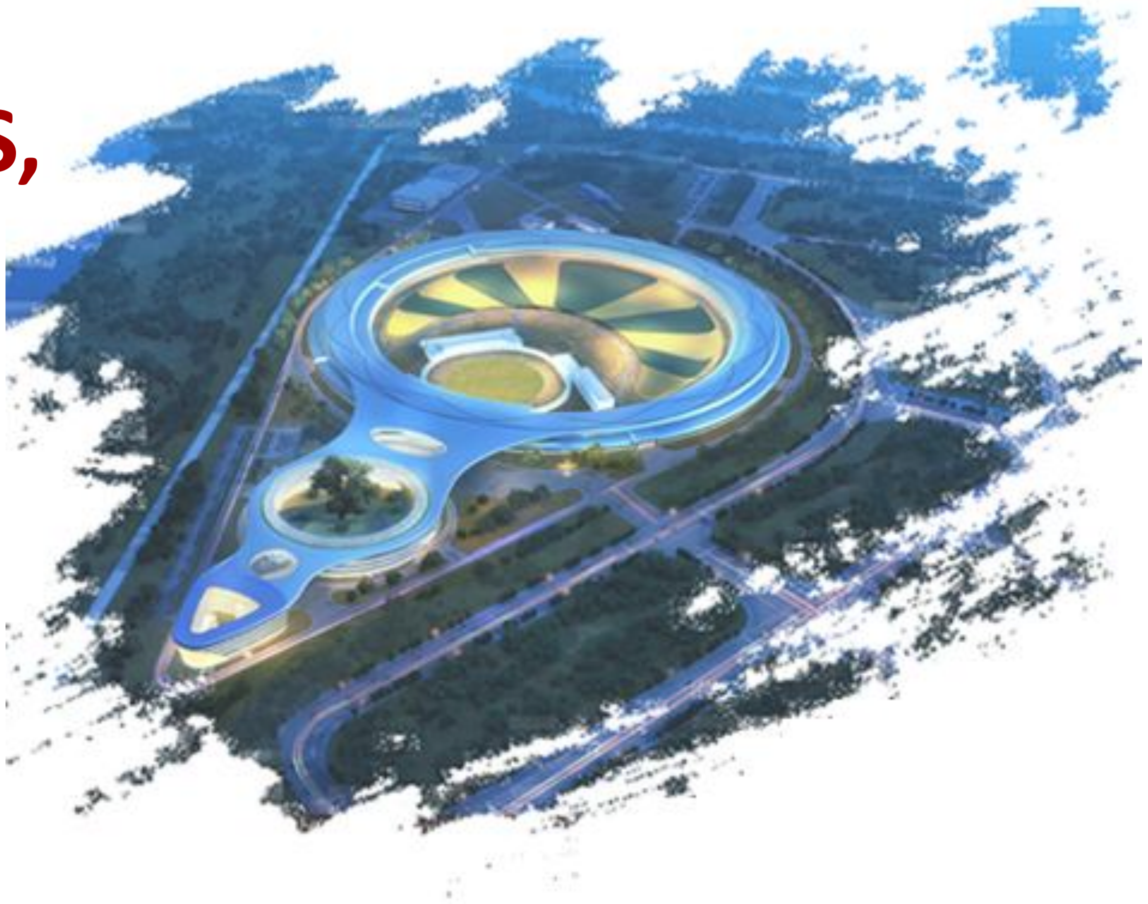
Progress of the experiment operating software system (ARPES, XPCS, RIXS) at HEPS



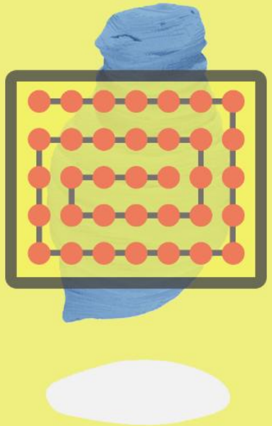
Lingzhu Bian
HEPS Software Team

12/08/2025

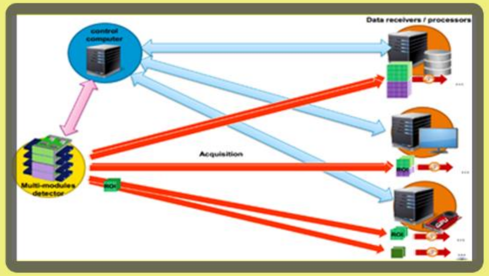
HEPS/MAX IV Control System Meeting

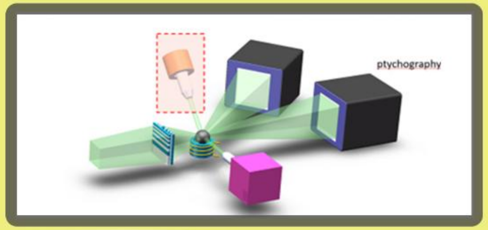
Drastic increase in data and experiment complexity

1 Nano & macro probe

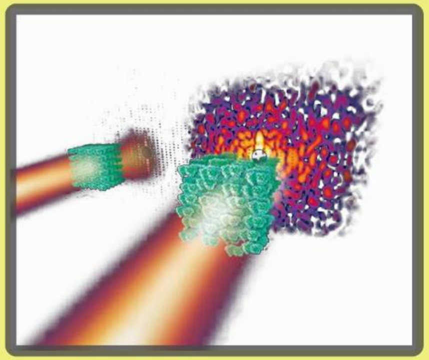


2 High throughput & Multi-modal

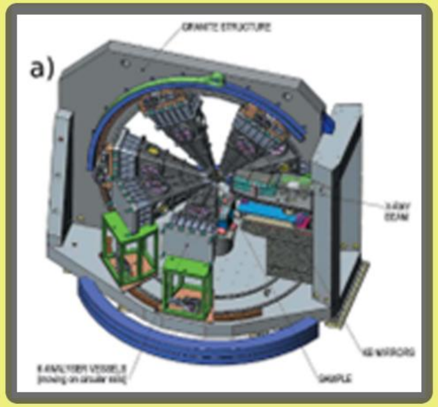




3 In situ & dynamic experiments



4 beamline automation & intelligent control



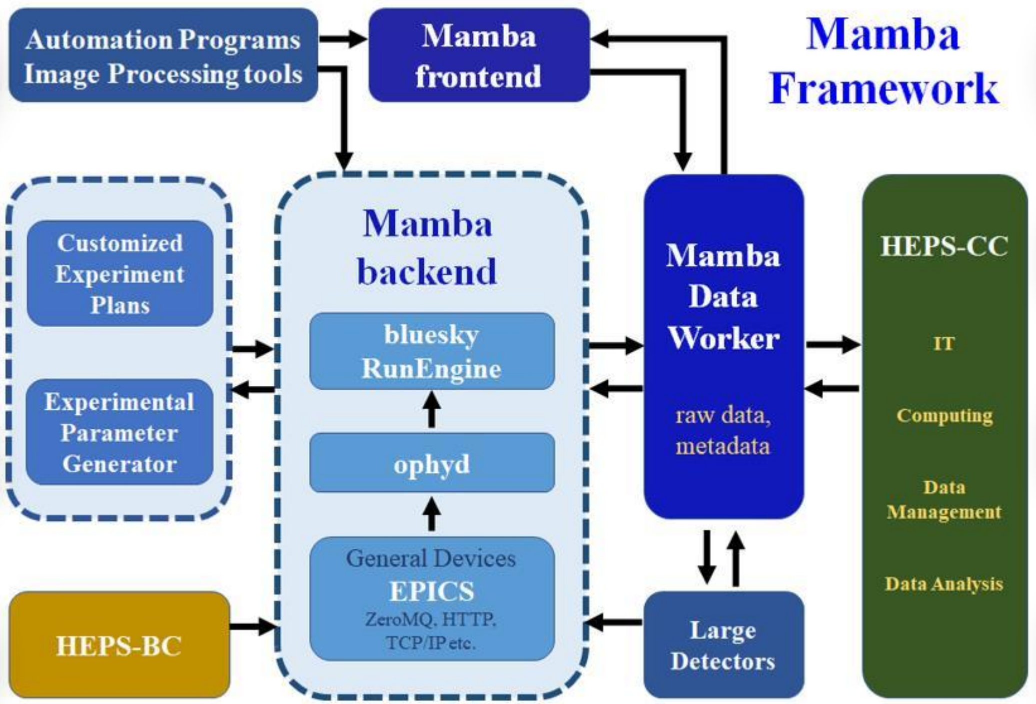
5 National data mangementpolicy

- **X-ray flux orders of magnitude brighter,**
- **Detectors are orders of magnitude larger and faster, single beamline generate up to *Pb* /run,**
- ***In situ* and *dynamic* experiments require real-time feedback and autonomous control,**
- **Data and software infrastructure for big science project**

