^2$
Beam flux (ph/s)	- Tuned Undulator: $>1.0 \times 10^{13}$ (@10 keV) - Tapered Undulator: $>1.0 \times 10^{12}$ (@10 keV)	$> 1.0 \times 10^{12}$ (@33 keV)	- Tender-B: 1.5×10^{12} - Soft-B: 6.3×10^{11}	- micro-ARPES: $>1.0 \times 10^{13}$ - nano-ARPES: $1.0 \times 10^{11} \sim 1.0 \times 10^{12}$

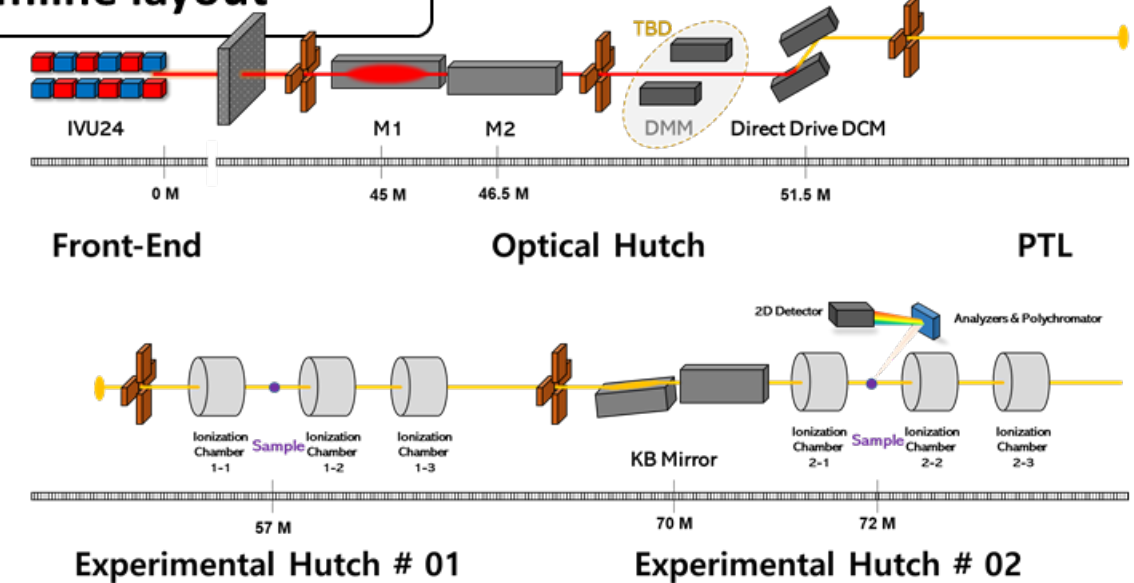
Thank You For Your Attention

Studying reaction dynamics on sub-second time scales and states of electrons

Principle and application



Beamline layout



Specification

Photon Source

In Vacuum Undulator 24

Energy Range

4 ~ 40keV

Energy resolution

Si (111): 1.4×10^{-4}

Si (311): 3.0×10^{-5}

Beam flux (ph/s)

Tuned Undulator:
 6.8×10^{13} (@10 keV)

Tapered Undulator:
 2.4×10^{12} (@10 keV)

Beam size (μm^2)

H $\times$ V, FWHM

Focused mode: $10 \times 10 \mu\text{m}^2$ Unfocused mode: $1 \times 0.8 \text{ mm}^2$

Measurement time

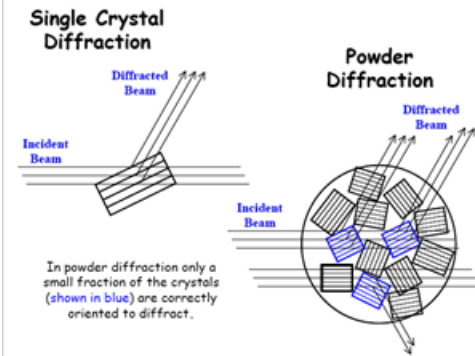
XAS : 1 ~ 20 min
Quick XAS : > 1 s
XES : a few min

Feature of Beamline

- By utilizing the IVU24, the ID23 beamline provides advanced spectroscopies, including Quick XAS, operando/in-situ XAS, HERFD-XAS, and XES.
- Such capabilities are expected to support research on both national strategic technologies and fundamental academic science.

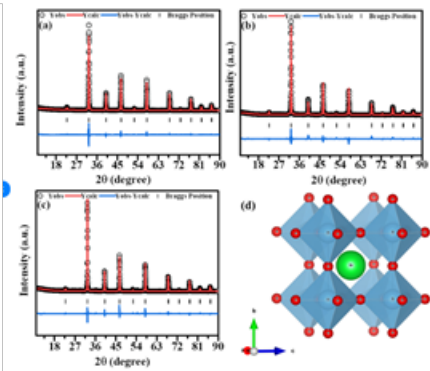
Analysis of microstructure and phase transition of crystalline materials with high resolution

Principle and application

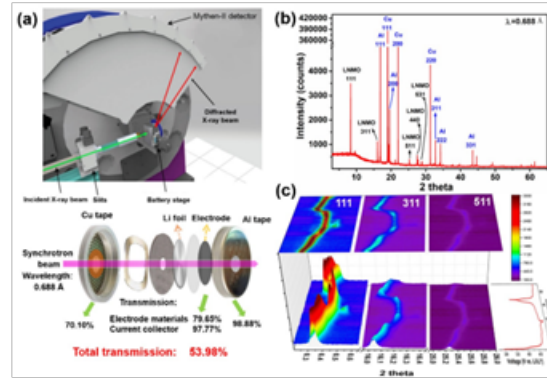


Information obtained from Powder diffraction

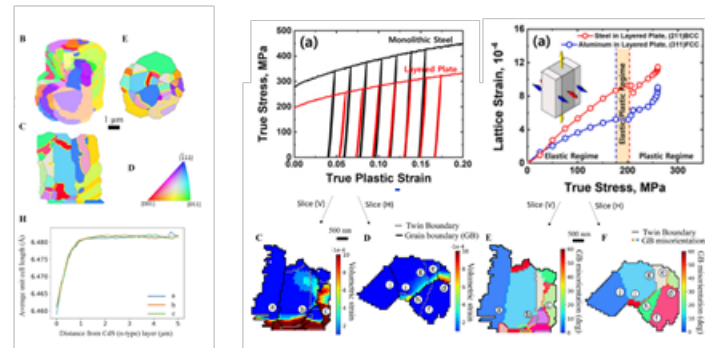
- Peak Position
- Peak Intensities
- Peak Shapes and Widths



Analysis of microstructure with high resolution



Batteries & Supercaps 2021, 4, 380–384

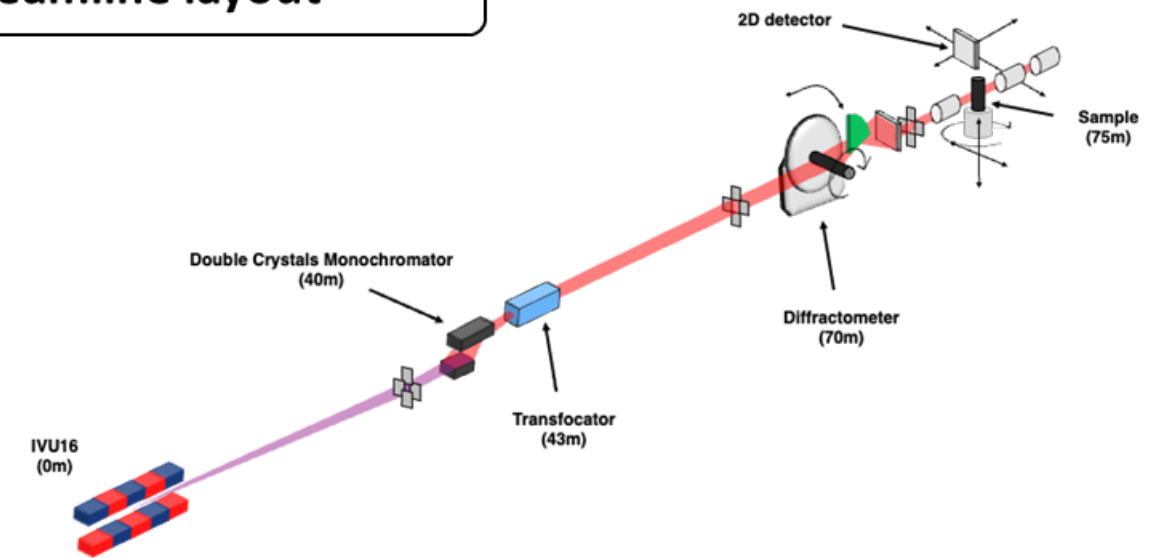


In-situ/Operando of crystal structure behavior/mapping

Feature of Beamline

- Delivers a beam with low divergence and low harmonic order, exceeding 20 keV via an insertion device for high-resolution powder diffraction (HRPD) above 30 keV.
- Utilizes HRPD as the primary technique, with an automated sample changer for enhanced efficiency and additional analysis via dedicated experimental setups.
- Supports varied sample environments (temperature, gas, atmosphere) with real-time XRD analysis.

Beamline layout



Specification

Photon Source

In Vacuum Undulator 16

Energy Range

6 ~ 45keV (optimized: 33.5)

Energy resolution

$< 2 \times 10^{-4}$

Beam flux (ph/s)

$\sim 1 \times 10^{12}$

Beam size (μm^2)

Natural: 1200×600

H × V, FWHM

Focused: 150×100

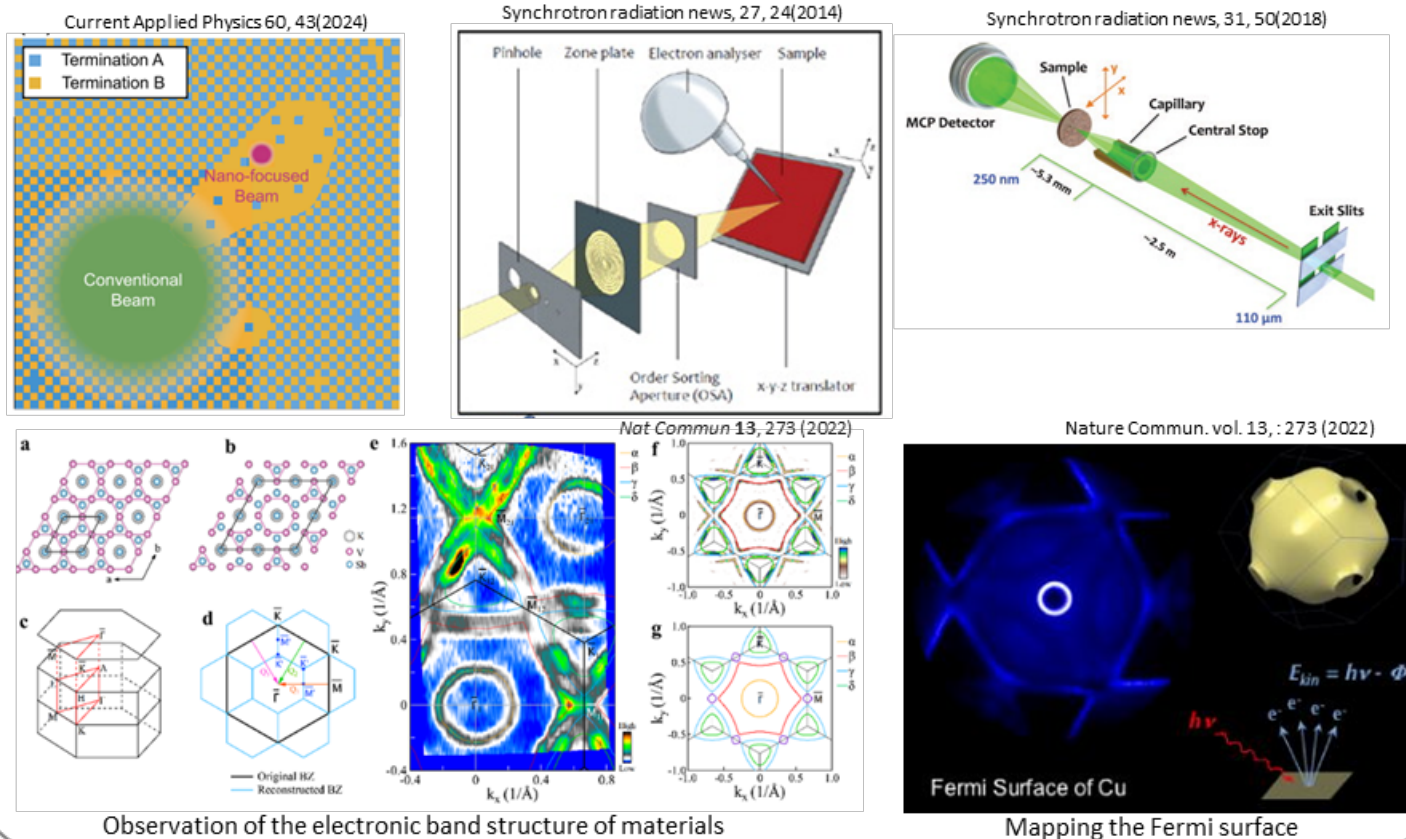
Measurement time

(0.02° step / 0.5s)

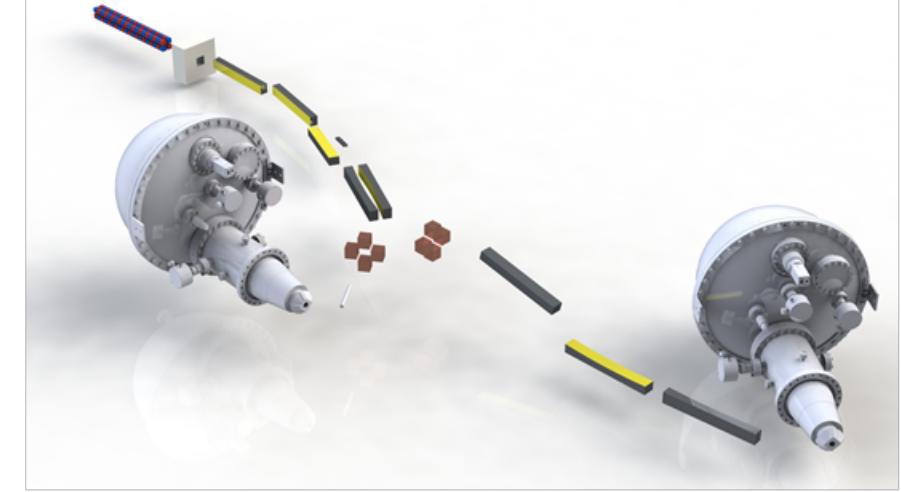
~ 15 min

Mapping of the Fermi surface and observation of the electronic band structure of materials

