AI for Science in HEPS

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1. Background: 4th-generation synchrotron source

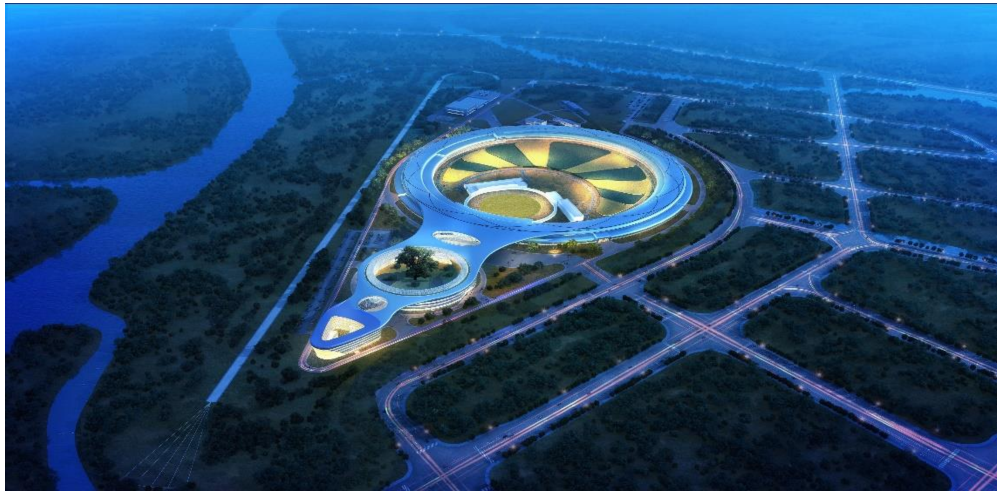
MAX IV Laboratory 2016

ESRF-BES 2020

SIRIUS3 2020

In China, two 4th-generation synchrotron radiation facilities are being constructed:

High Energy Photon Source – HEPS 2025



Hefei Advanced Light Facility – HALF 2028

- **Multidisciplinary Research Platforms**
- **Major Science and Technology Infrastructure**

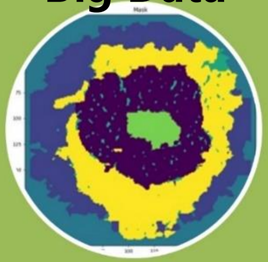
1. Background: High Energy Photon Source (HEPS)

- ➢ The beam energy is **6 GeV**
- ➢ The brightness is more than **1×10^{22}** phs/s/mm^2/mrad^2/0.1% BW
- ➢ The horizontal emittance of the electron beam becomes better than **60 pm•rad**
- ➢ More than **90** high-performance beamlines and stations can be constructed
- ➢ Provide highly brilliant and highly coherent X-rays with photon energy up to **300 keV**

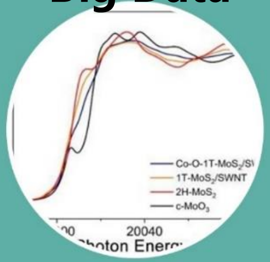
2. Multimodal Data Analysis Demand

- **Urgent demand for the application of 4th generation synchrotron source including HEPS**

Image Big Data



Spectroscopy Big Data



Diffraction Big Data

Data volume ~ 3 PB/day
Urgent need: dedicated artificial intelligence algorithms to achieve scientific big data mining