HEPS

A new generation synchrotron experiment operating software system (*Mamba*)

- **Beamline automation**
- **Real-time feedback and autonomous control**
- **Custom experimental procedures and commands for all experiment methods**
- **Smart *in-situ* experiment**



- **Friendly GUIs**
- **Easy experiment mode switch**
- **Fast and multi-modal DAQ**
- **Rich metadata, high interoperability**
- **Multi-dimensional, accurate, fast fly scans**

Mamba: a systematic software solution for beamline experiments at HEPS. ***Journal of Synchrotron Radiation***, 2022

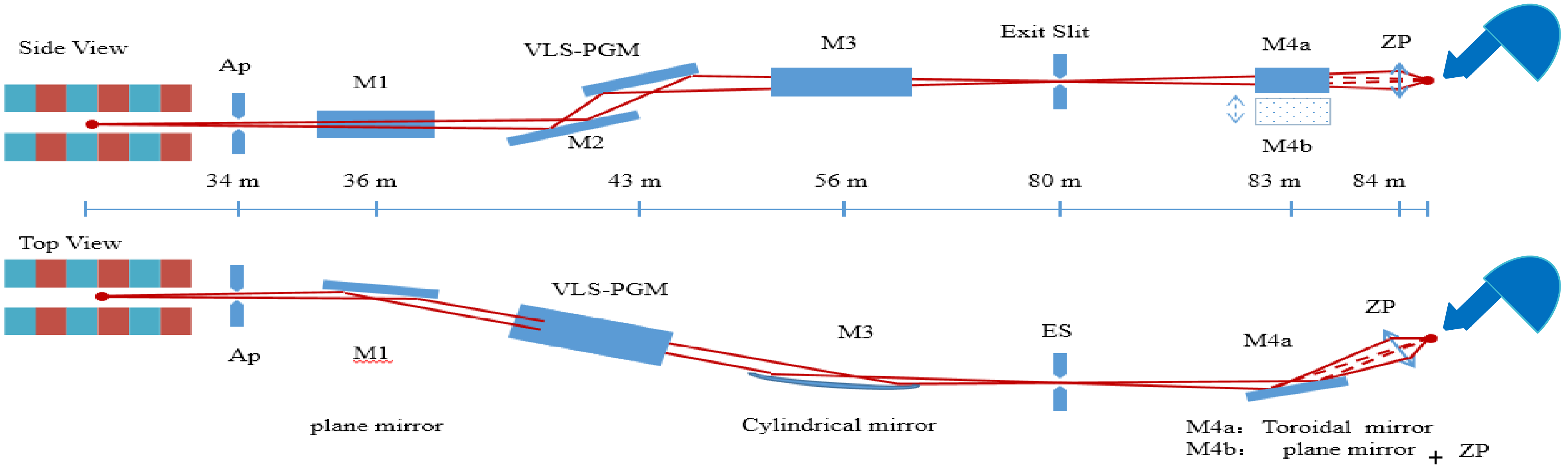
Outline

- Experiment Control and Data Acquisition System
  - High-resolution Nano Electronic Structure Spectroscopy Beamline (HiNESS/ARPES)
  - X-ray Photons Correlation Spectroscopy (XPCS)
  - Resonant inelastic scattering (RIXS)

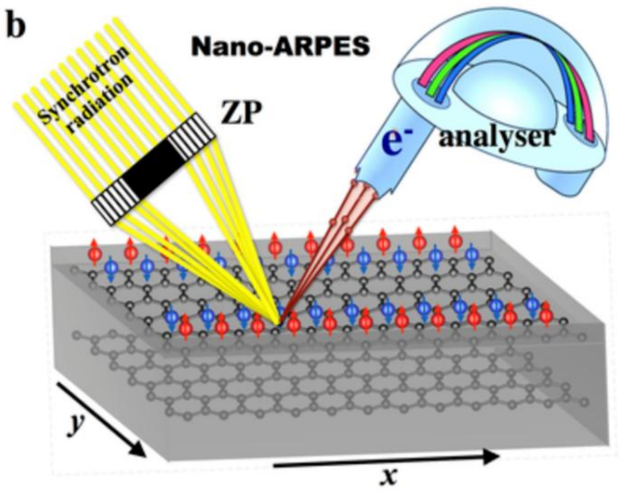
- Machine Learning on Data Analysis and Data Acquisition
  - Unsupervised clustering on ARPES spatial mapping dataset

- Summary and Prospects

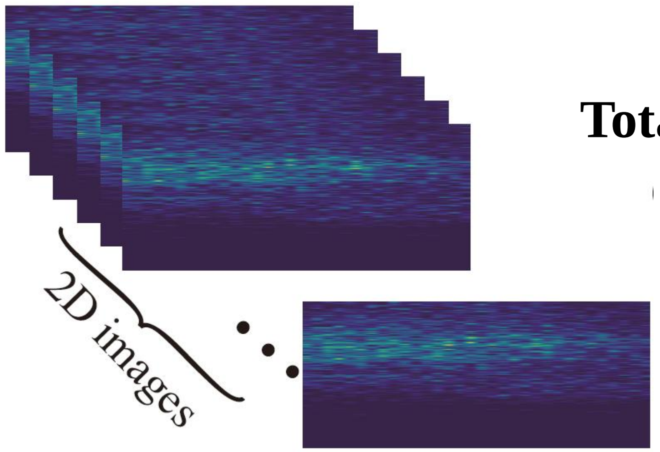
High-resolution Nano Electronic Structure Spectroscopy Beamline



Introduction-ARPES

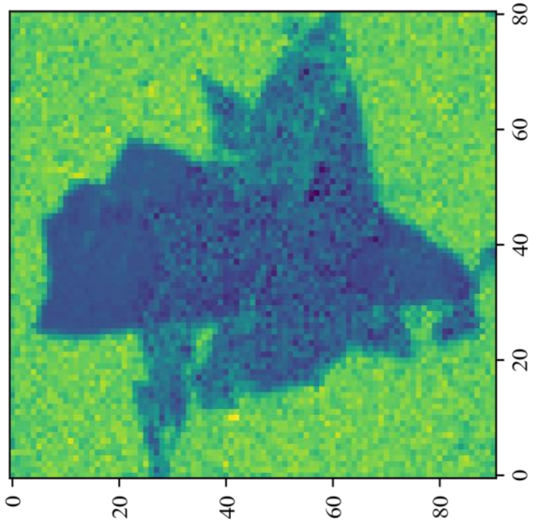


photoelectric effect
beam size to micro/nano-meter



electronic structure (E_k Vs angle) at different spatial point

Total integration



electronic structure distribution in the real space

- ARPES is a powerful tool to observe electronic structures in solid-state materials
- Spatially resolved ARPES (μ-ARPES, n-ARPES) promotes the measurements into relatively inhomogeneous surfaces
- Usually, first perform a coarse real-space scan to locate regions of interest (ROI), then conduct a high-resolution scan at the selected positions.
- However, positioning of the ROI on surface currently relies on manual inspection—time-consuming, labor-intensive, and requiring experiment interruption.