Principle and application



Beamline layout



Specification

Photon Source

Elliptically Polarizing Undulator 98

Branch

Micro ARPES

Nano ARPES

Energy Range

0.1 ~ 2 keV

100~200 eV

Energy resolution

< 5×10^{-5} (below 200eV)< 10^{-4}

Beam flux (ph/s)

 $\sim 10^{12}$ $\sim 10^{11}$ Beam size (μm^2)
H $\times$ V, FWHM

5 x 5

0.1 x 0.1

ARPES analyzer Energy resolution

< 1.8meV FWHM

ARPES analyzer Acceptance angle

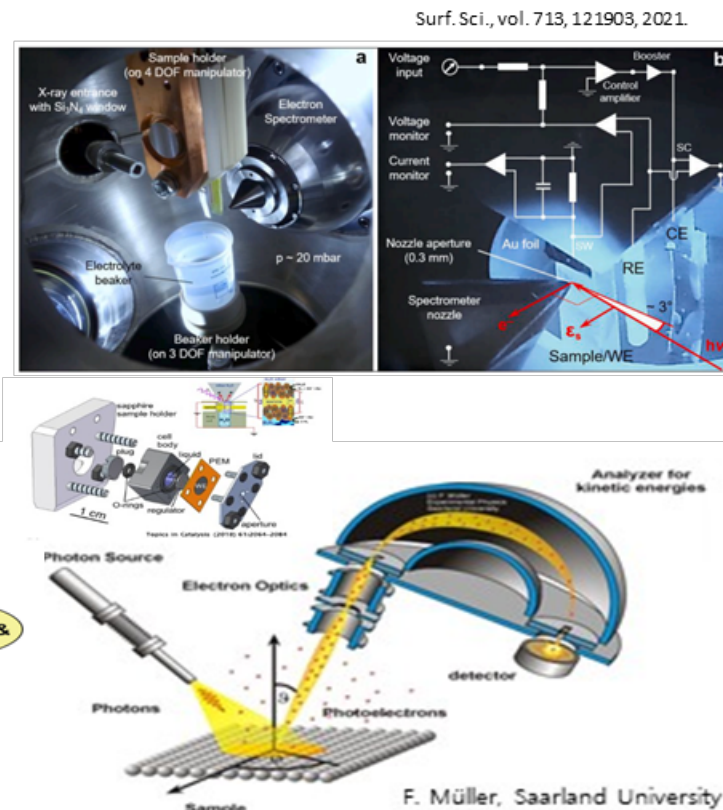
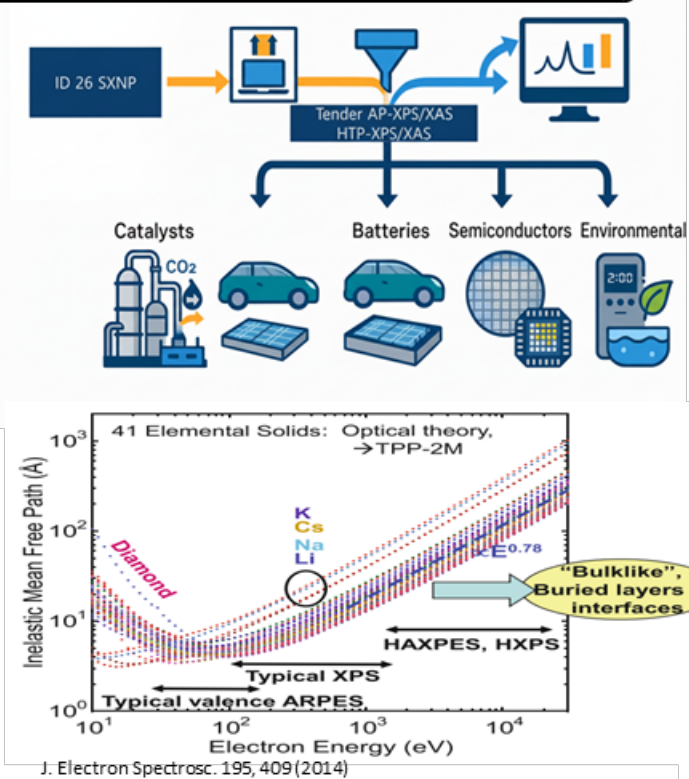
38°

Feature of Beamline

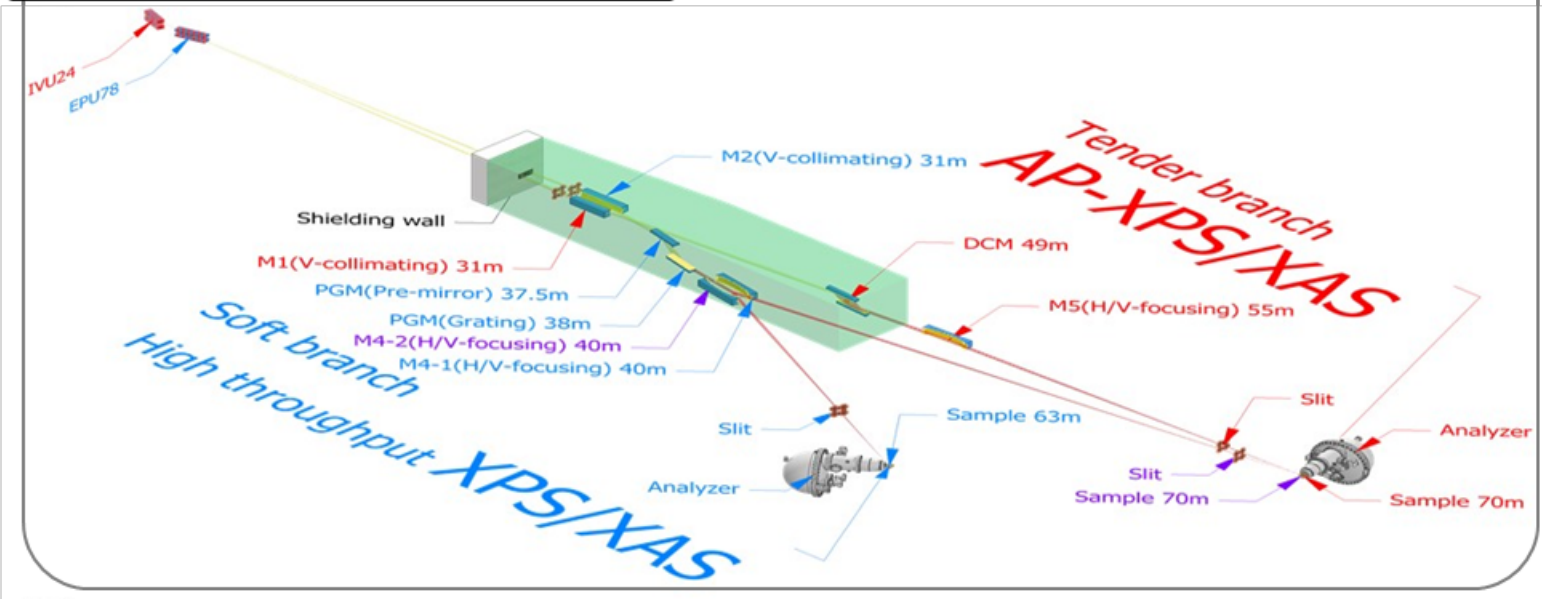
- Enables to observe the electronic band structure, which indicates physical properties, such as electrical, optical and magnetic characteristics.
- From various polarization modes of the undulator, Enables the analysis of magnetic properties and asymmetrical electronic structures
- Operates with two end stations: Micro ARPES (beam size: 5 x 5 μm) and Nano-ARPES (beam size : 100 x 100 nm)

Probing the electronic structure, chemical states, and nanoscale morphology of materials

Principle and application



Beamline layout



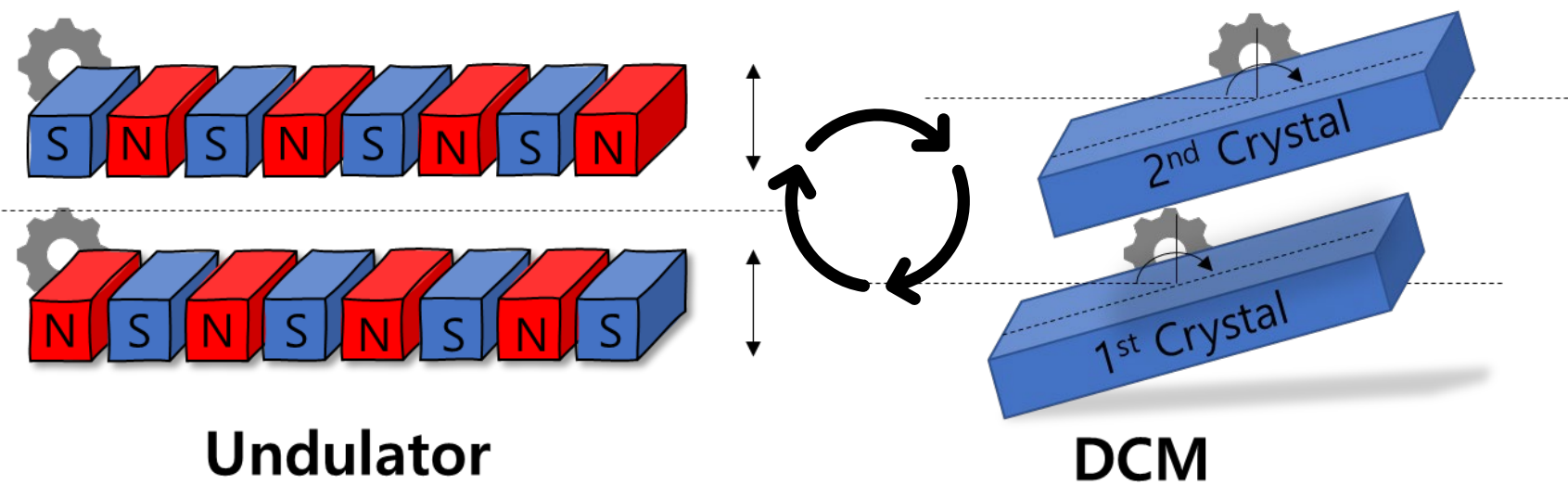
Specification

Branch	Tender X-ray	Soft X-ray
Undulator	In Vacuum Undulator 24 (1.5m)	Elliptically Polarizing Undulator 78 (2m)
Energy Range (mainly)	2-5keV	0.1 – 2keV
Energy resolution	< 10 ⁻⁴ (at 4 keV)	1 x 10 ⁻⁴ ~ 2 x 10 ⁻⁴
Beam flux (ph/s)	~ 1 x 10 ¹⁴	~ 6 x 10 ¹³
Beam size (μm ²) H x V, FWHM	12 x 5μm ²	10 ~ 400μm ²

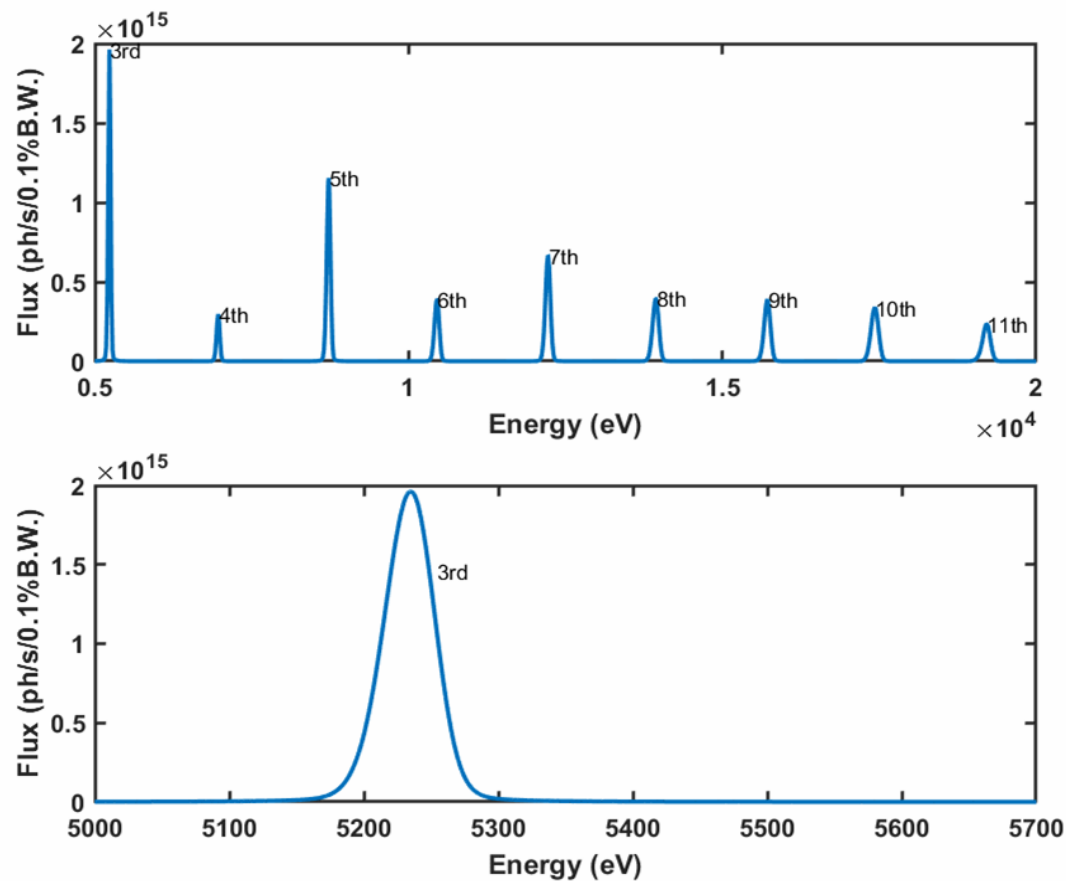
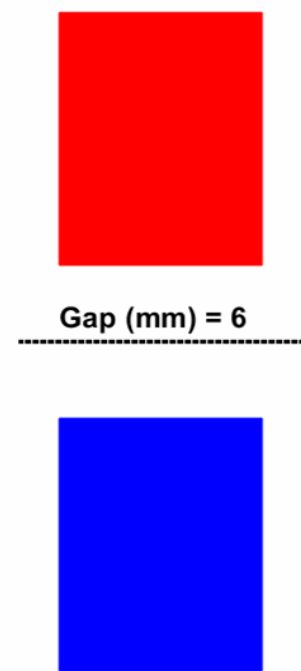
Feature of Beamline