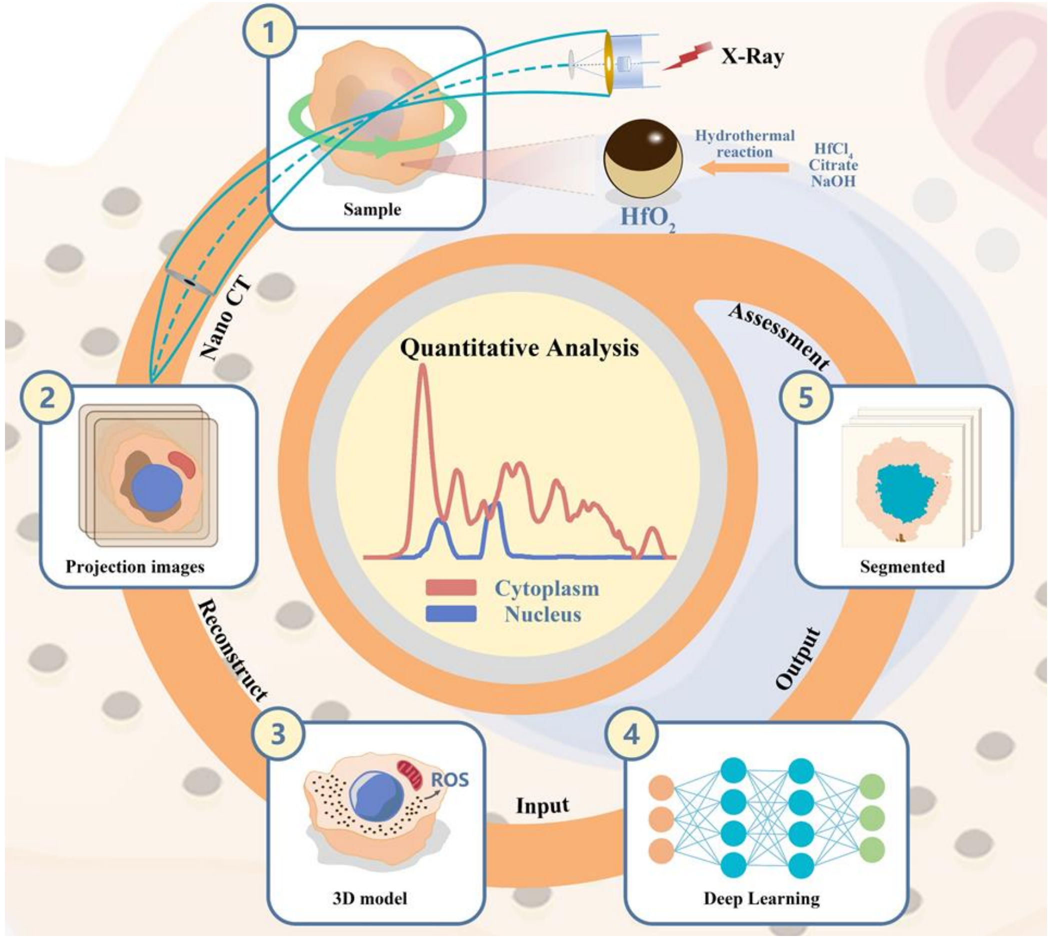
2. Multimodal Data Analysis Demand

- “AI for Science” Case Studies and Their Deployment
- More “AI for Science” Case Studies and Based on LLM

2.1 Image Data Analysis by AI Aiding

Image

Quantitative three-dimensional imaging analysis of HfO_2 NPs in single cells via deep learning aided Nano-CT



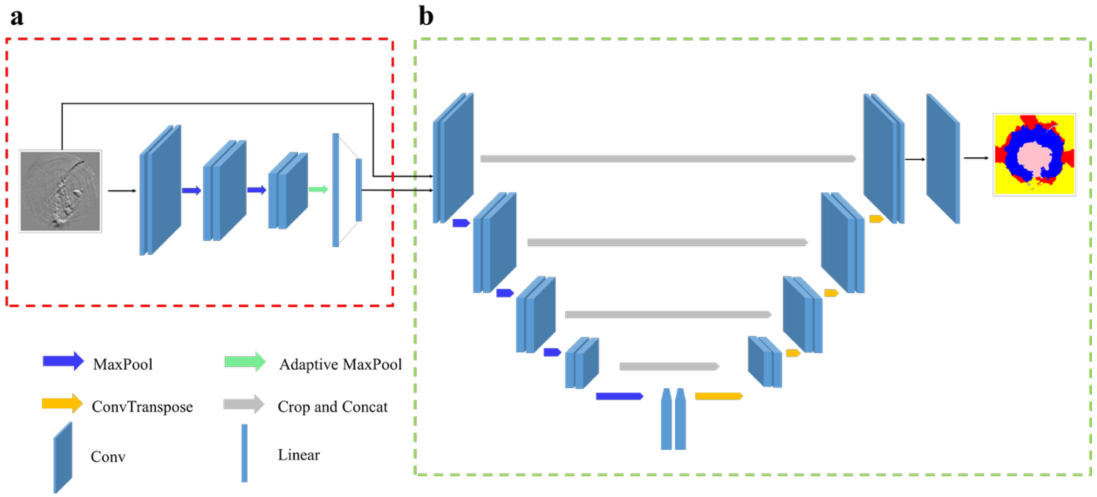
https://github.com/LinaZhaoAIGroup/Nano-CT