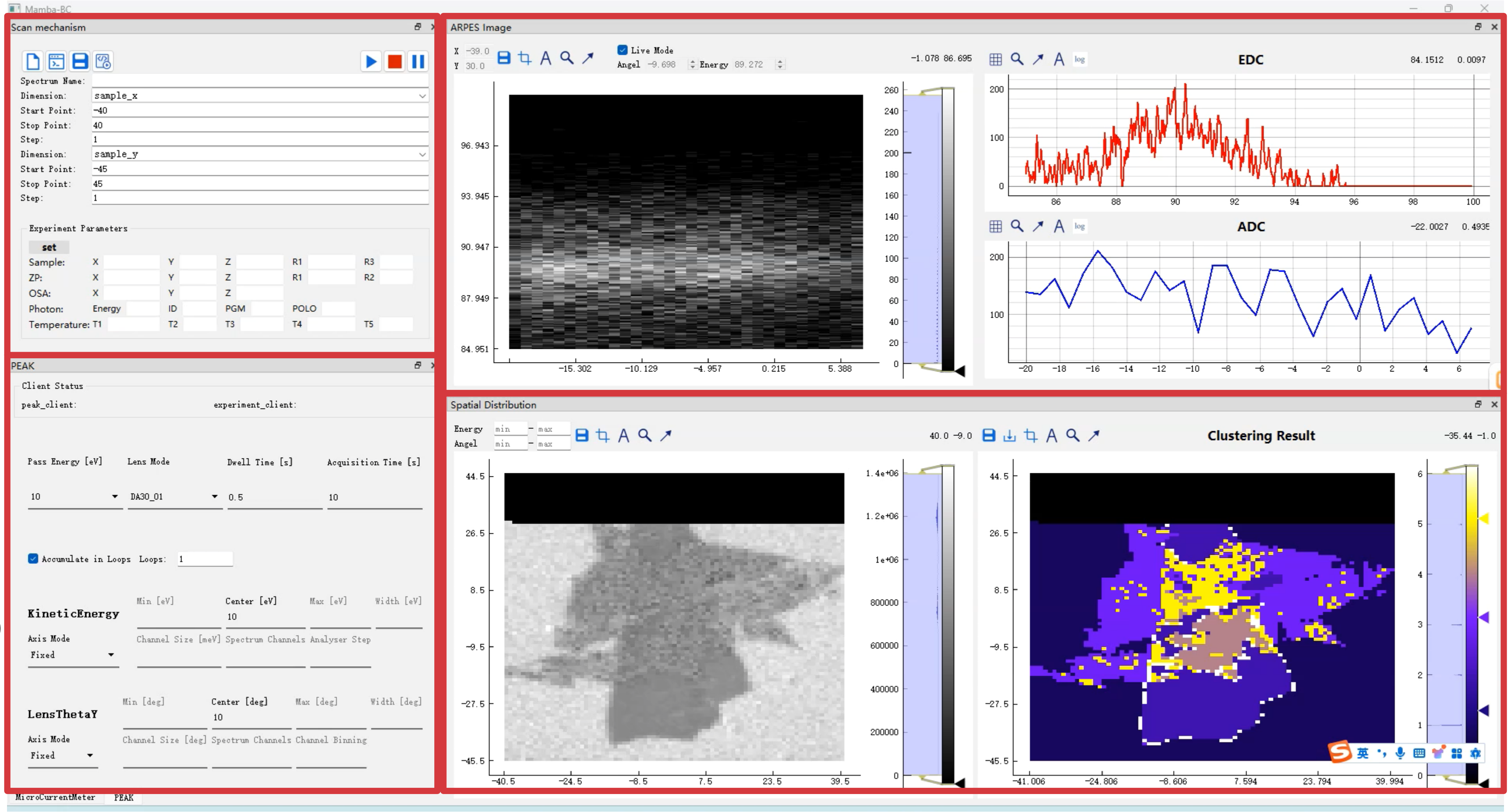
This situation can be improved in the Experiment Control and Data Acquisition Software

Experiment Control and Data Acquisition Software

Real-time 2D image display with EDC/ADC analysis.

Motor setting
Scan setting

Energy Analyzer Control （PEAK）



Embedded clustering algorithm for real-time segmentation of distinct electronic-structure regions on the sample surface.

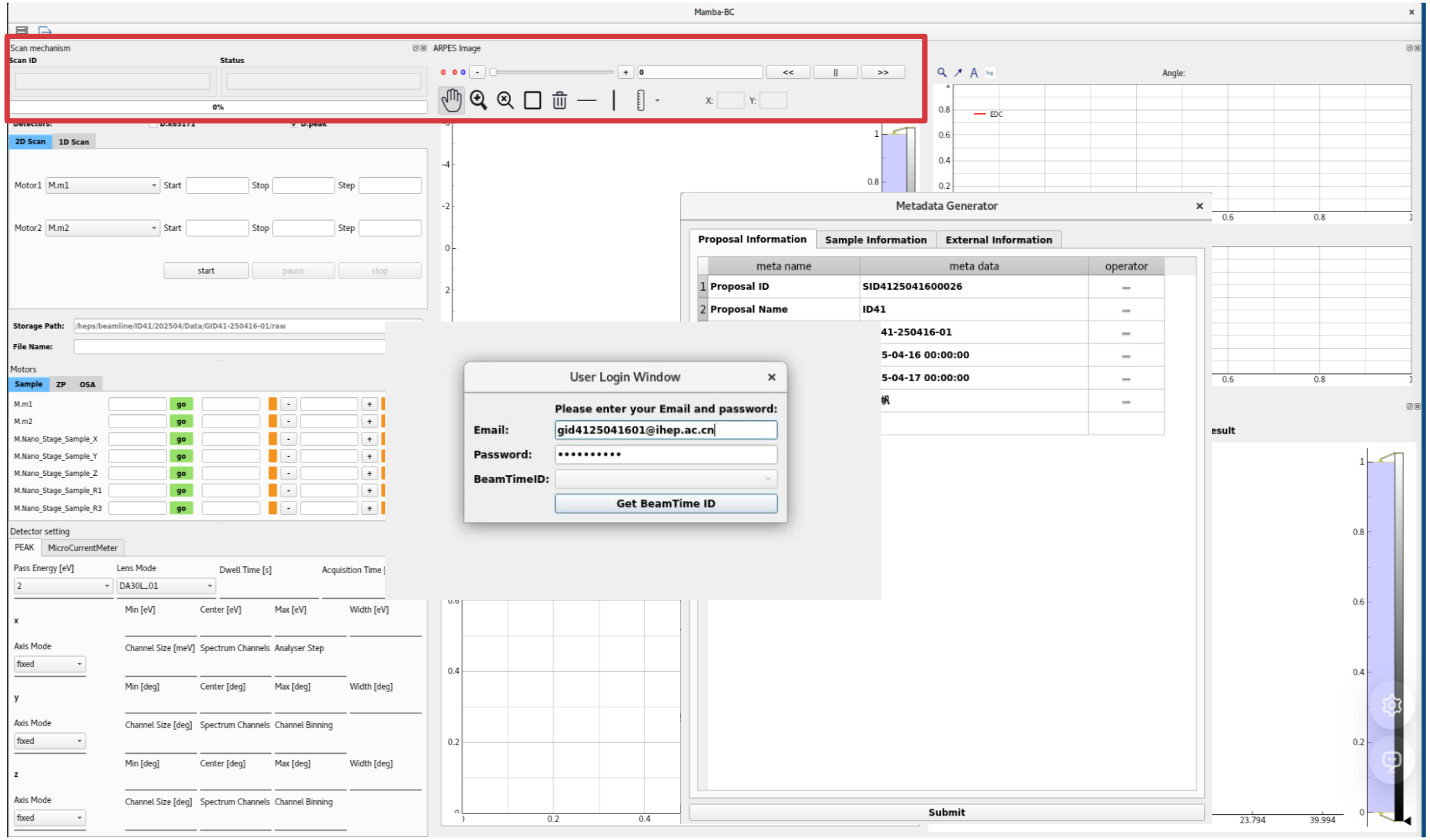
Developed a Python IOC to enable synchronized scanning between the analyzer and motors.

Analysis and visualization of distinct electronic phases on the sample surface
Supports synchronized ROI selection with scan parameters

Experiment Control and Data Acquisition Software

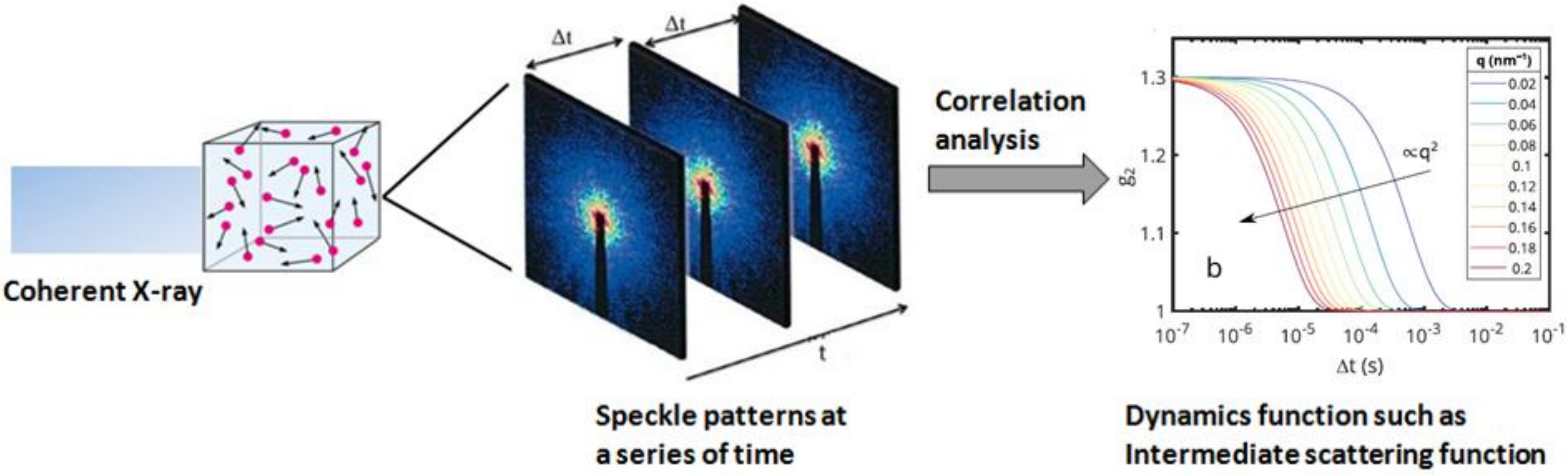
The latest version, untested

- Add user login/logout and experiment metadata information (proposal information, sample information) module.
- Add experiment status monitoring: ScanID, detector status, progress bar, etc.
- Add historical-data loading: the front end can retrieve cached experiment data by spectrum index, or play the entire dataset forward (from first to last record) and backward (from last to first).