- Canted insertion devices (IVU24 + EPU78)
First adoption of canted design in Korea
Energy coverage: 0.1–5 keV (soft → tender X-ray)
- Broad experimental environments
From ultra-high vacuum to ambient pressure
- Versatile Exp. in (AP)XPS/XAS
- - in-situ Operando Spectroscopy + Microscopy

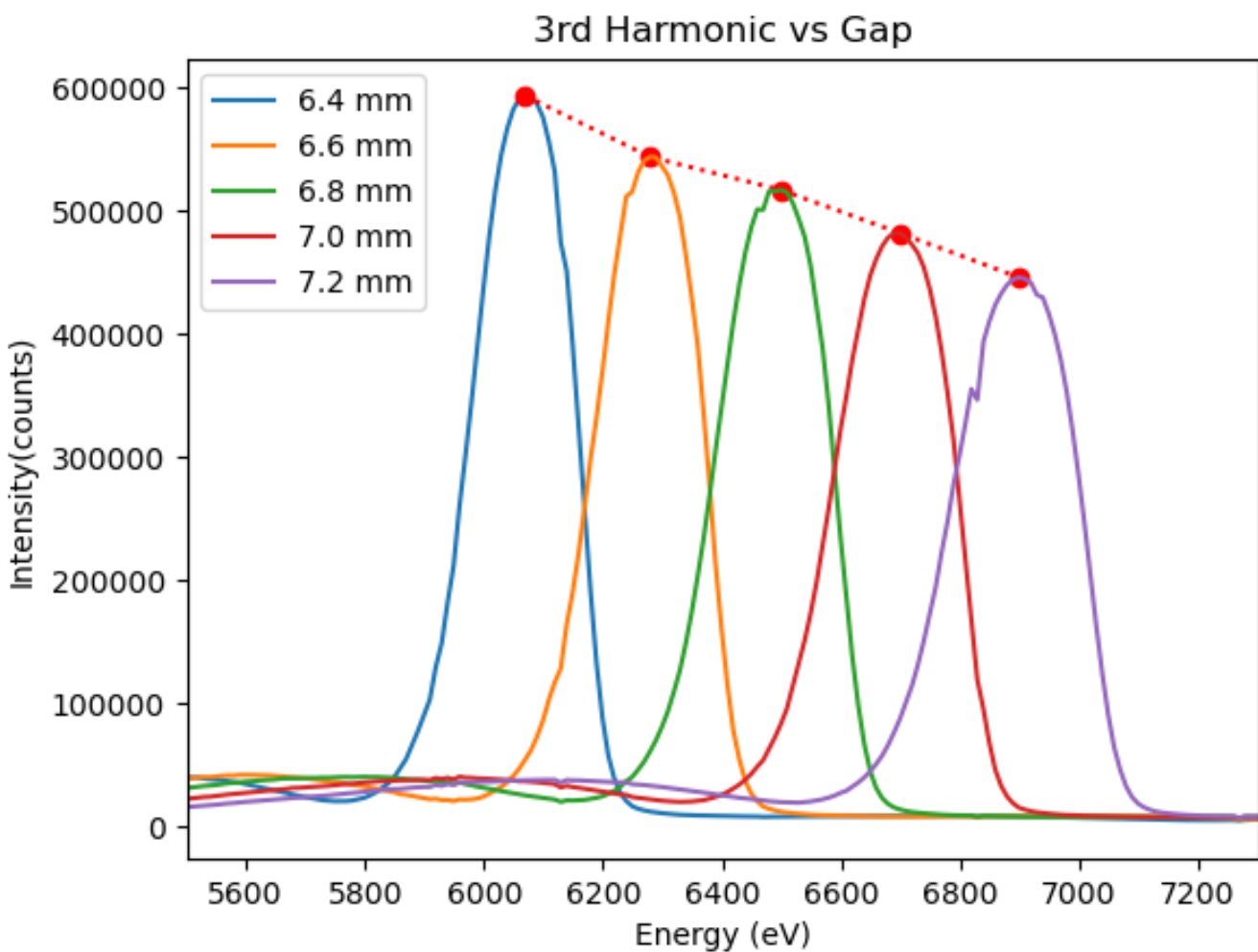
Normal Mode (Gap Scan)



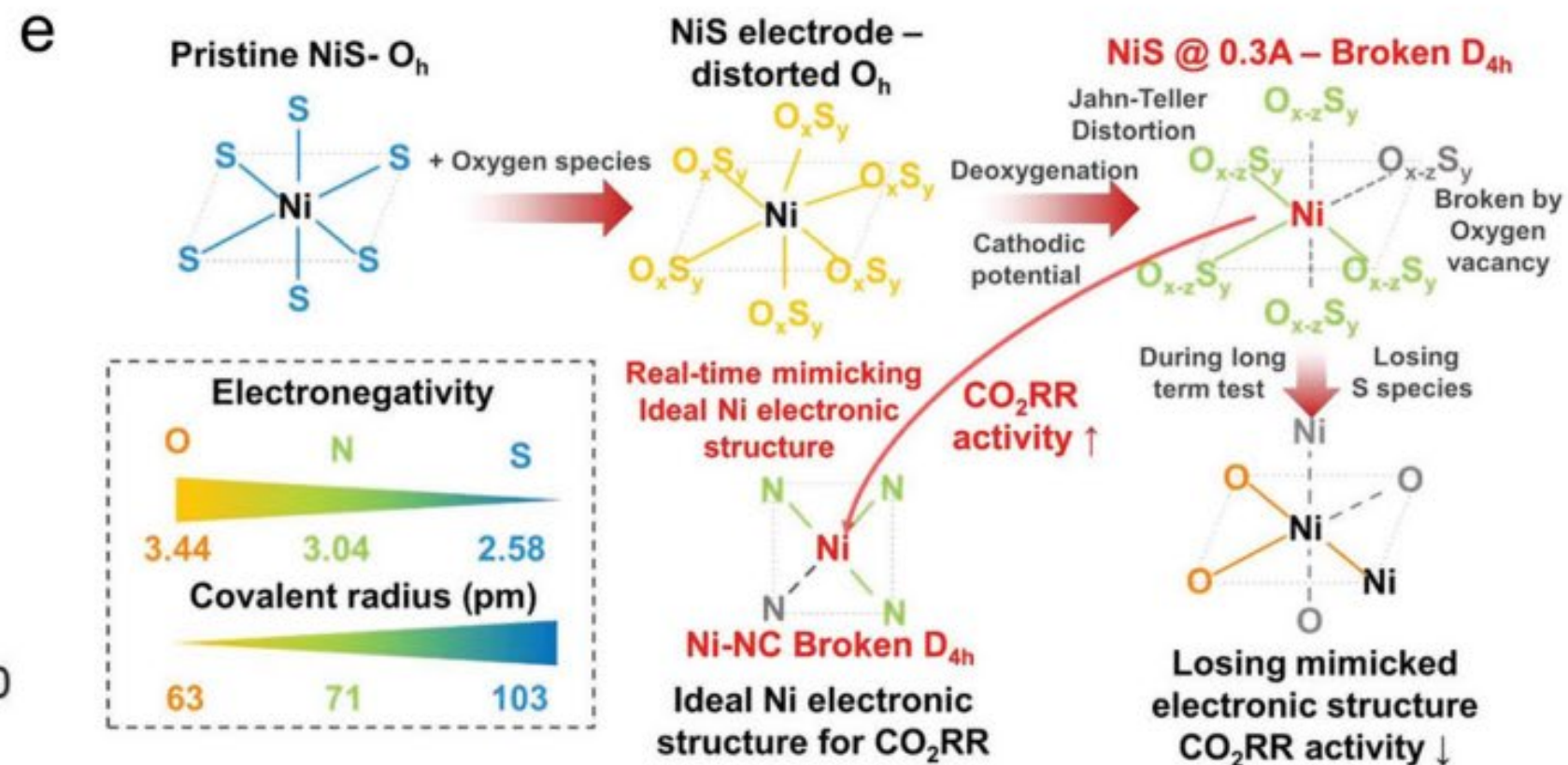
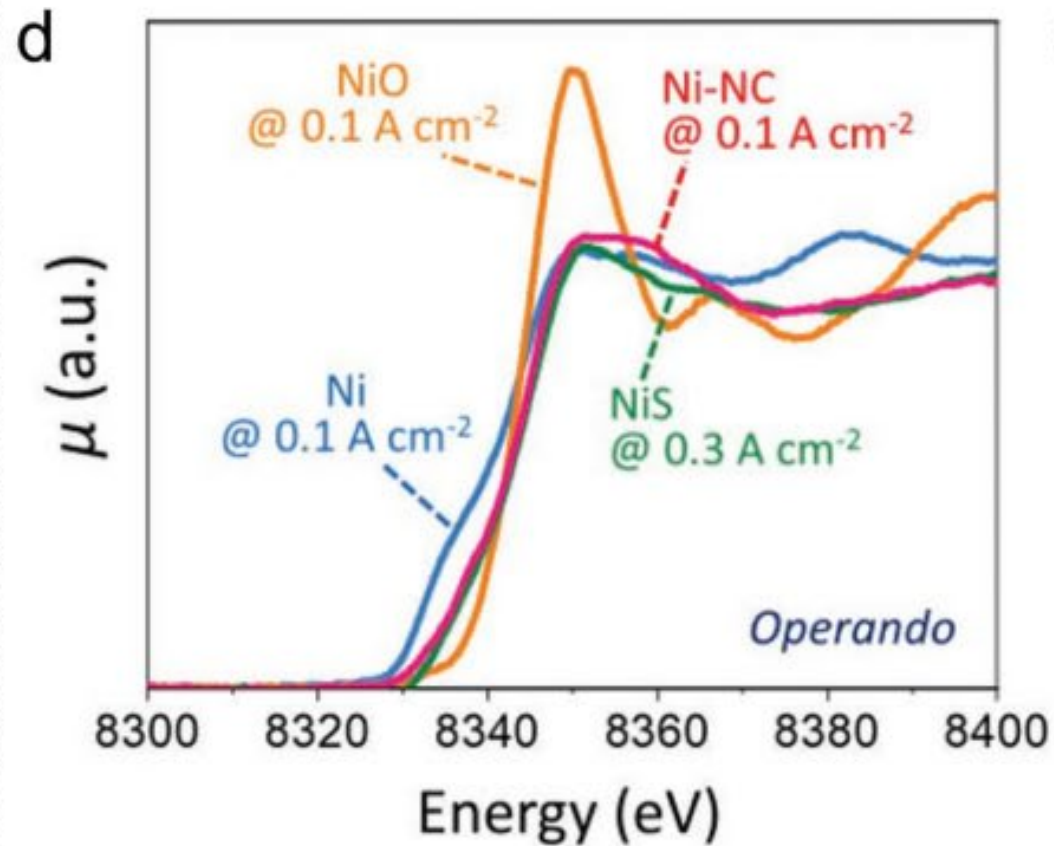
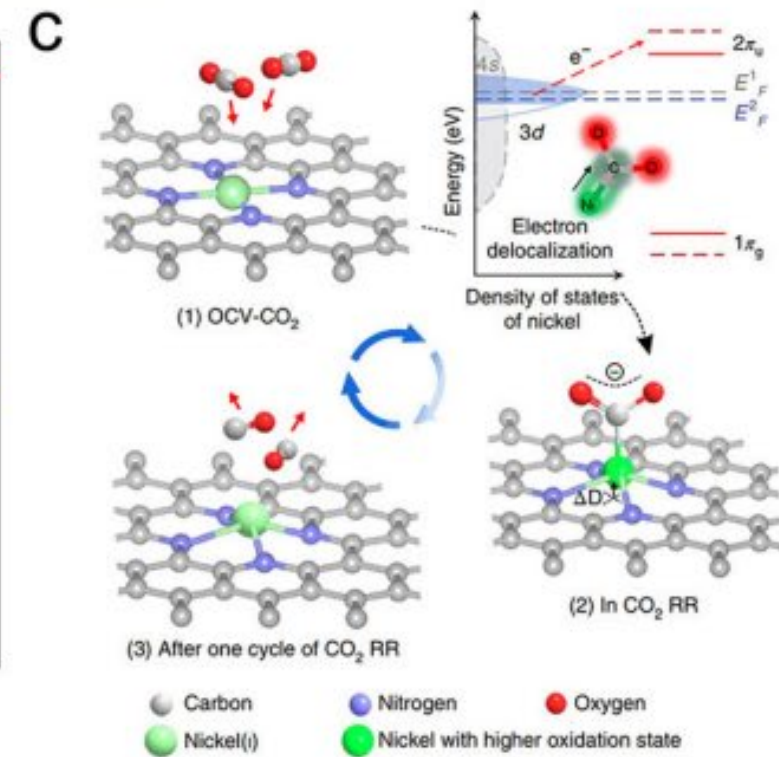
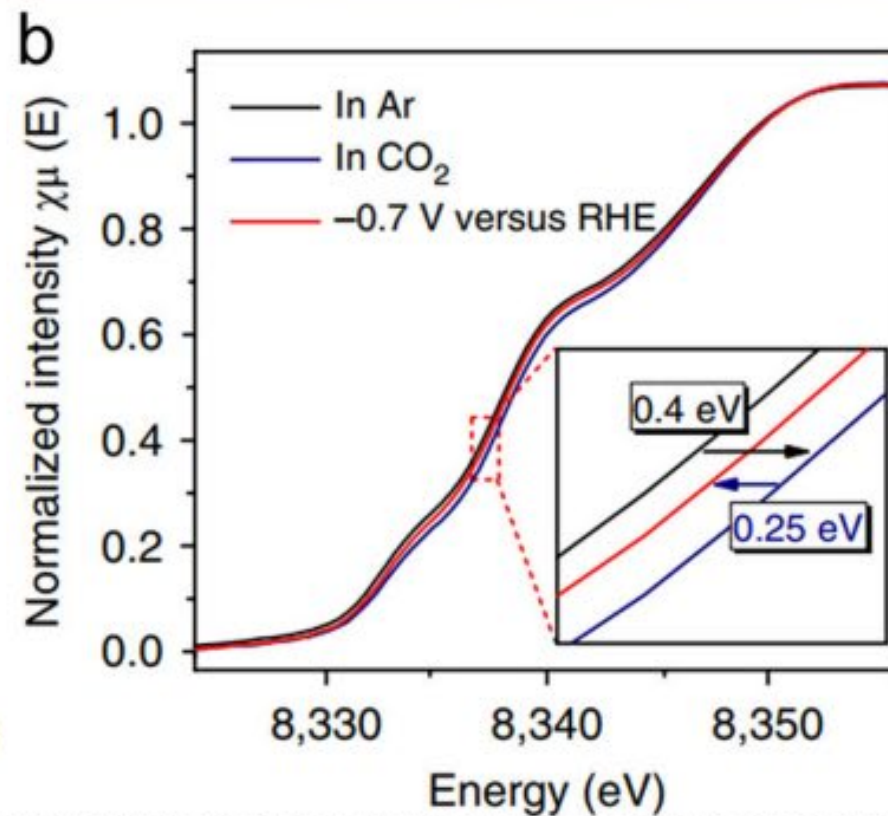
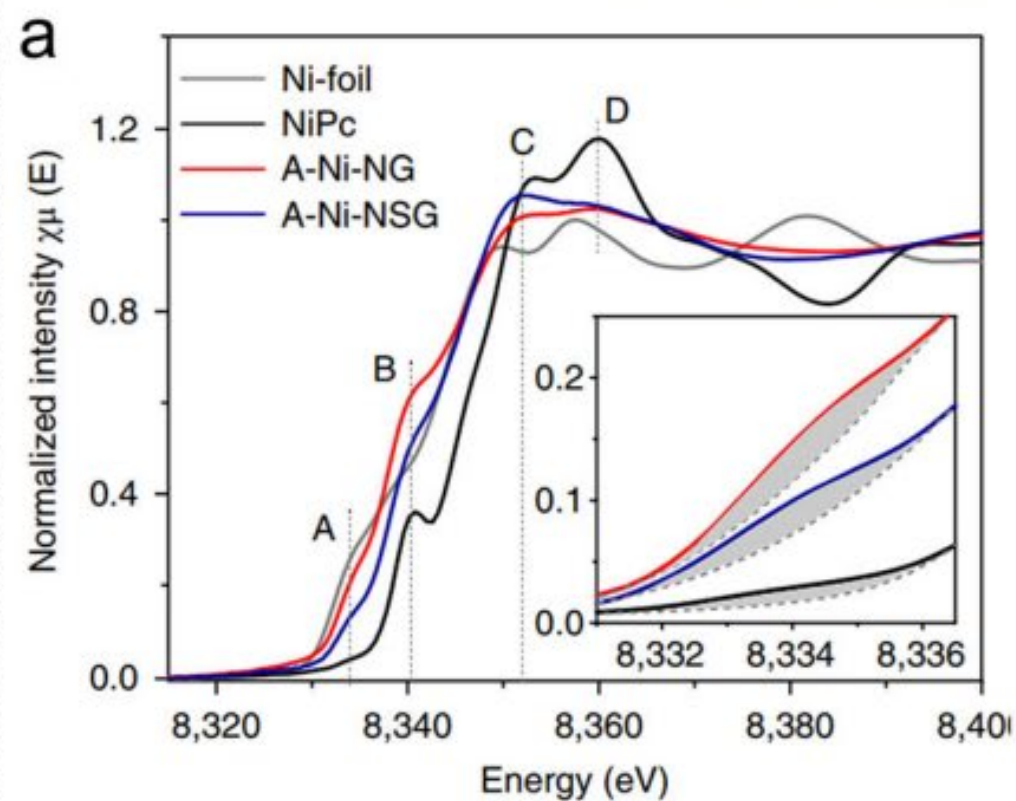
Korea-4GSR IVU24 Gap Scan Simulation