2.1 Image Data Analysis by AI Aiding

Image

Quantitative three-dimensional imaging analysis of HfO_2 NPs in single cells via deep learning aided Nano-CT

Training dataset: 284 images (>300 pixels)



The comprehensive layout of the CSUNet network

Comparison test results of different models

model	PA (%)	mPA (%)	mIoU (%)	class IoU (%)		
				Nucleus	Cytoplasm	HfO_2 NPs
U-Net	99.17	97.66	95.84	98.10	99.28	89.73
TransUnet	99.70	99.10	98.81	99.24	99.68	96.68
DeepLabV3+	98.47	90.55	67.95	97.29	98.81	73.34
SwinUnet	99.53	98.51	96.56	99.00	99.62	93.18
CSUNet	**99.83**	**99.60**	**99.33**	**99.70**	**99.88**	**98.42**

Zuoxin Xi, …, Lina Zhao*, ***ACS Nano*** 18, 22378, **2024**.

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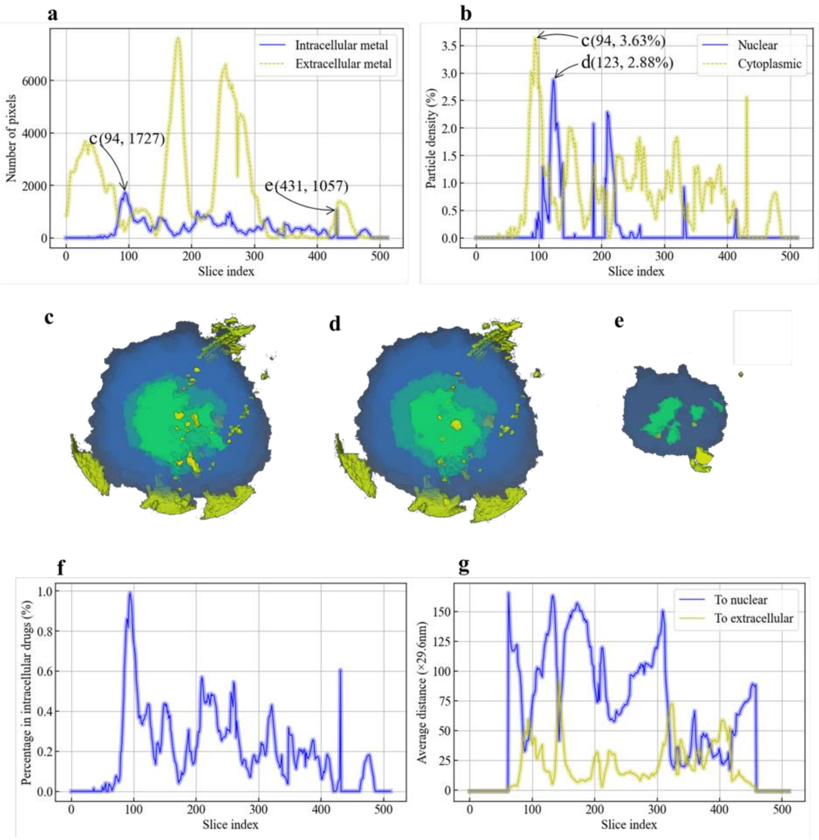
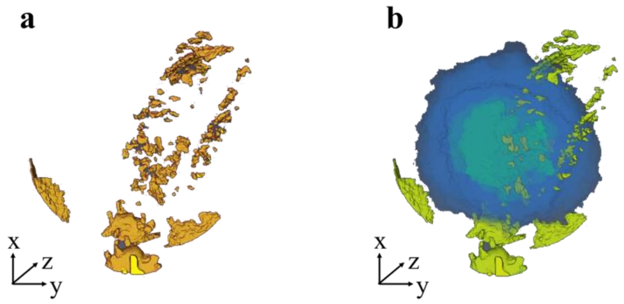