Acquisition rate can reach 50 Hz.
All data are stored in HDF5 format.

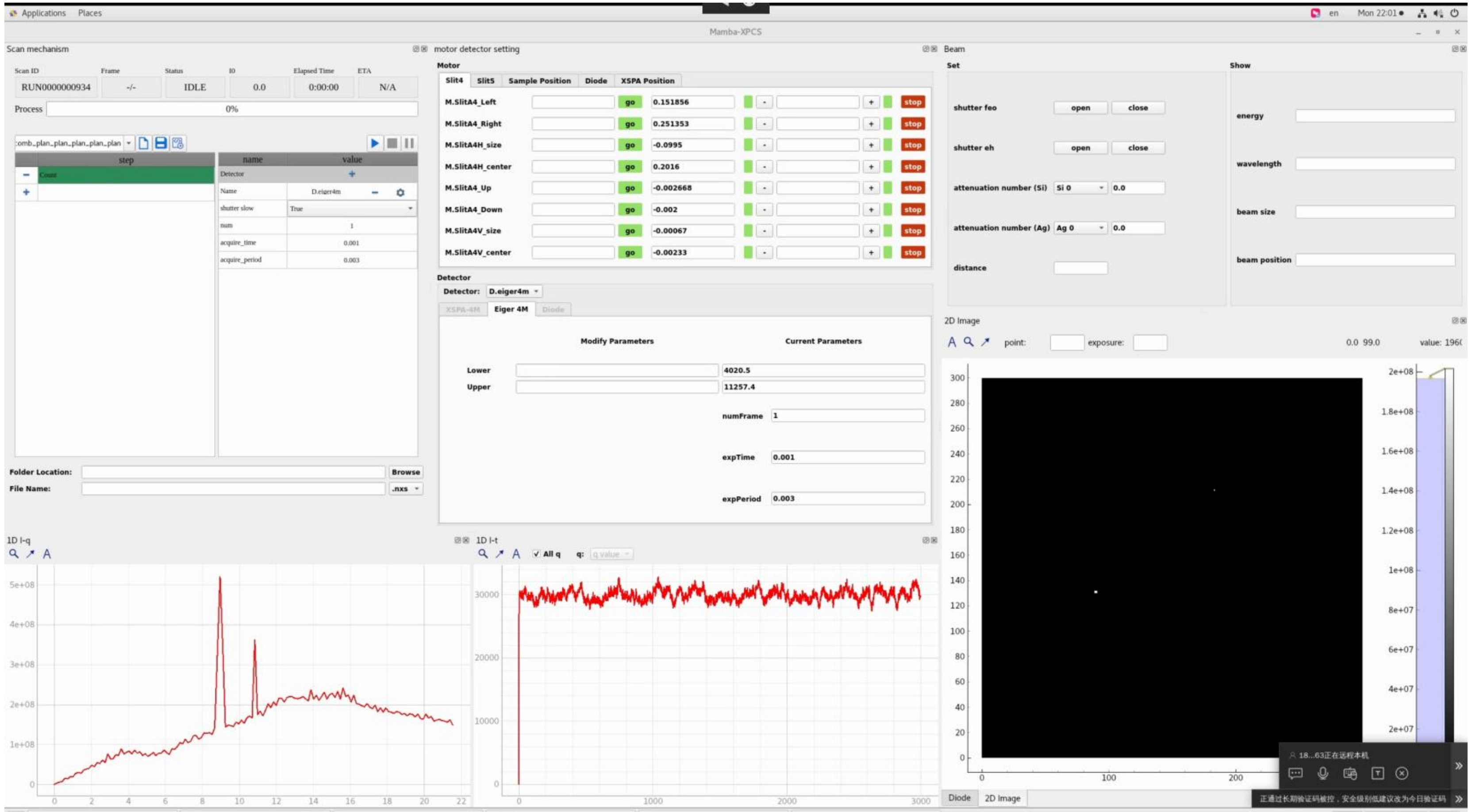
X-ray Photons Correlation Spectroscopy (XPCS)



Experiment Control and Data Acquisition Software

- **Scan Sequence Module**
  - ➢ supports count, step-scan, move, and sleep operations.
  - ➢ Users can queue multiple plans at once;
  - ➢ for every plan, motor position, exposure time, frame time, frame rate, and shutter state can be configured independently.
- Provides real-time 2D image display along with calculation and visualization of 1D I–q and I–t plots.
- The Eiger detector enables high-frame-rate acquisition at **16–18 GB/s （~2 kHz）.**

XPCS: multi-segment measurements with short times and high throughput.



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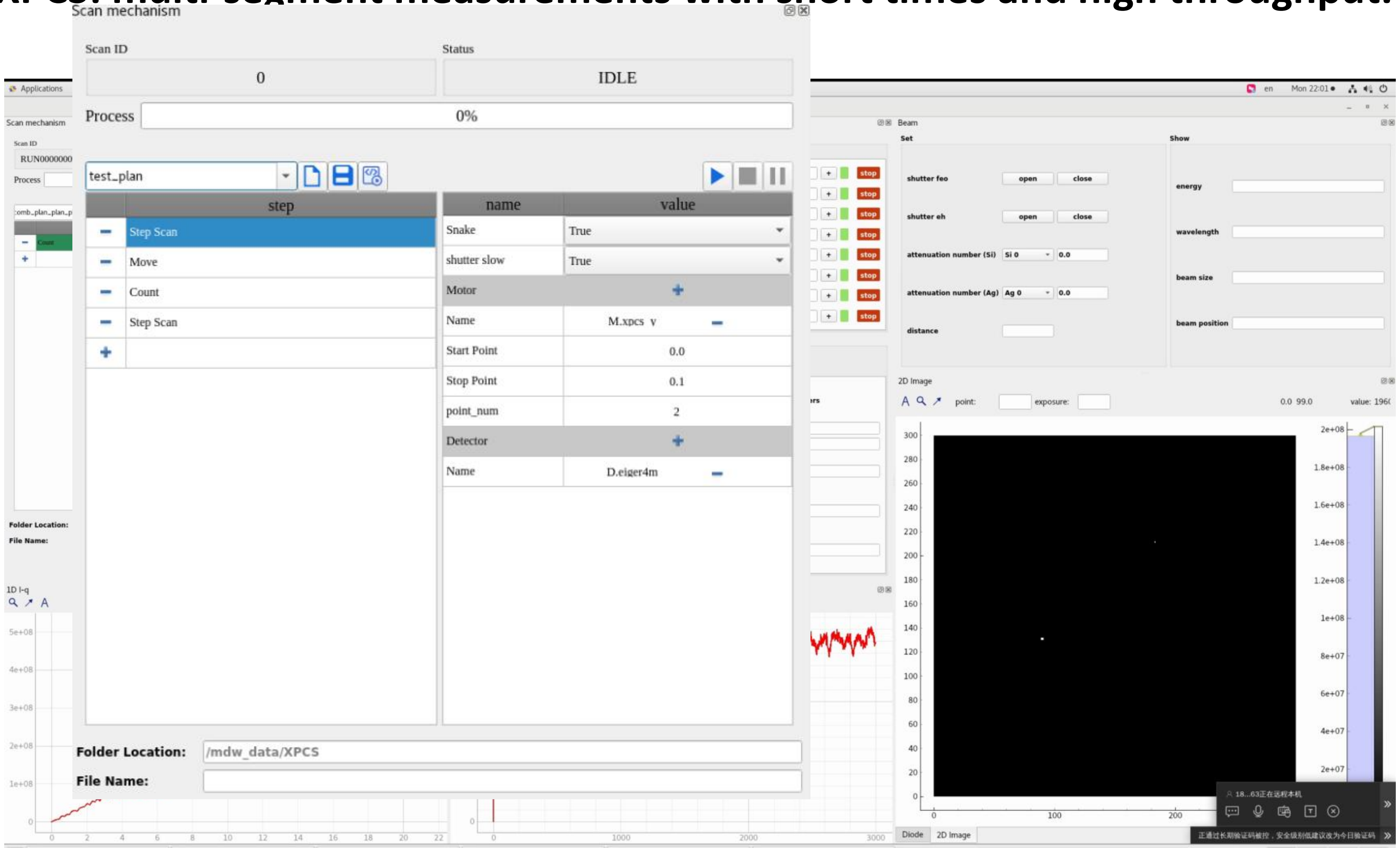