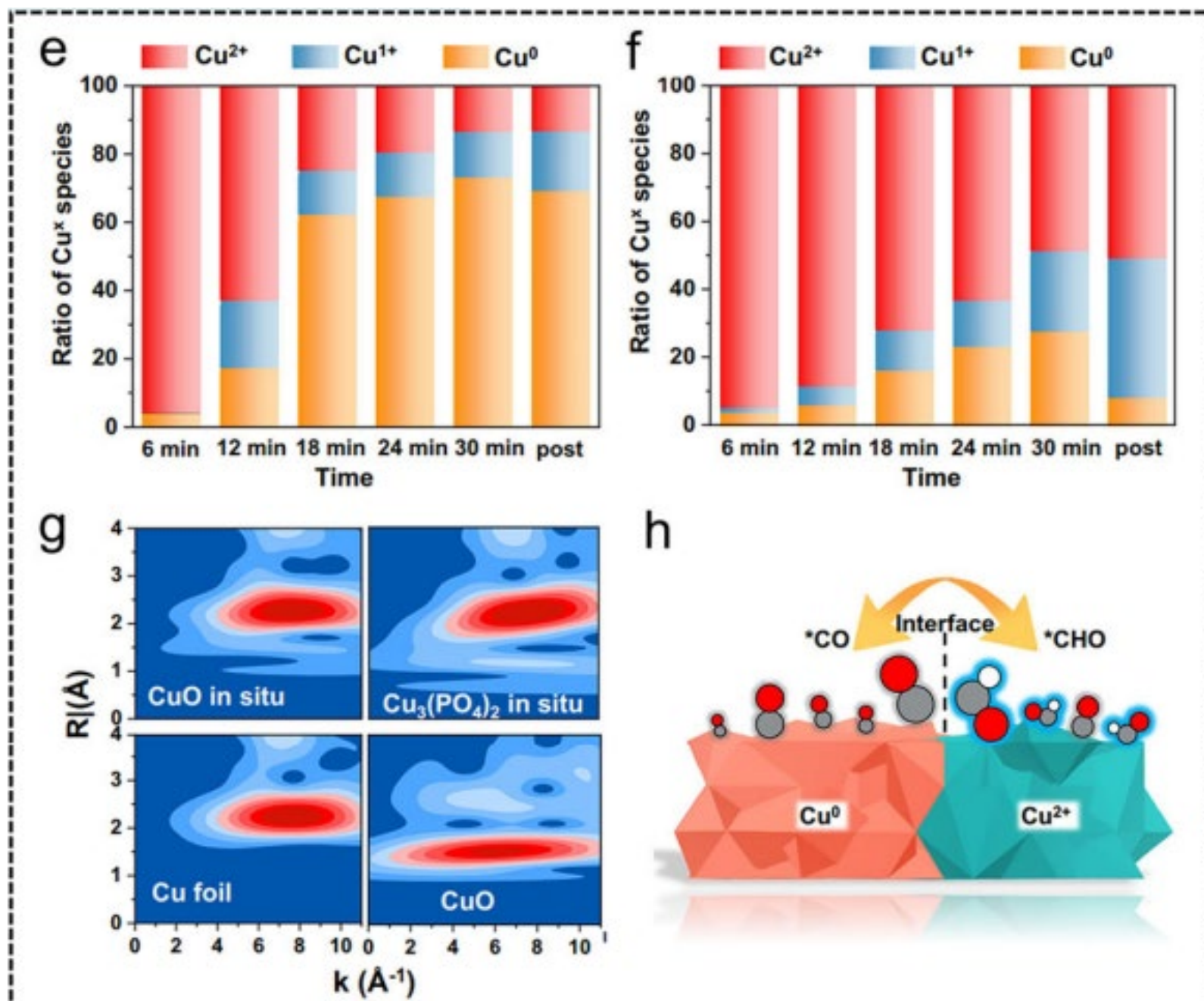
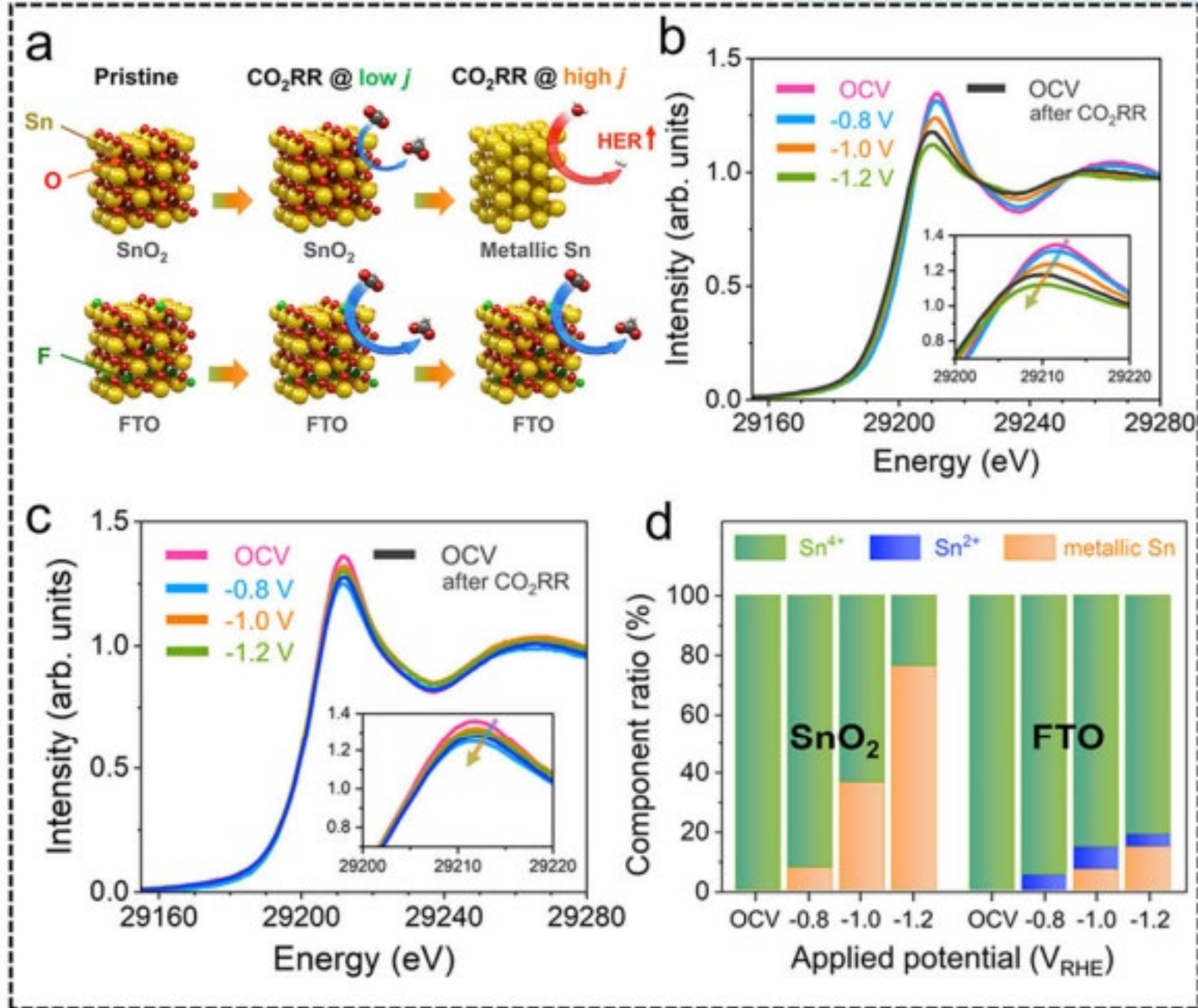