Visualization of the 3D structure for MCF-7 cells and HfO_2 NPs.

Quantitative analysis of metal NP uptake by cancer cells: basis for nanomedicine design

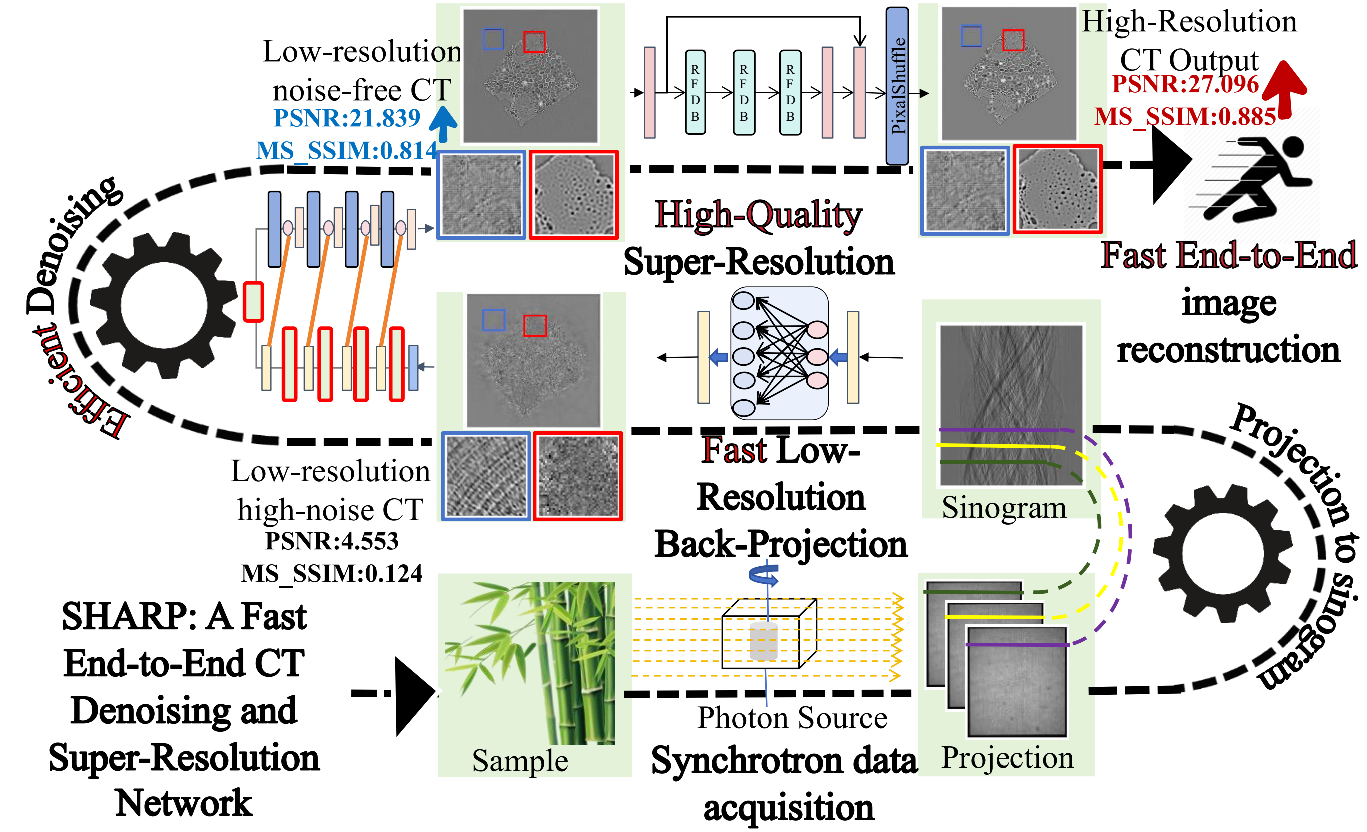
Zuoxin Xi, ..., Lina Zhao*, ***ACS Nano*** 18, 22378, **2024**.