Experiment Control and Data Acquisition Software

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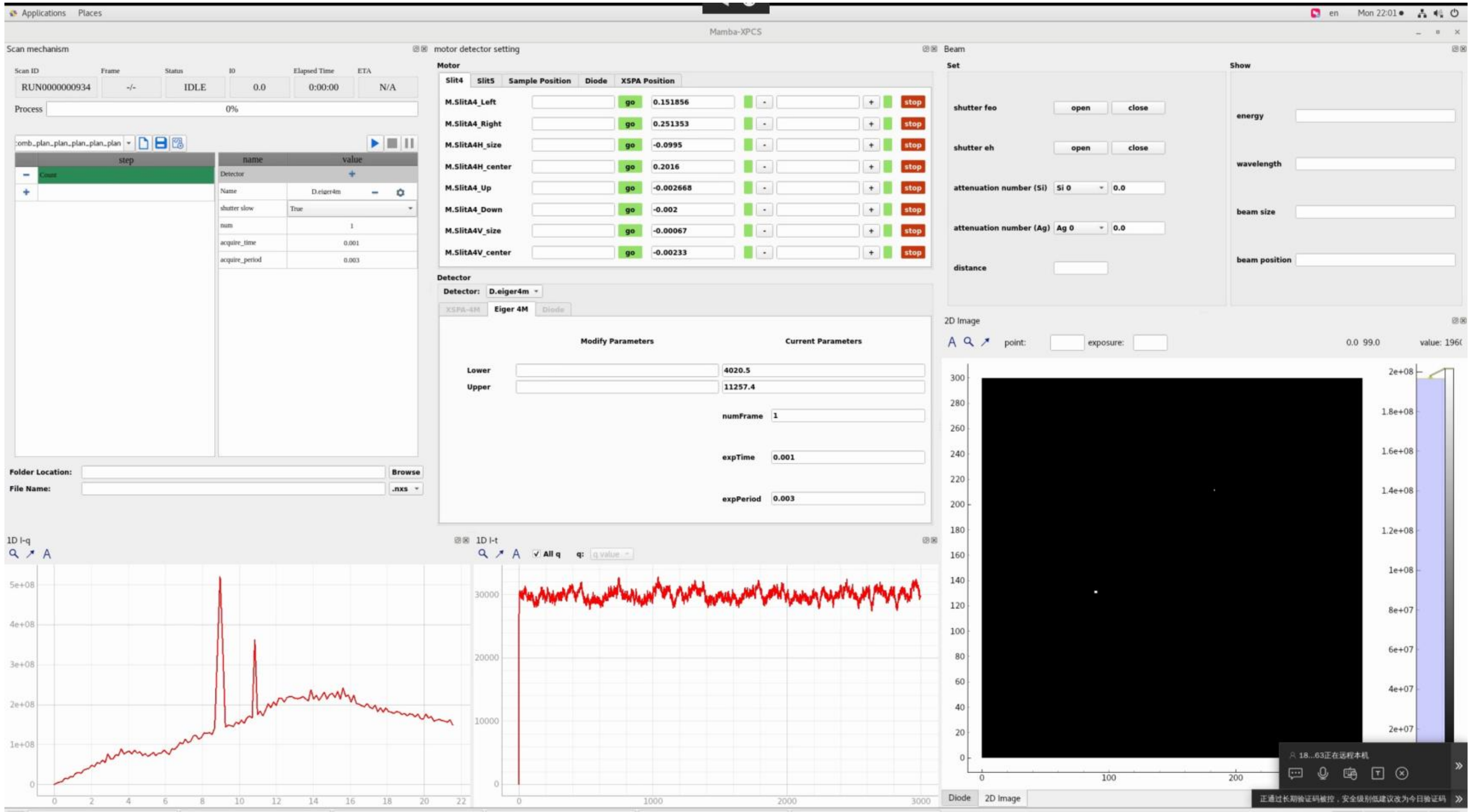
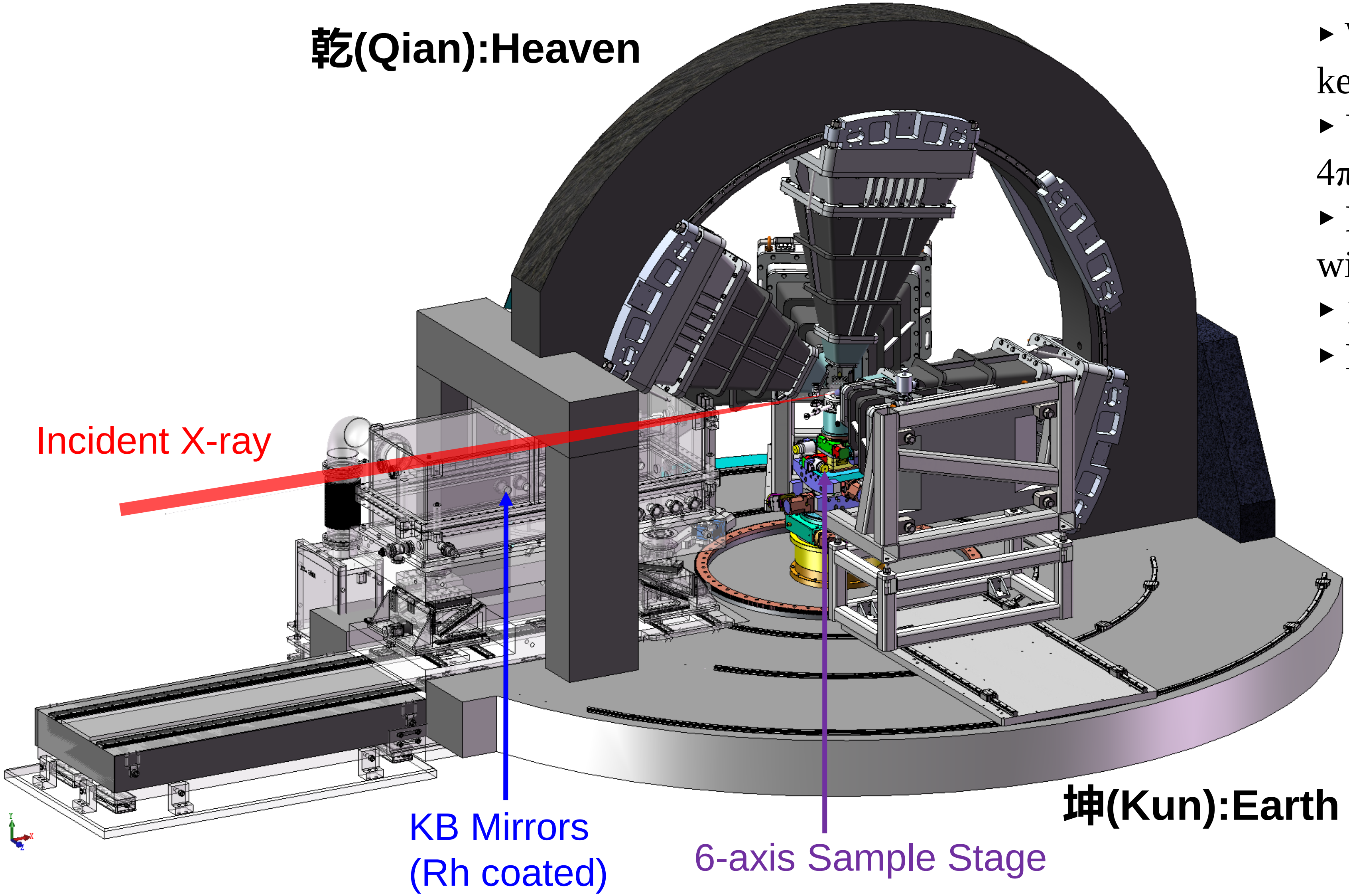