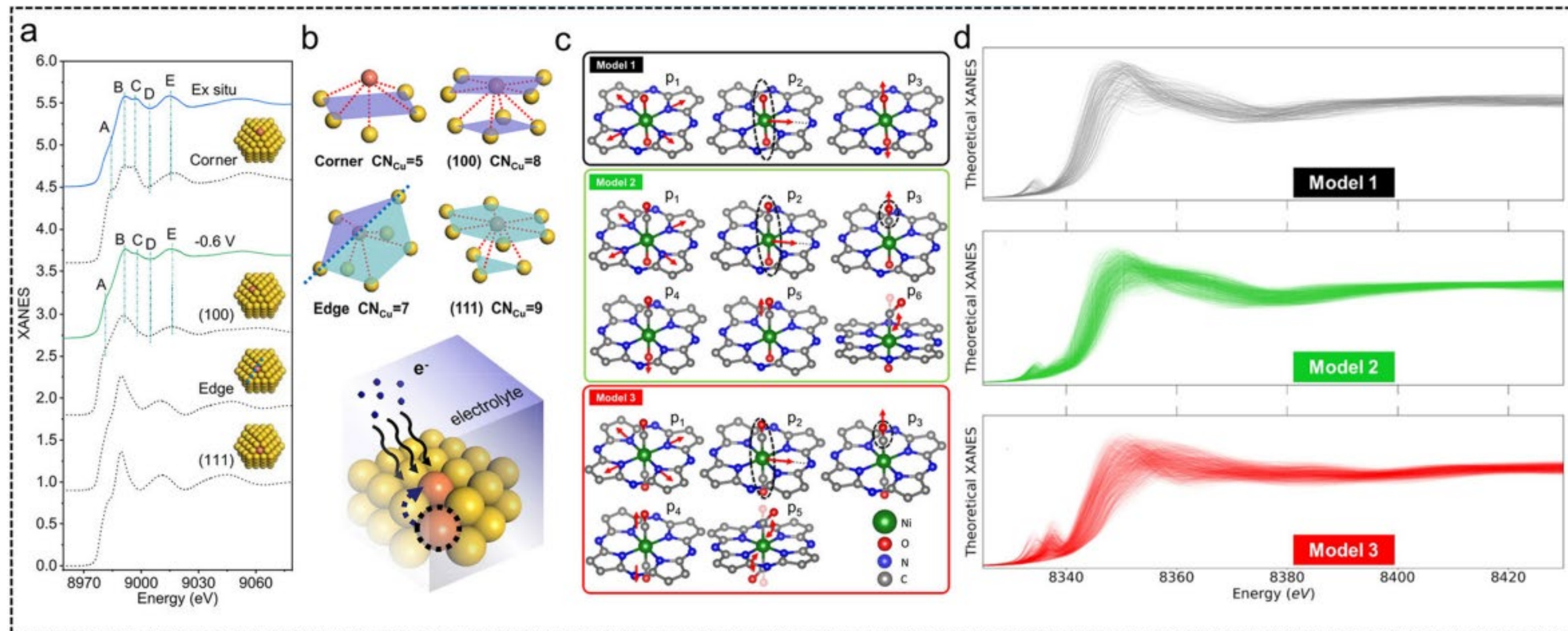
PAL PLS-II IVU20 Gap Tuning

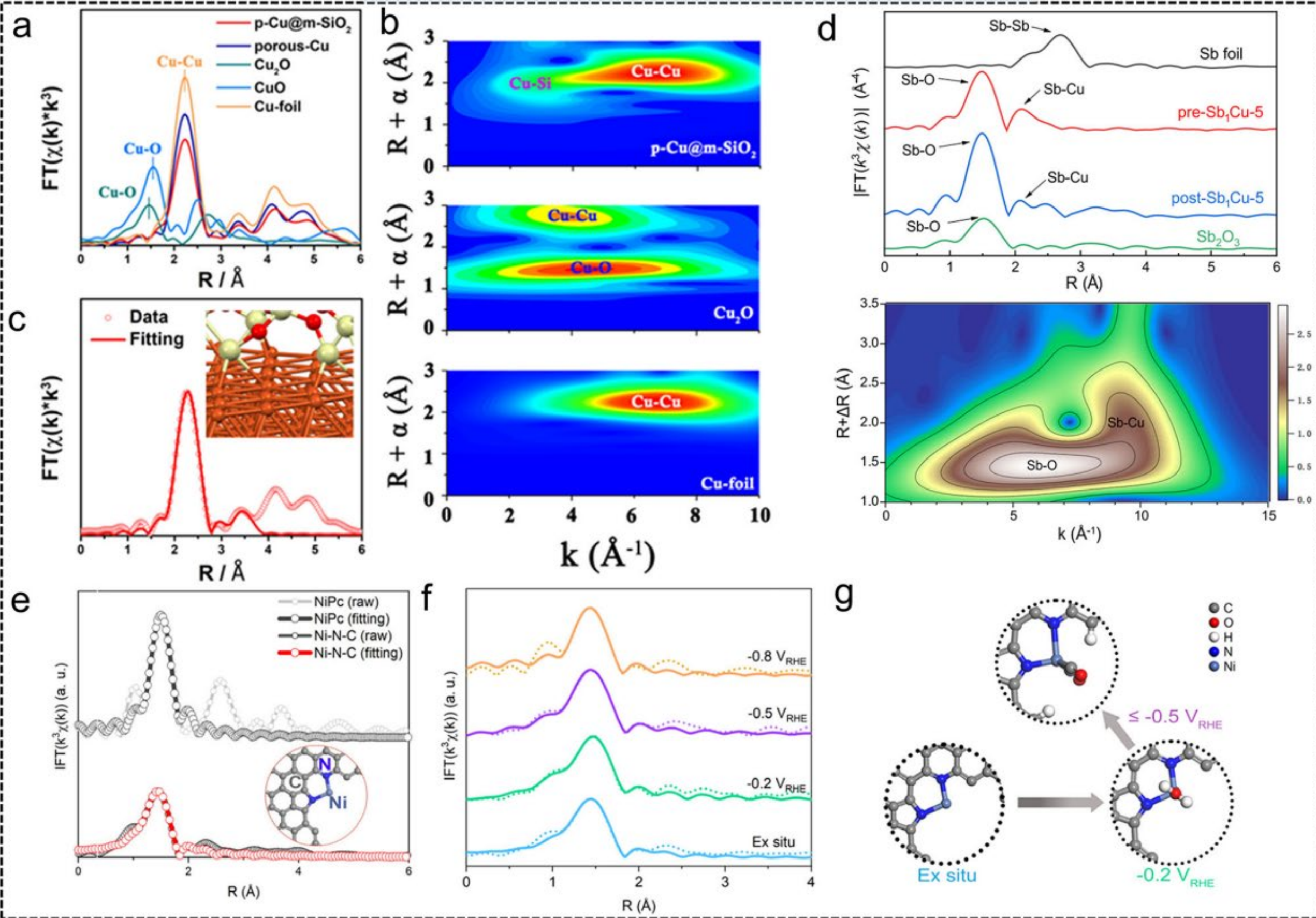


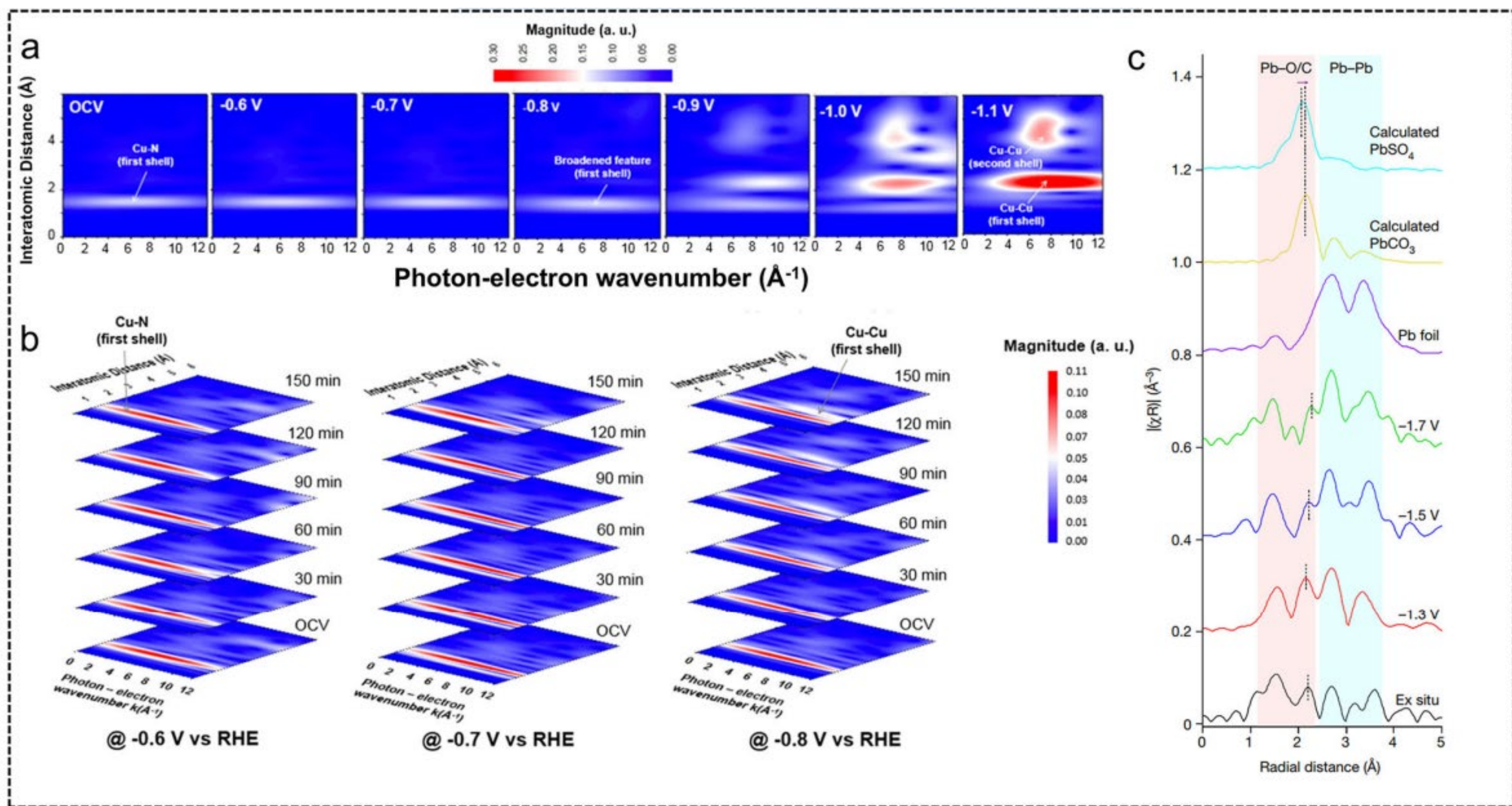
- By synchronizing the DCM and the undulator — a process known as a gap scan — a high-flux beam can be delivered to the experimental hutch.

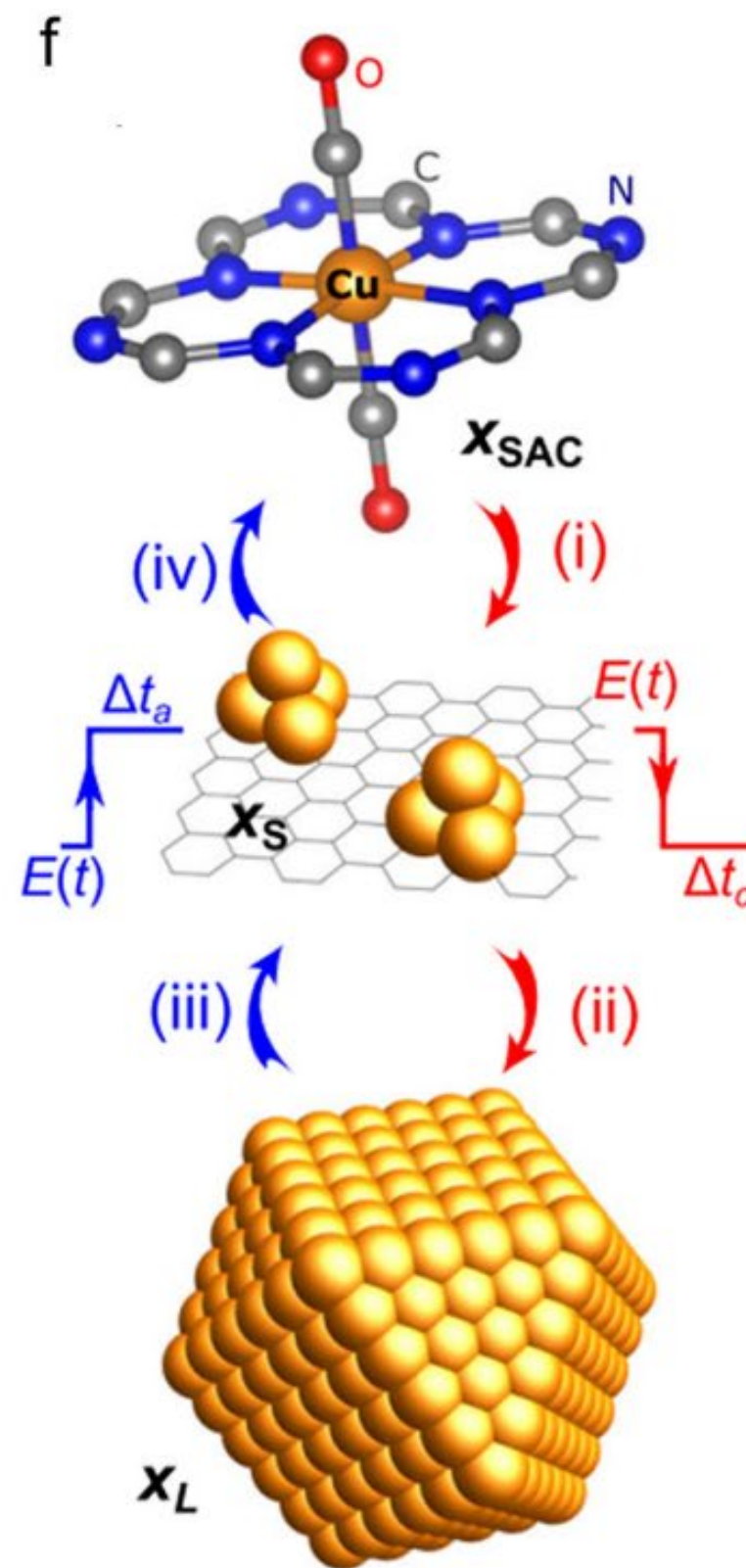
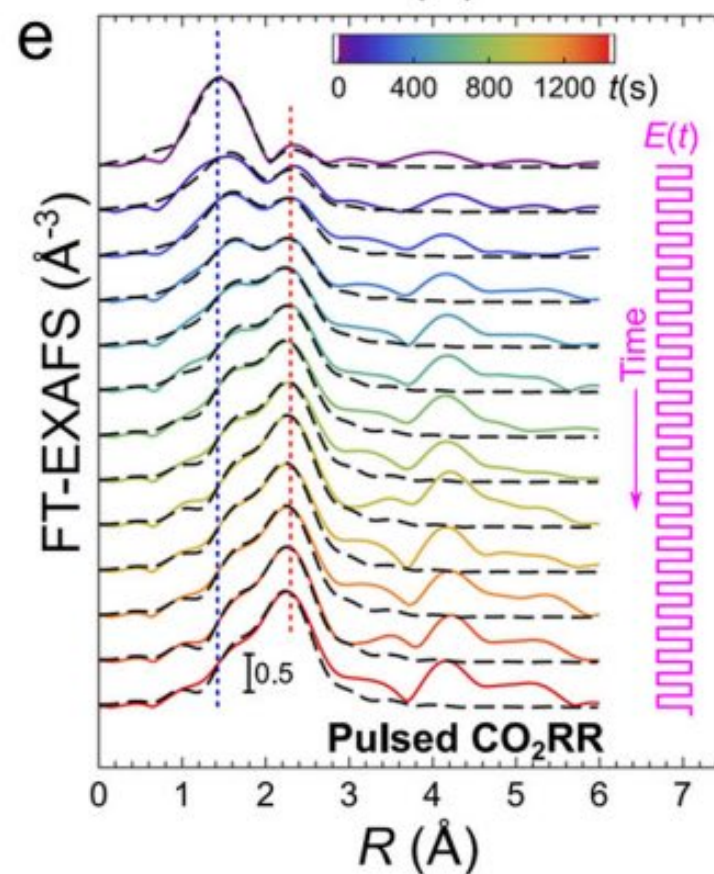
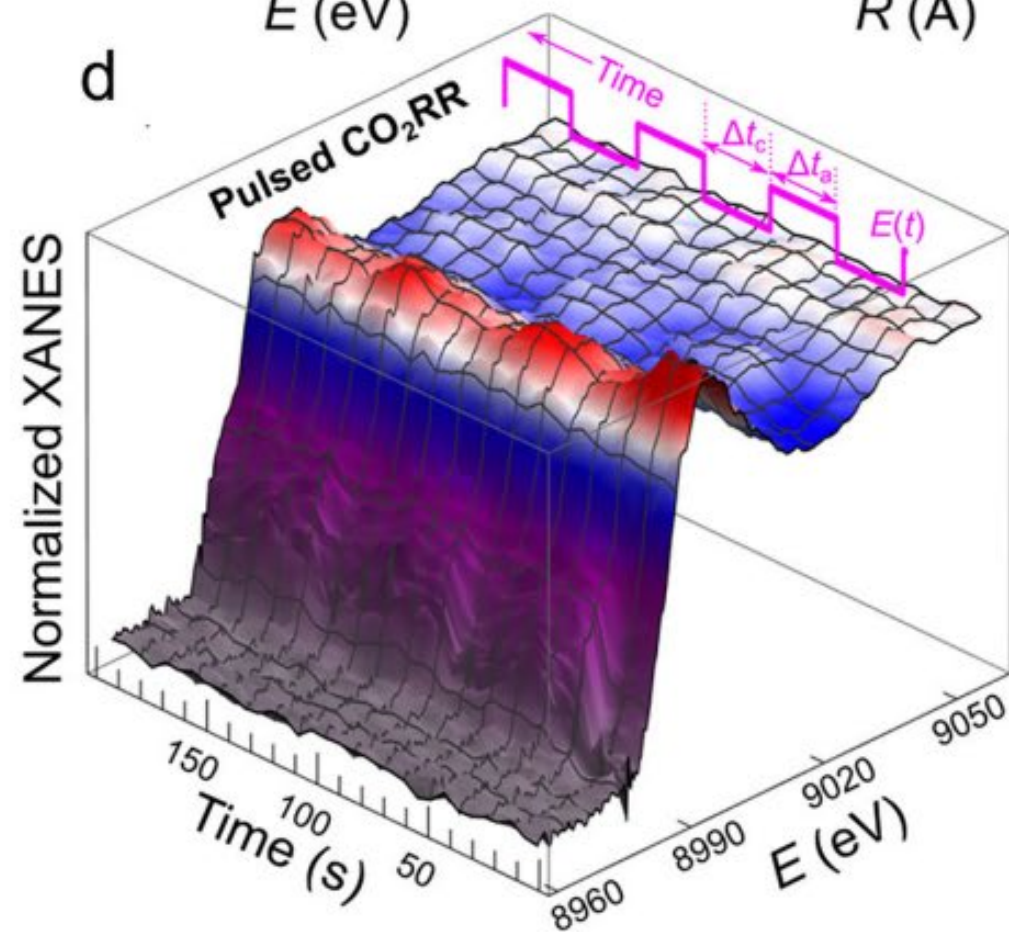
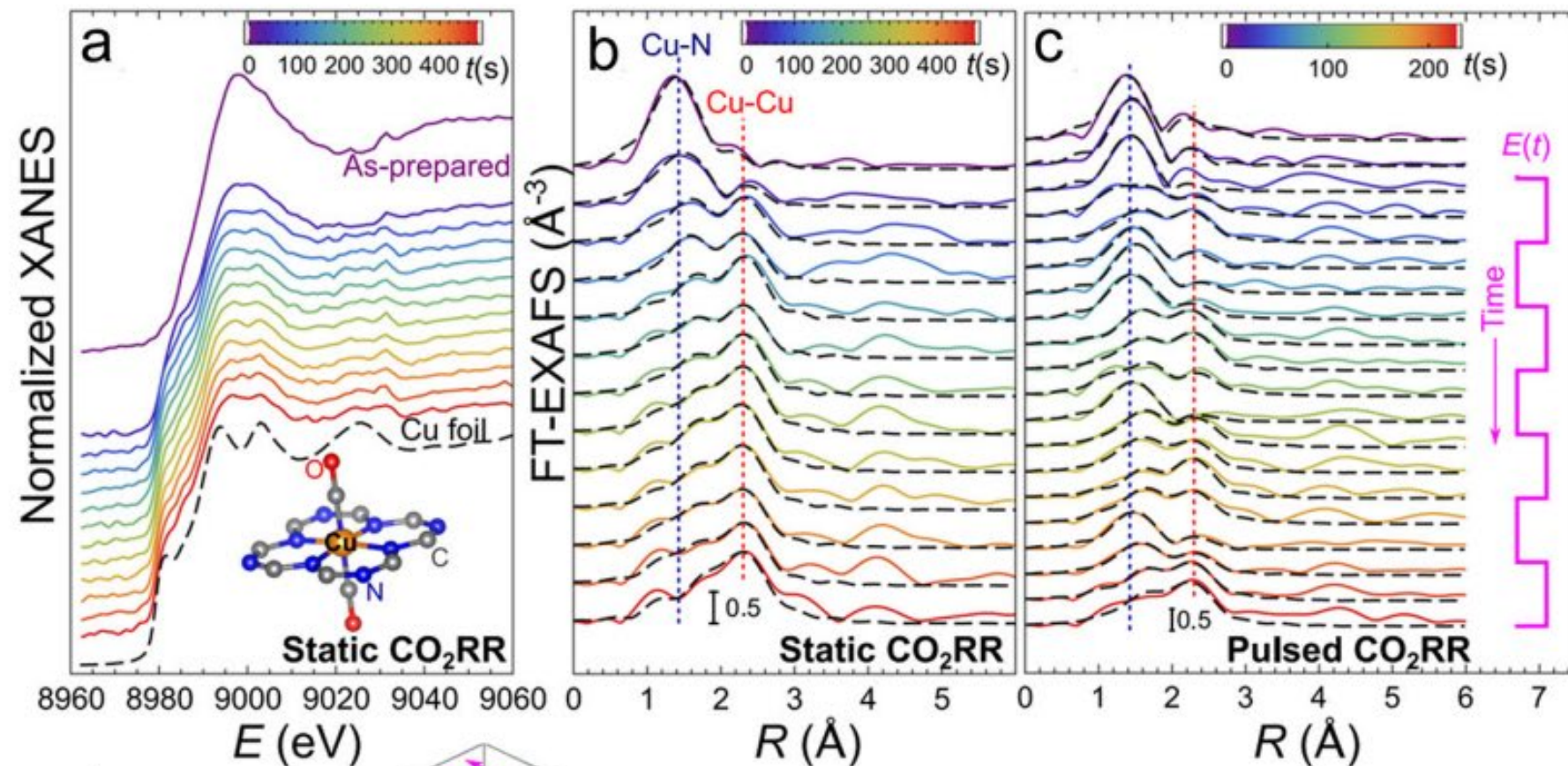