2.2 SHARP: Fast, High-quality Synchrotron CT Reconstruction

Research Background

✦SRCT offers μm-level, non-destructive 3D imaging.

✦High-pixel data (TB-scale) makes reconstruction bottleneck—fast, accurate algorithms are critical.



SHARP：

Super High-Resolution Artifacts Removal and Back-Projection

What's New

✦Unified end-to-end pipeline that maps sinograms directly to tomograms.

✦Low-res latent reconstruction plus super-res upscaling slashes compute and artifacts.

Under Review

2.2 SHARP: Fast, High-quality Synchrotron CT Reconstruction

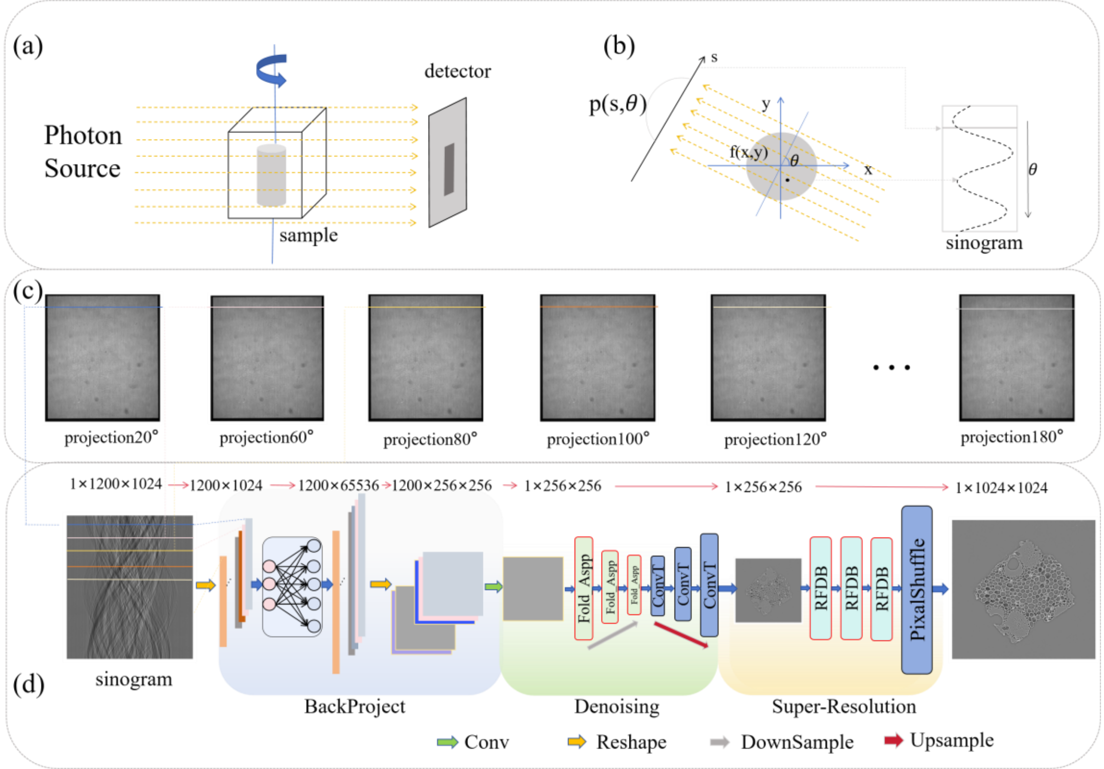
Three-Stage End-to-End Pipeline

✦FC Back-Projection: maps raw sinograms to a low-res latent image, slashing parameters while keeping structure.