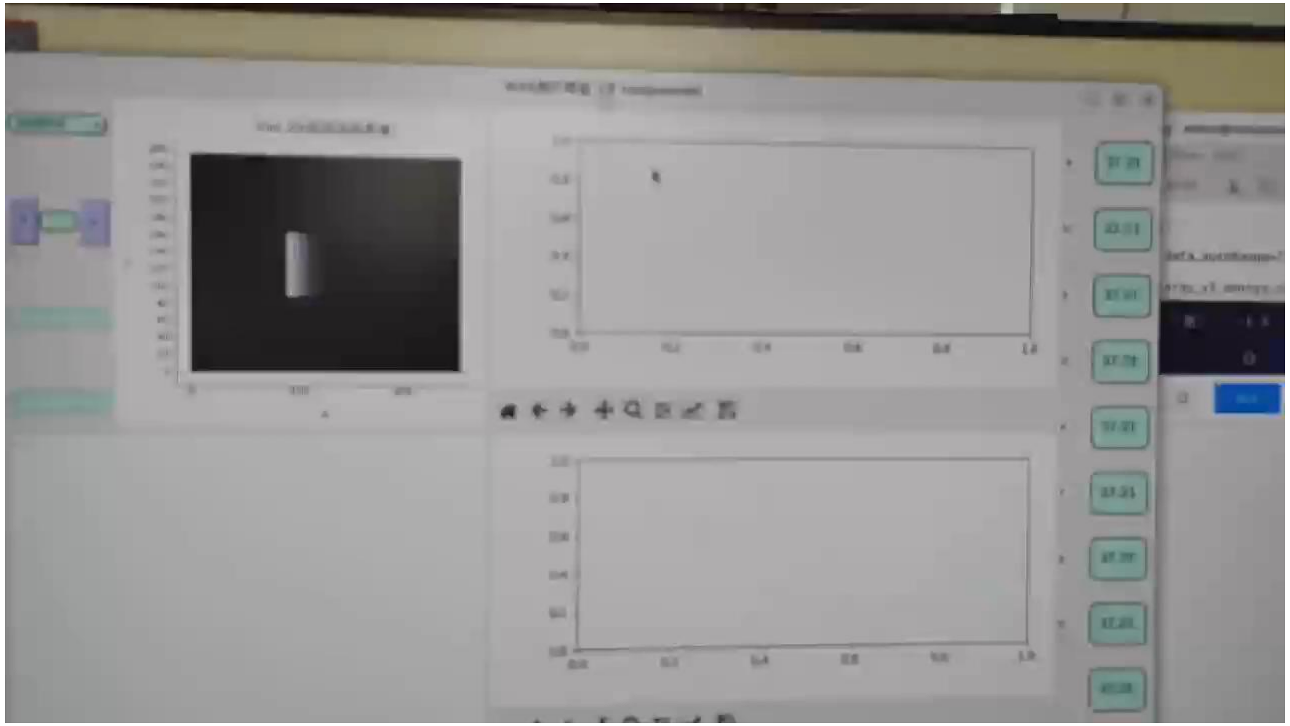
Resonant inelastic scattering (RIXS)

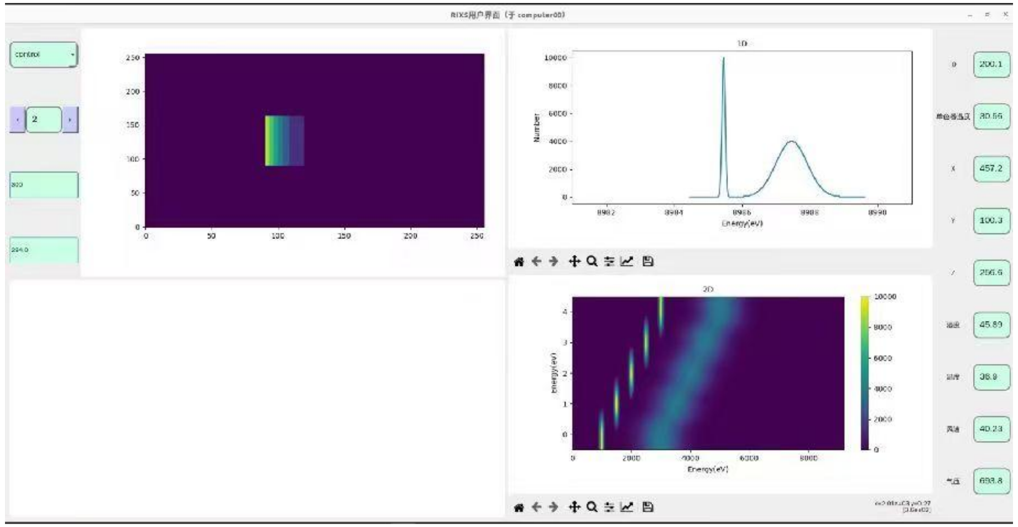
Spectrometer “Qiankun(乾坤)”



- Working energy: **~10 keV Si(660)**; ~13 keV Si(880); ~16 keV Si(10 10 0)
- Up to 15*6=90 analyzers to cover ~5.6% 4πSr
- Energy resolution ~0.7 eV @~10 keV with 1 m Rowland circle
- 140 mm space for sample environment
- High-resolution IXS/RIXS/XES modes