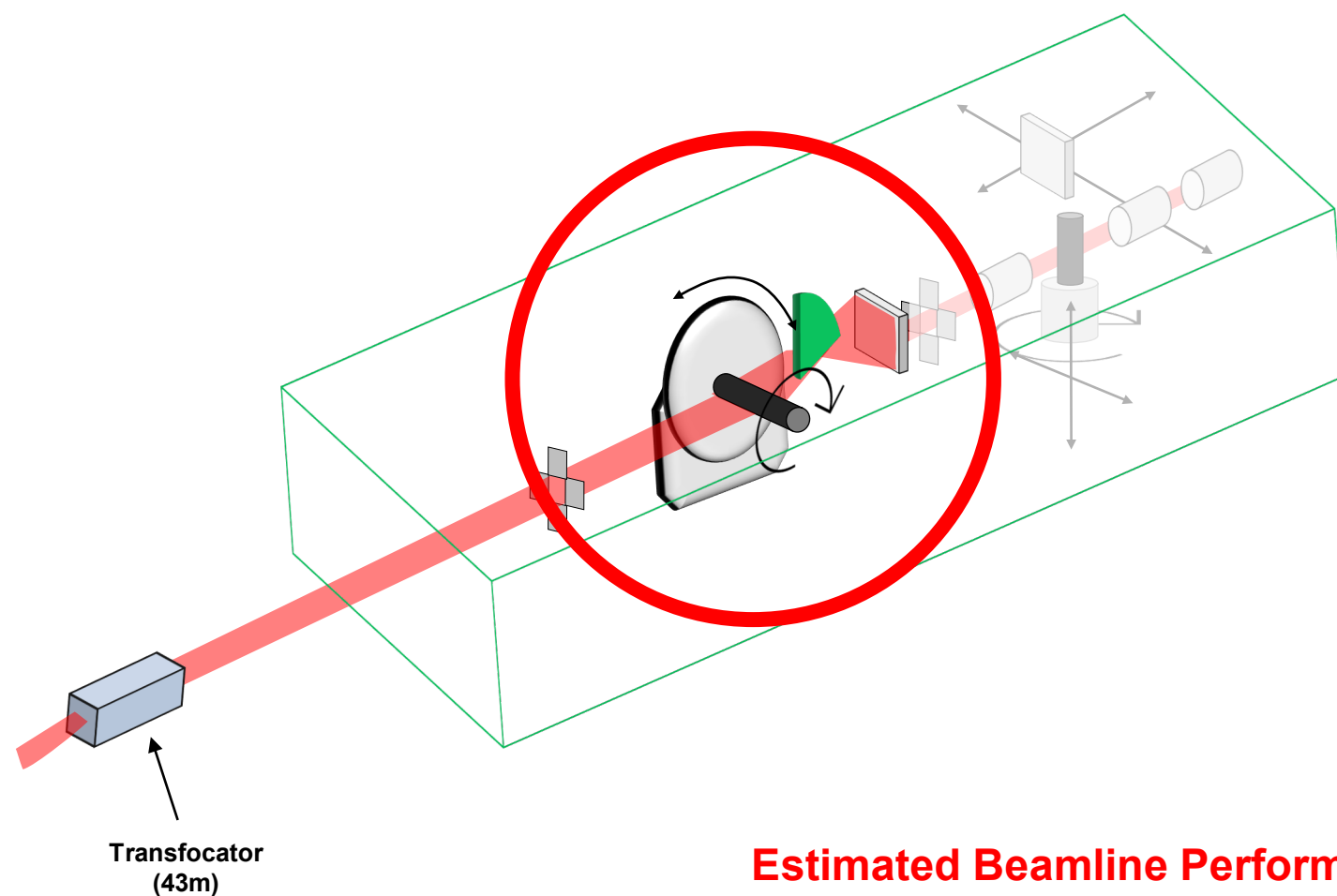








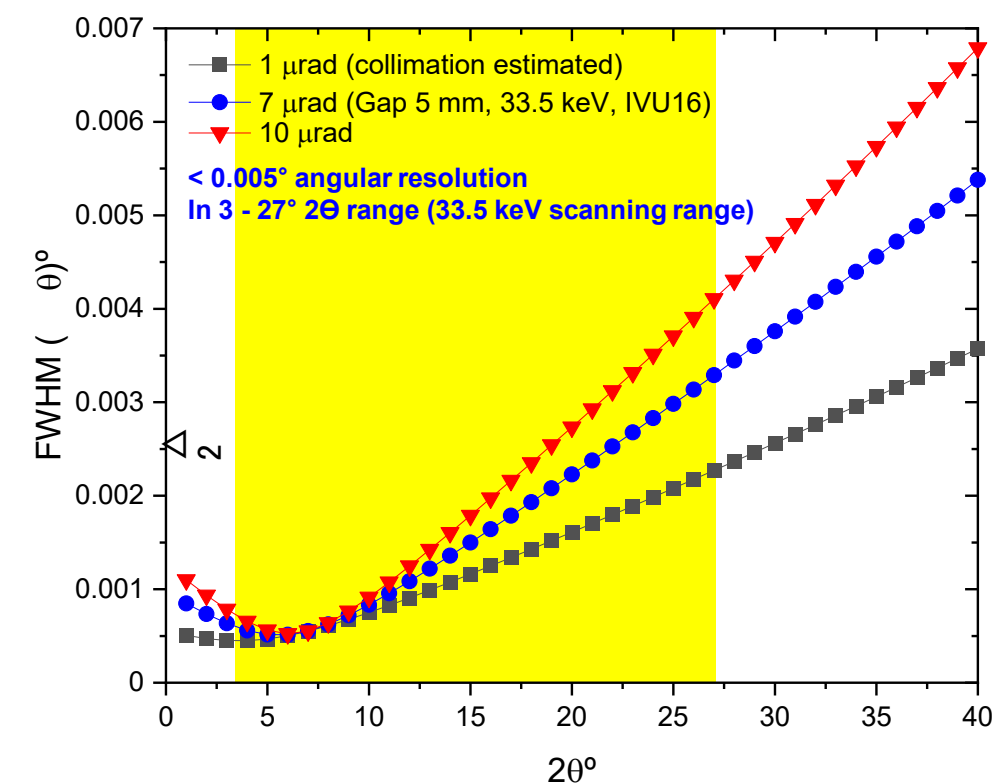
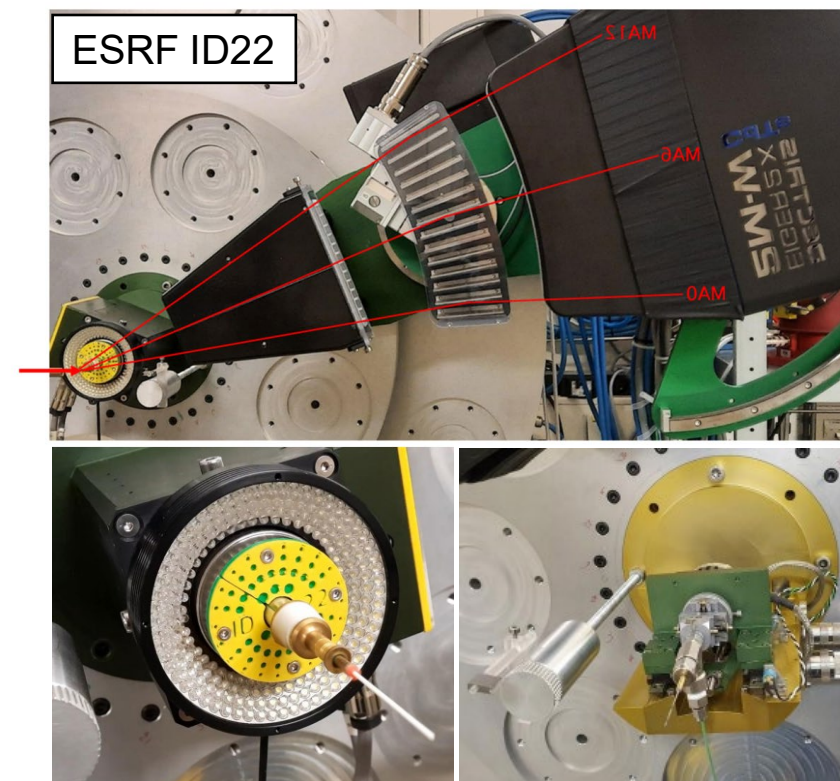