✦U-Net Denoiser: multi-scale encoder-decoder removes noise & ring artifacts.

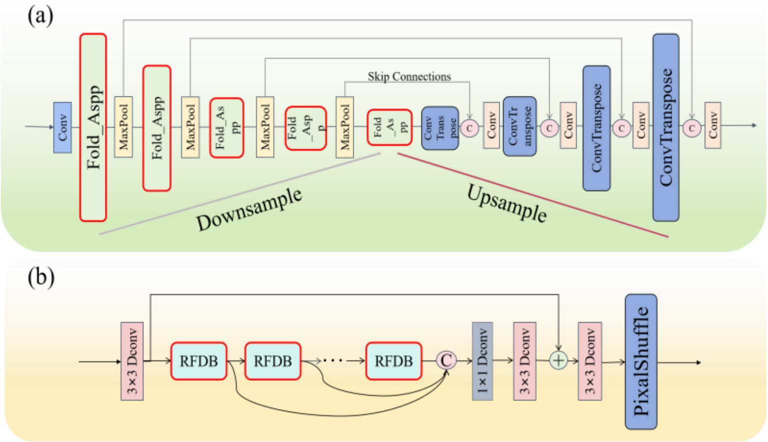
✦RFDN Super-Resolution: residual feature distillation upsamples to full resolution with fine detail.

Why It's Different



✦Consolidates the traditional pipeline into a single end-to-end network.

✦Performs reconstruction in a low-resolution latent space, then restores full detail via super-resolution—achieving high throughput while effectively suppressing artifacts.



2.2 SHARP: Fast, High-quality Synchrotron CT Reconstruction

How We Tested (Ablation Experiments)

✦Sequentially disabled one of the three modules while keeping the others fixed.

✦Compared image quality and visual artifacts to the full SHARP network.

Back-Projection Module	Denoising Module	Super-Resolution Module	Metrics		
			RMSE↓	PSNR(db)↑	MS_SSIM↑
Fully Connected	Fold_Aspp+ U-Net	RFDN	**0.0724**	**22.863**	**0.845**
/	Fold_Aspp+ U-Net	RFDN	0.0801	21.962	0.822
Transposed Convolution	Fold_Aspp+ U-Net	RFDN	0.0782	22.159	0.826
Fully Connected	/	RFDN	0.0784	22.145	0.828
Fully Connected	U-Net	RFDN	0.0735	22.636	0.833
Fully Connected	CNN	RFDN	0.0741	22.639	0.836
Fully Connected	Fold_Aspp+ U-Net	Linear Interpolation	0.0917	20.768	0.811
Fully Connected	Fold_Aspp+ U-Net	Pixel shuffle	0.0891	21.036	0.770

Take-aways

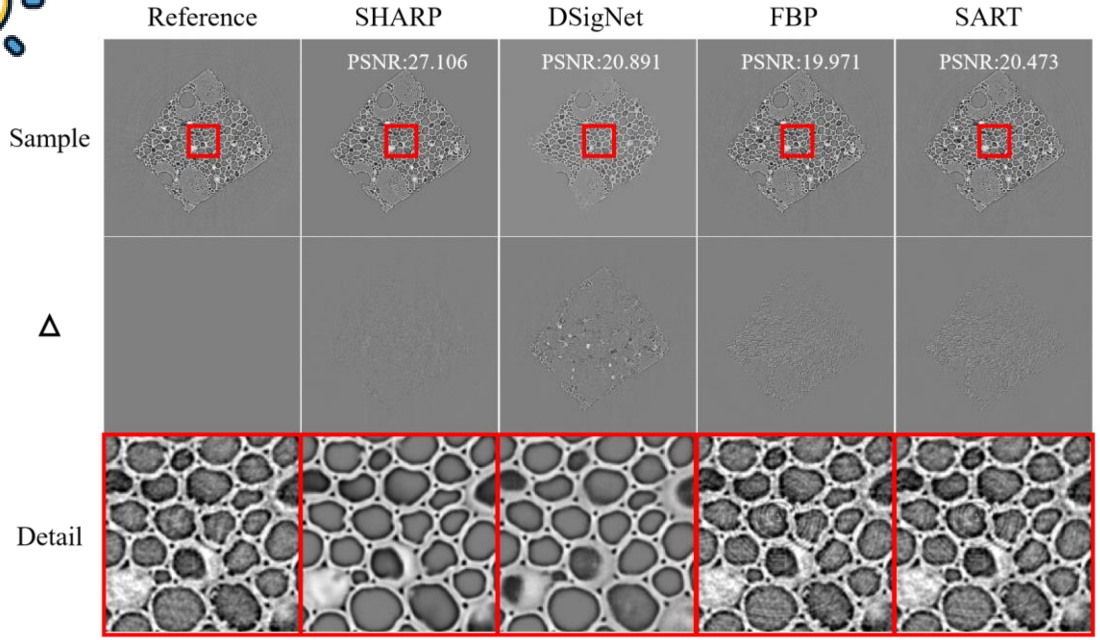
✦FC Back-Projection delivers ~2 % MS-SSIM gain over transposed convolution, improving structural fidelity.