Experiment Control and Data Acquisition Software

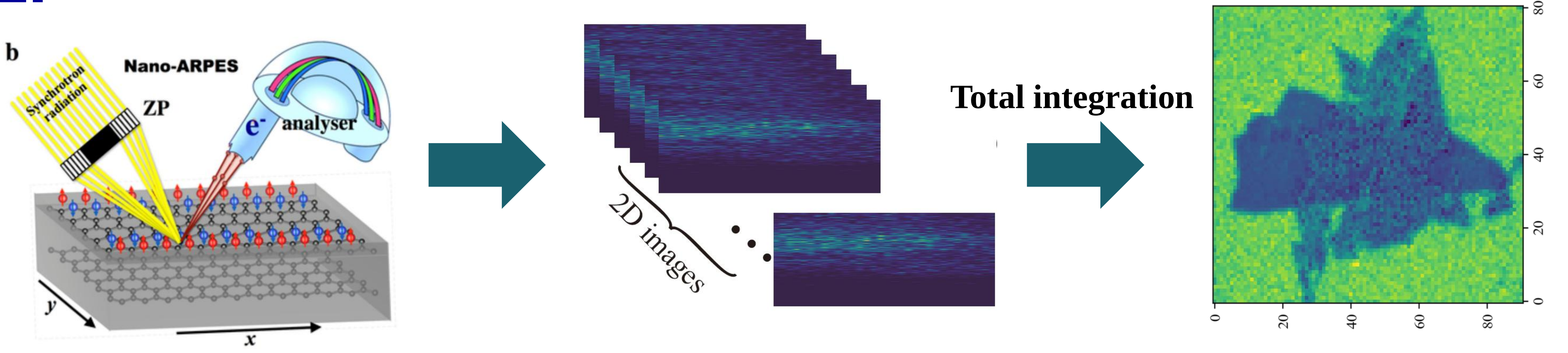




Virtual Beamline-Based

Unsupervised clustering on ARPES spatial mapping dataset

Introduction-ARPES



photoelectric effect
beam size to micro/nano-meter

electronic structure (E_k Vs angle) at different spatial point

electronic structure distribution in the real space

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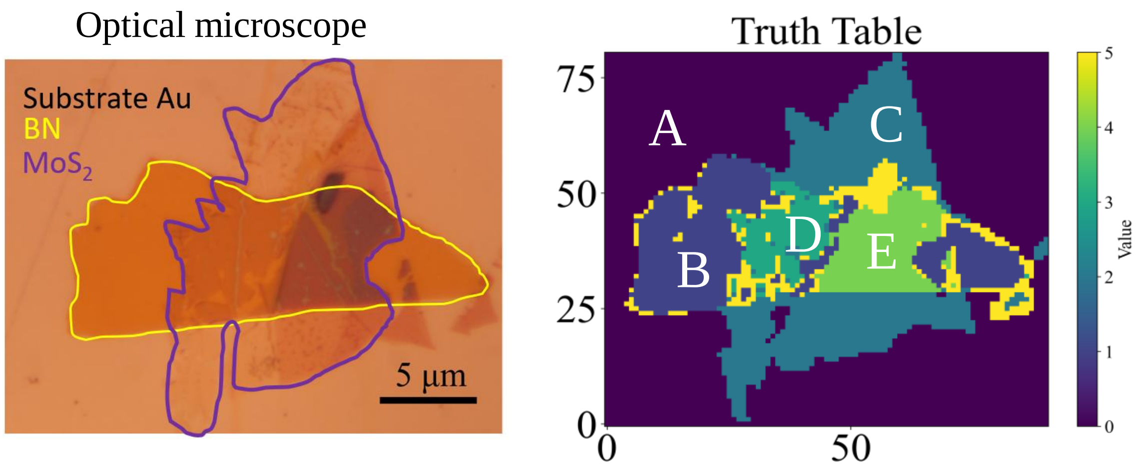
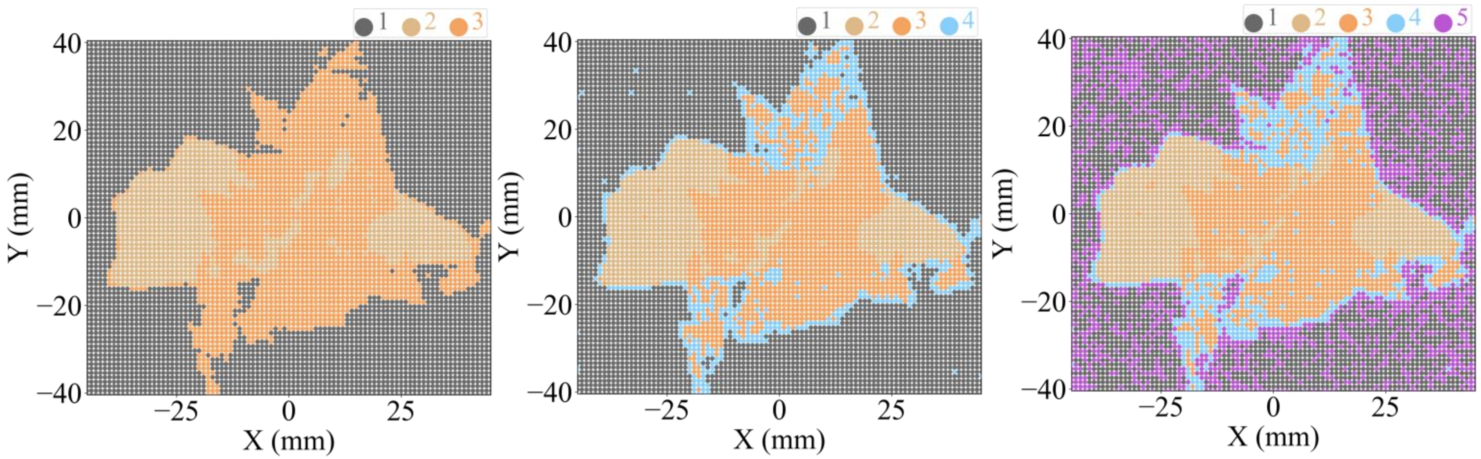
- Spatially resolved ARPES (μ-ARPES, n-ARPES) promotes the measurements into relatively inhomogeneous surfaces
- Usually, first perform a coarse real-space scan to locate regions of interest (ROI), then conduct a high-resolution scan at the selected positions.
- However, positioning of the ROI on surface currently relies on manual inspection—time-consuming, labor-intensive, and requiring experiment interruption. **Call for a more efficient way based on machine learning**

Unsupervised clustering on ARPES analysis

- Unsupervised clustering such as K-means, shows strong capabilities in categorizing the spatial mapping dataset. [npjQuantum Mater. 7, 24 (2022)] **Automatic on the order of seconds**
- Difficult to distinguish subtle differences caused by different layers and substrates.



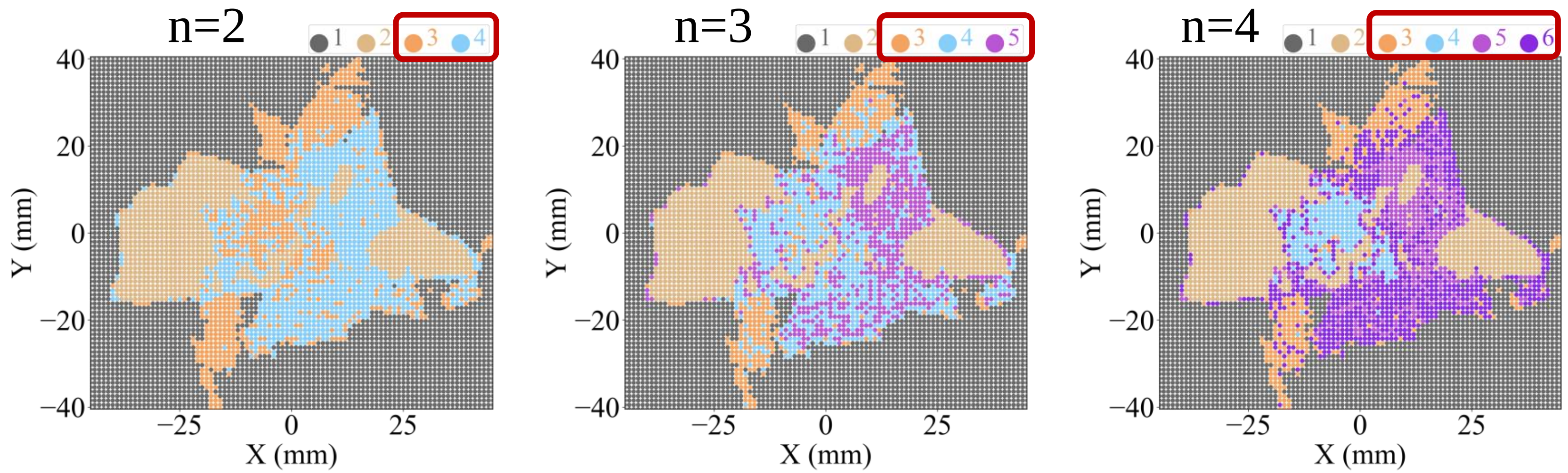
ARPES sample Au/BN/MoS_2
from top to bottom being MoS_2, BN and Au
A: Au **B**: BN
C: MoS_2 on Au （**MoS2-Au**）
D: monolayer MoS_2 on BN （**1-MoS_2**）
E: multilayer MoS_2 on BN （**m-MoS_2**）

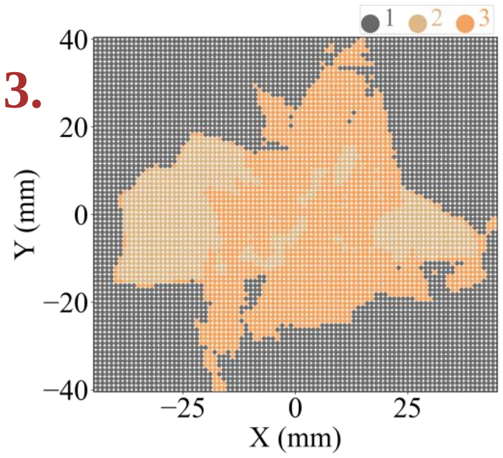


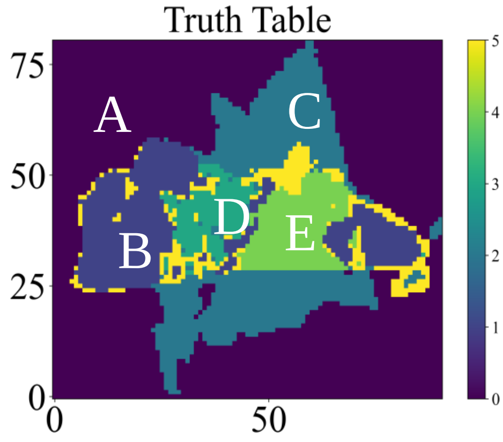
K-means clustering results
- effectively recognizes the areas of MoS_2, BN and Au **n=3 case**
- but different categories of MoS_2 (**CDE partitions**) are not distinguished.