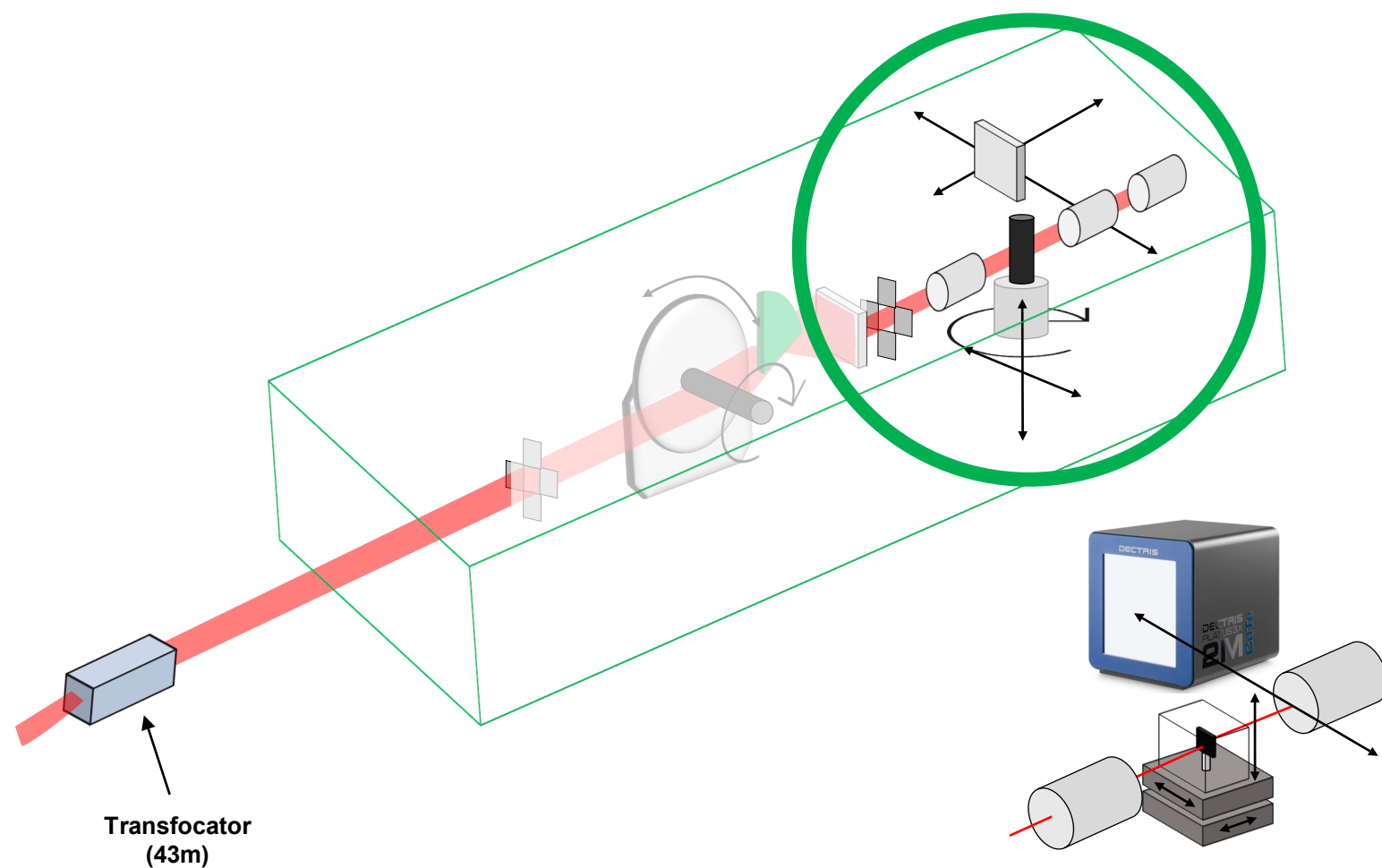


Estimated Beamline Performance for HRPD

Optimized energy : 33.5 keV (IVU16, Gap 6 mm)
 Sample Capillary (1, 0.5, 0.3 mm capillaries)
 Various Capillary holding mode (Spinning, In-situ, ...)
 2θ Scanning range $3^\circ \sim 40^\circ$ (Optimized $5^\circ \sim 30^\circ$)
 (d-spacing $\sim 1 - 8 \text{ \AA}$)
 Angular resolution $< 0.005^\circ$
 Measuring time 15 min / sample
 (0.02° step scan, expose time 0.5s)

*MAC crystals information
 2° interval 13 crystals with single axis

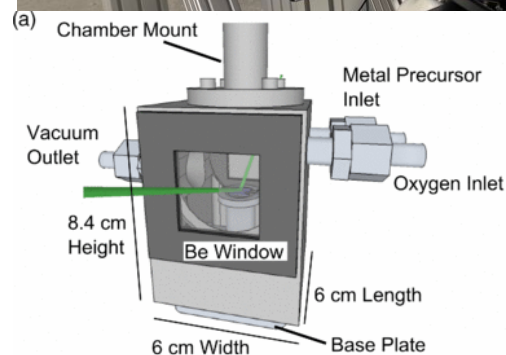




MAX IV DanMax



NSLS, X18A



SDD	MAX 2 θ	Angular Resolution	d-spacing range (@33.5 kev, half ring)
500 mm	37.47°	0.074°	0.5 – 4.3 Å (2 $\theta_{\min}$ = 5°)
1000 mm	18.74°	0.037°	1.1 – 8.6 Å
2000 mm	9.37°	0.019°	2 – <16 Å

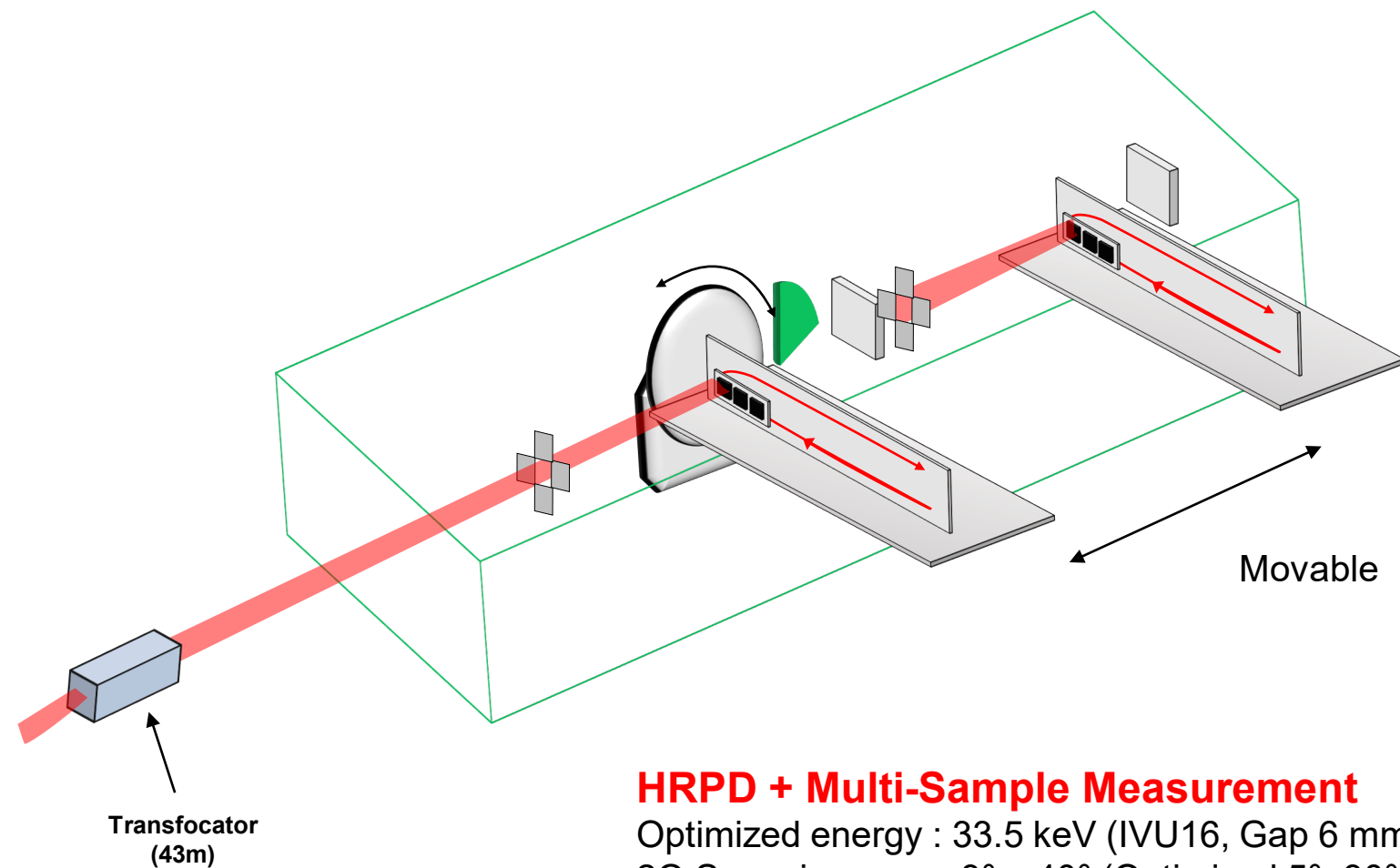
*PILATUS4 X 4M (estimated with values of 327 mm active area in height, 150 μ m pixel size, 0.5 mm sample thickness)

Estimated Beamline Performance for 2DXRD

Optimized energy : > 20 keV (depending on detector)
 2 θ Max canning range 10° ~ 40° (depending on SDD)
 SDD range 500 – 2000 mm

Angular resolution range (0.006 – 0.08° in the range of 500-2000 mm SDD)

Measuring time < 1 min / sample



HRPD + Multi-Sample Measurement

Optimized energy : 33.5 keV (IVU16, Gap 6 mm)

2 θ Scanning range 3° ~ 40° (Optimized 5°~30°)

(d-spacing ~1 – 8 Å)

Angular resolution < 0.005°

Measuring time 15 min / sample

2DXRD + Multi-Sample Measurement

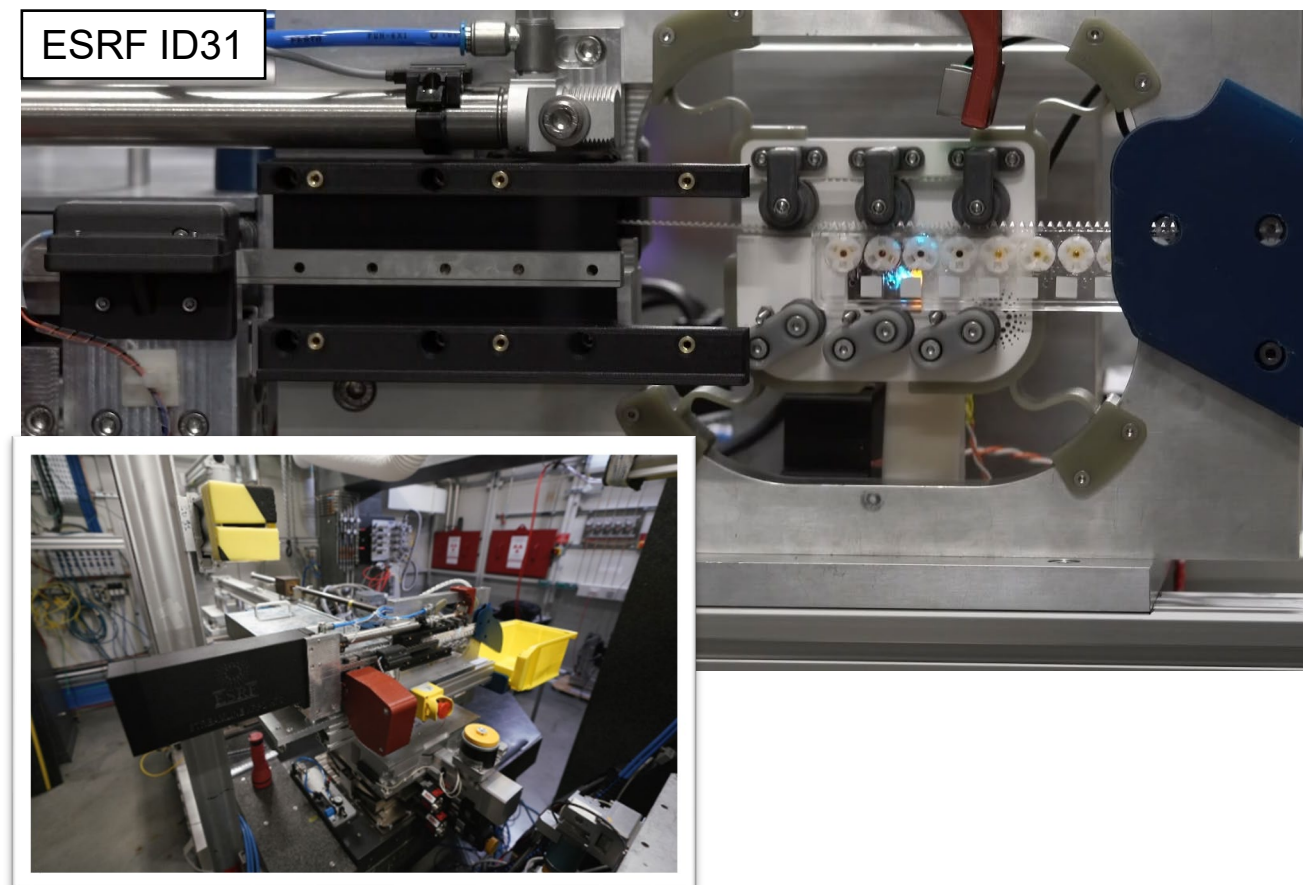
Optimized energy : > 20 keV (depending on detector)

2 θ Max canning range 10° ~ 40° (depending on SDD)

SDD range 500 – 2000 mm

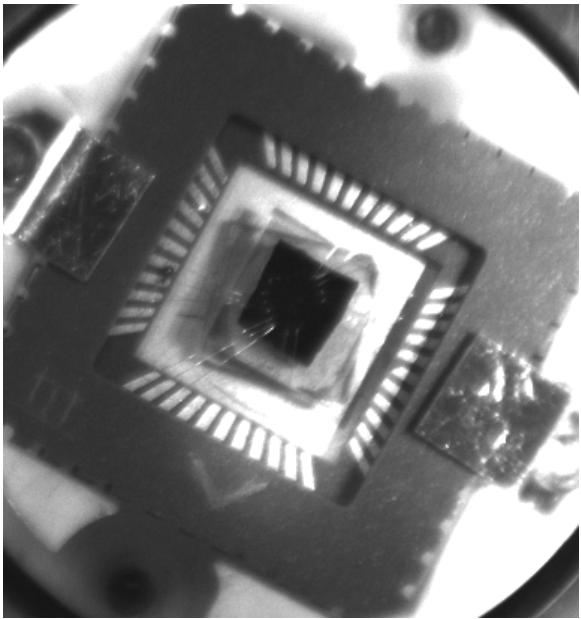
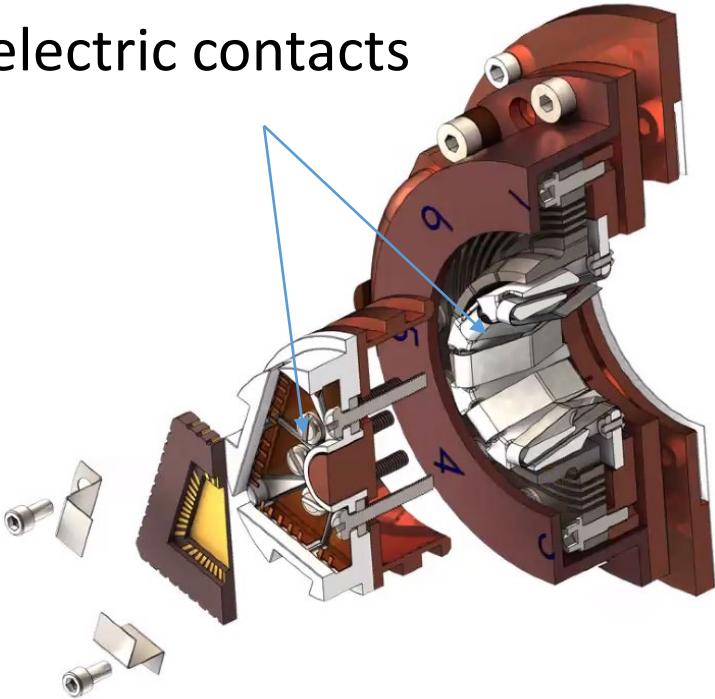
Angular resolution range (0.006 – 0.08° in the range of 500-2000 mm SDD)

Measuring time < 1 min / sample

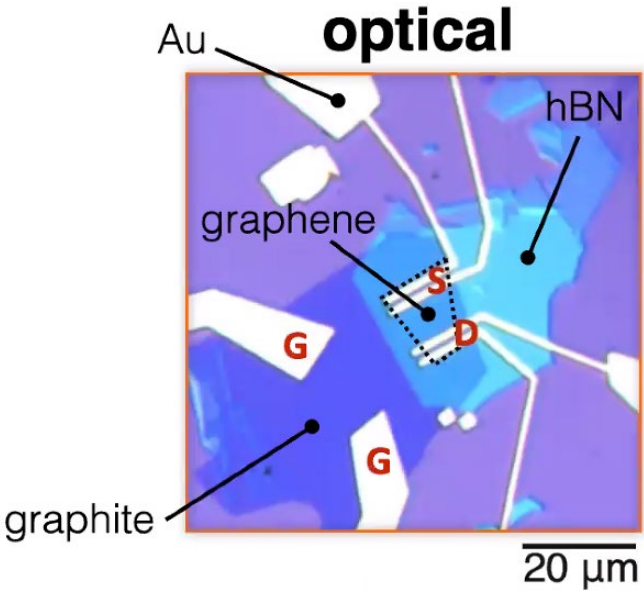


In-operando measurement

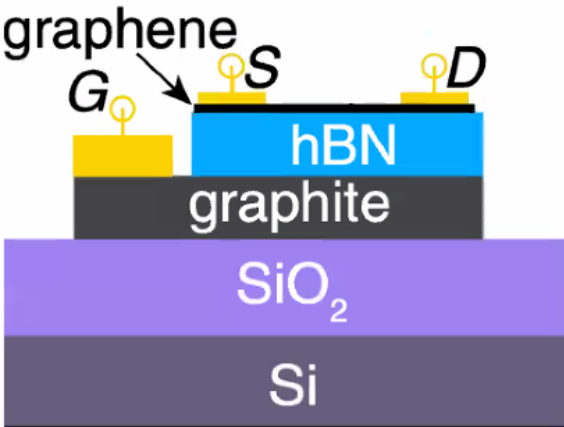
8 electric contacts



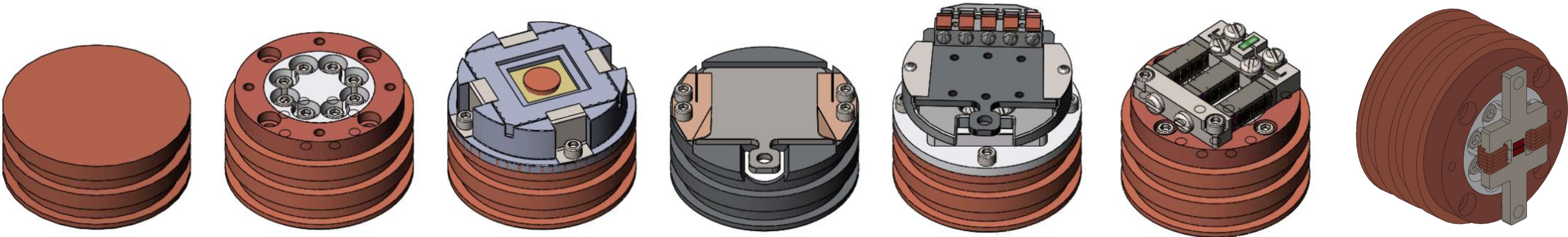
Wire bonding to device



Transport / gating capability



Strain controller



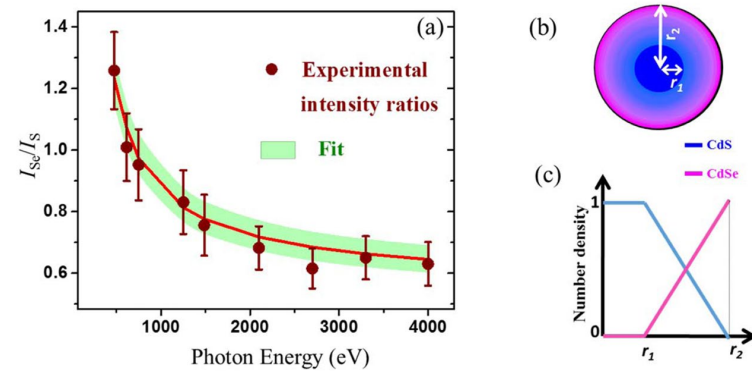
Transport / Gating

Transport / Gating
general sample holder

Magnetic field inducer

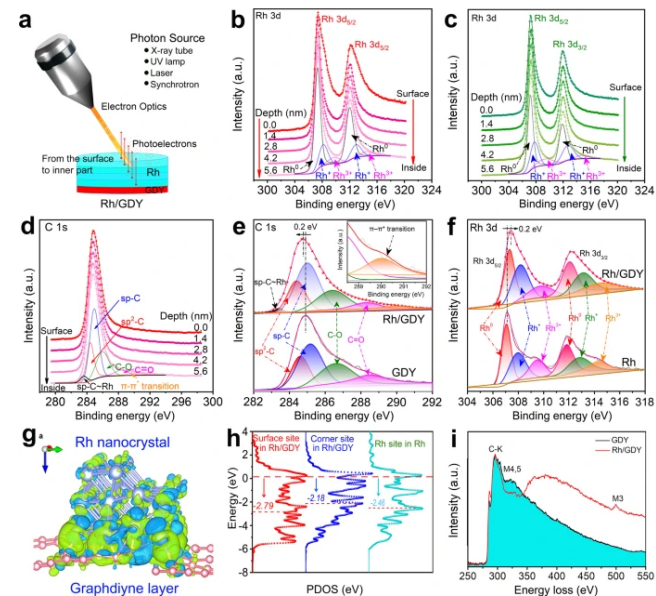
❖ Tender AP-XPS/XAS

- Tender Energy [2 ~ 5keV (+ 0.1 ~ 3 keV)]
- Tender Ambient Pressure XPS and XAS



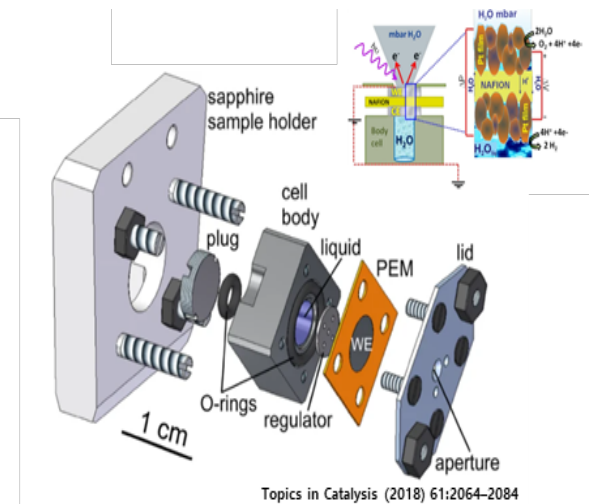
J. Phys. Chem. C **118**, 15534 (2014)

Energy-dependent depth resolution



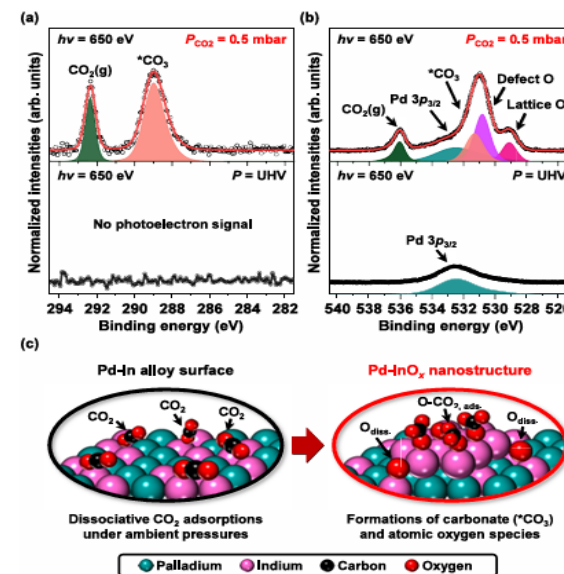
Nature Communications **13**, 5227 (2022)

Depth profiling experiments



Top Catal **61**, 2064 (2018)

Electro chemical

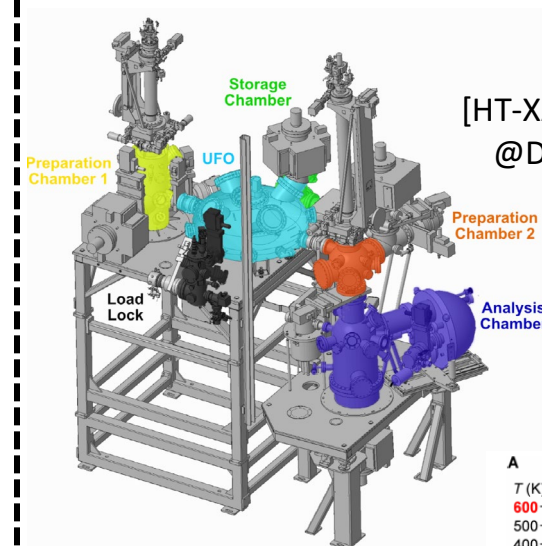


J. Phys. Chem. Lett. **16**, 4131–4138 (2025)

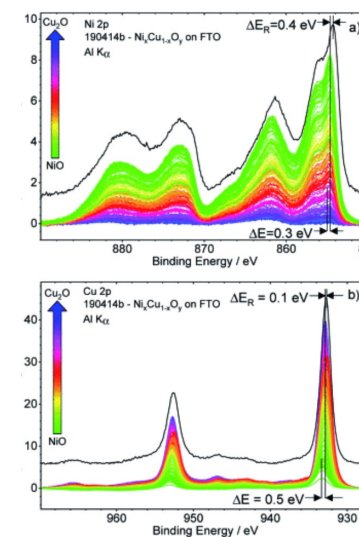
CO₂ Conversion

❖ Nano-XPS/XAS

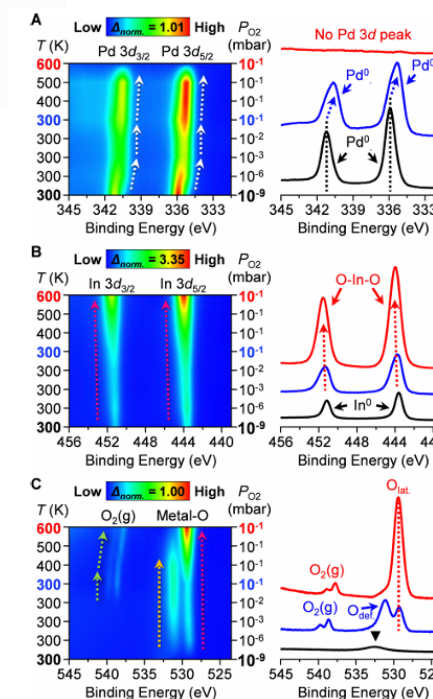
- Soft Energy (0.1 ~ 3 keV)
- High-throughput XAS(XPS)
- Beam focusing(optional) to sub-micron size
- Automated sample measurement
- Open to accepting a candidate systems



[HT-XAS(XPS)
@DIAMOND B07)]

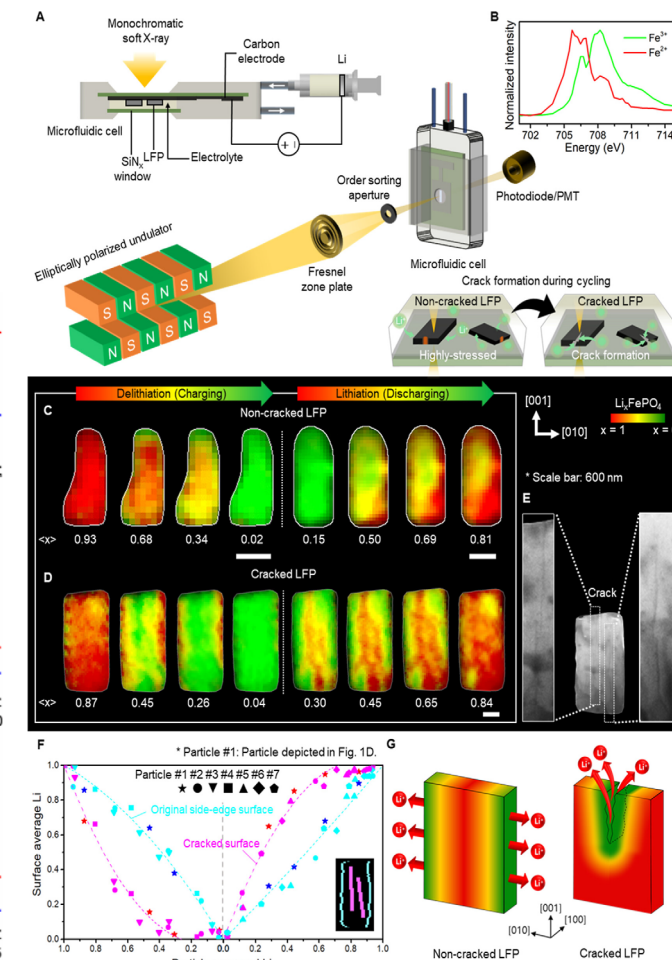


RSC Adv. **12**, 7996 (2022).



Chem. Commun. **61**, 14181 (2025).

In-situ/Operando Experiments



ACS Nano **19**, 9936 (2022).