Unsupervised clustering on ARPES analysis

Another K-means clustering only based on the ARPES images belonging to MoS_2, the **cluster 3.**
Result of cluster number (n) = 2/3/4:



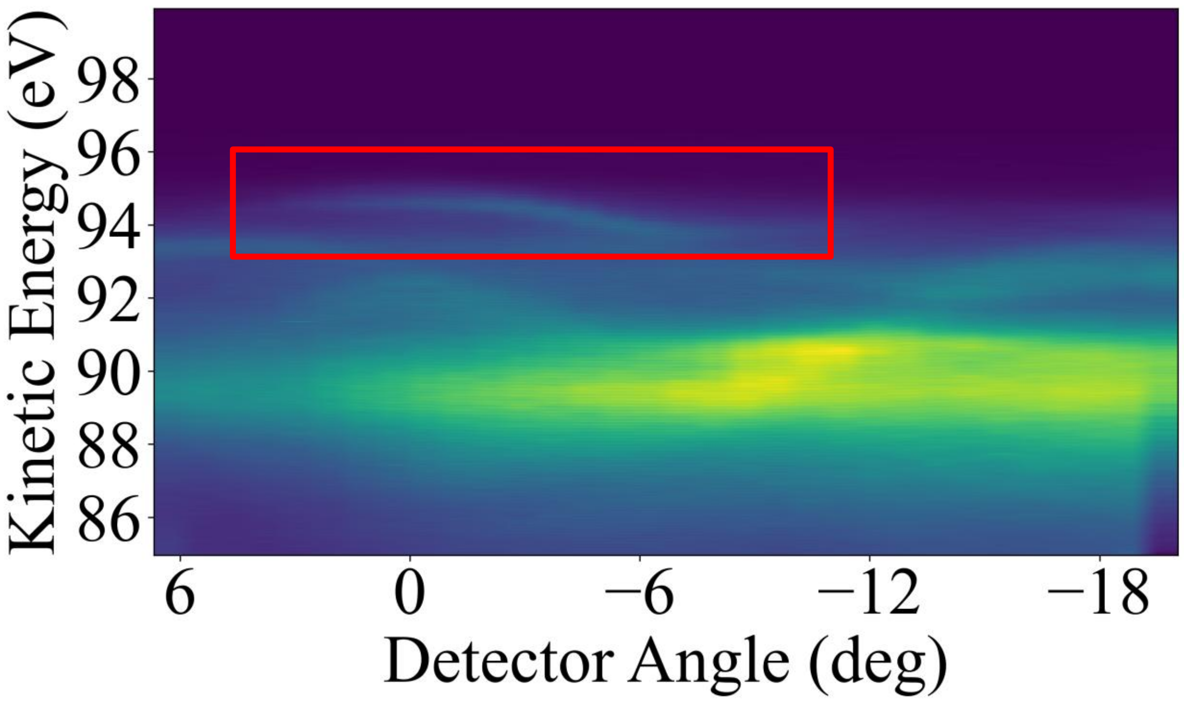




Partition	Accuracy(%)	Precision(%)	Recall(%)	F1(%)
Au	97.8	96.8	99.7	98.2
BN	98.9	95.9	95.1	95.5
MoS2-Au	86.7	92.0	30.4	45.7
1-MoS2	98.4	78.1	76.6	77.3
M-MoS2	94.0	47.0	47.0	47.0
Macro average	95.2	82.0	69.7	72.7

A: Au **B**: BN
C: **MoS2-Au**
D: **1-MoS2**
E: **m-MoS2**

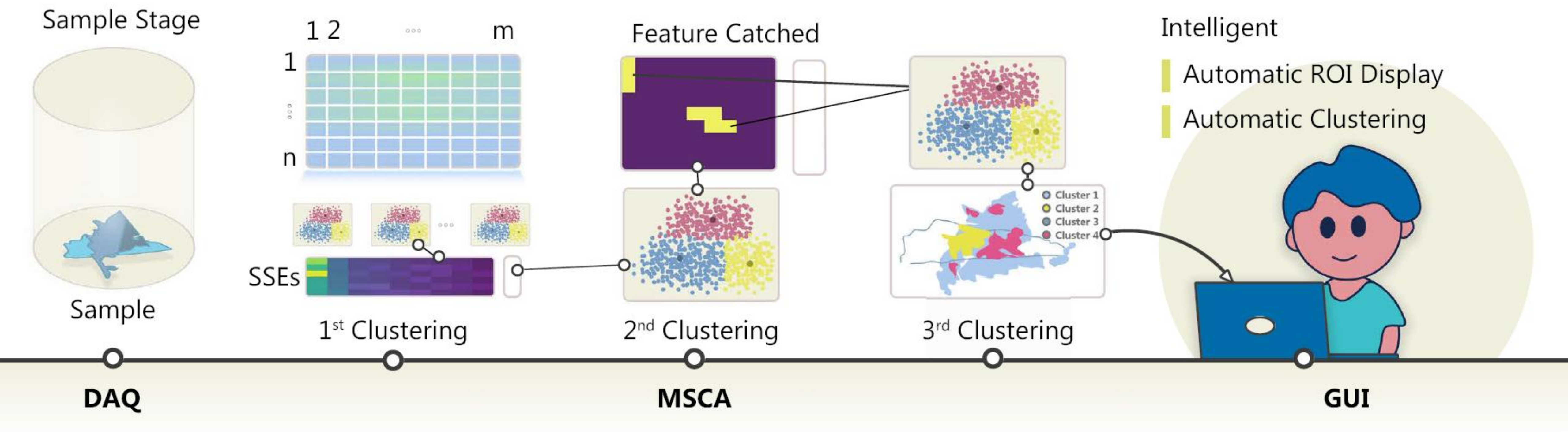
Unsupervised clustering on ARPES analysis



- The key region for distinguishing between different types of MoS_2 lies in specific energy band
- While the clustering input of K-means clustering is the whole 2D image (momentum space) of each spatial point, which would weaken the discrimination capability of the specific band

The key to achieving a fine clustering is to identify the specific band in the momentum space

Multi-Stage Clustering Algorithm(MSCA)



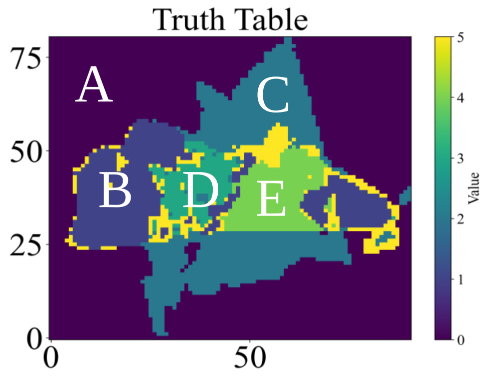
MSCA includes three clustering stages:

- 1st clustering: Divide the momentum space into different small cells and each cell go through a K-means clustering
- 2nd clustering: The clustering result of each cell serves as the input for a second clustering, the specific feature in momentum space will be captured
- 3rd clustering: A third K-means clustering based on the specific feature will achieve a fine clustering in real space

The performance of MSCA

The real space is divided into 6 partitions:

- Cluster 1-5 correspond well to partition A-E in truth table
- Cluster6:conjoint signal



A: Au **B**: BN
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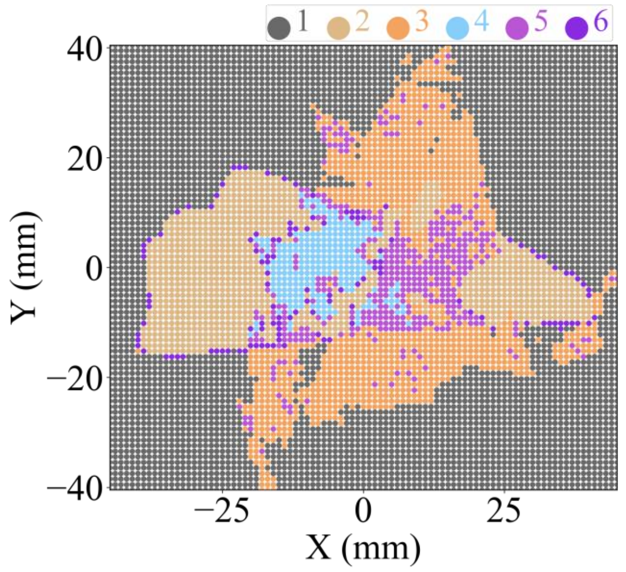
E: **m-MoS2**



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BN	98.9	95.9	95.1	95.5
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1-MoS2	99.1	89.3	84.4	86.7
M-MoS2	95.7	61.8	61.4	61.6
Macro average	97.2	86.9	83.9	85.3

Improvement: 2% 6% 20% 18%

Communications Physics 7, 398 (2024)

Summary and Prospects

- The software is currently under active development and optimization.
- The fully functional release will be ready for users by the end of this year.
- In parallel, we are also developing intelligent data-processing algorithms—such as denoising, clustering, and smart scanning, and the integration with DAQ system in HEPS (MAMBA)

Opening an era of efficient data collection!

MAMBA

Welcome to our homepage!