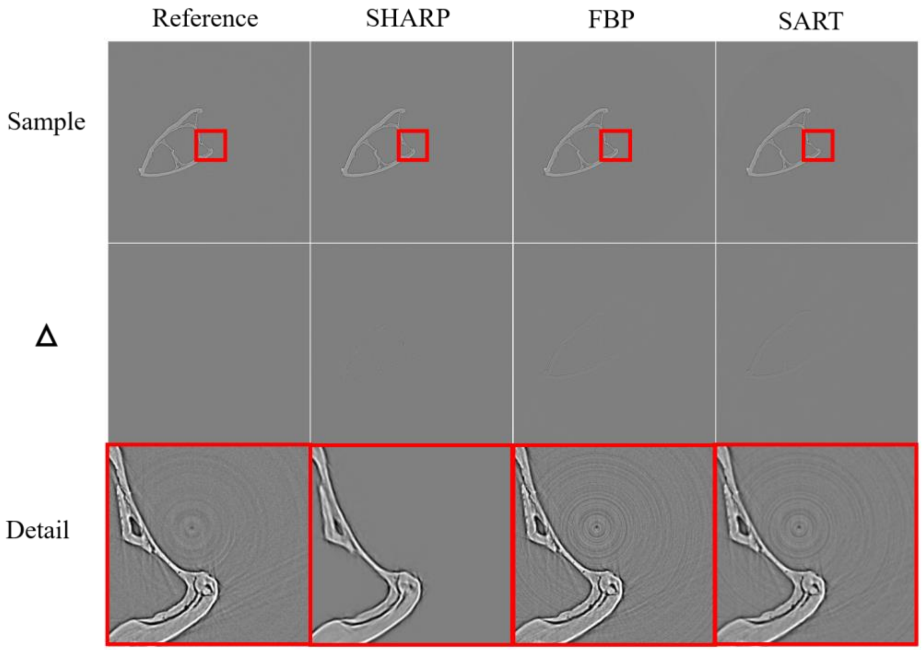
✦Fold-ASPP U-Net Denoiser is essential for removing rings/noise, adding ~0.7 dB PSNR.

✦RFDN Super-Resolution restores fine detail; simpler upsampling drops PSNR by >2 dB.

2.2 SHARP: Fast, High-quality Synchrotron CT Reconstruction

Experimental Results





Methods	number of Projections	Metrics			processing time (s)
		RMSE ↓	PSNR(db)↑	MS_SSIM↑	
FBP	1200	0.1036	19.687	0.834	13.77
SART		0.0990	20.086	0.839	101.36
DSigNet		0.0973	20.253	0.762	3.40
Ours		**0.0724**	**22.863**	**0.845**	**0.42**

Take-aways

✦Highest fidelity: best PSNR & MS-SSIM, virtually no artifacts.

✦Fastest reconstruction: ~30 × faster than FBP—providing rapid feedback during experiments.

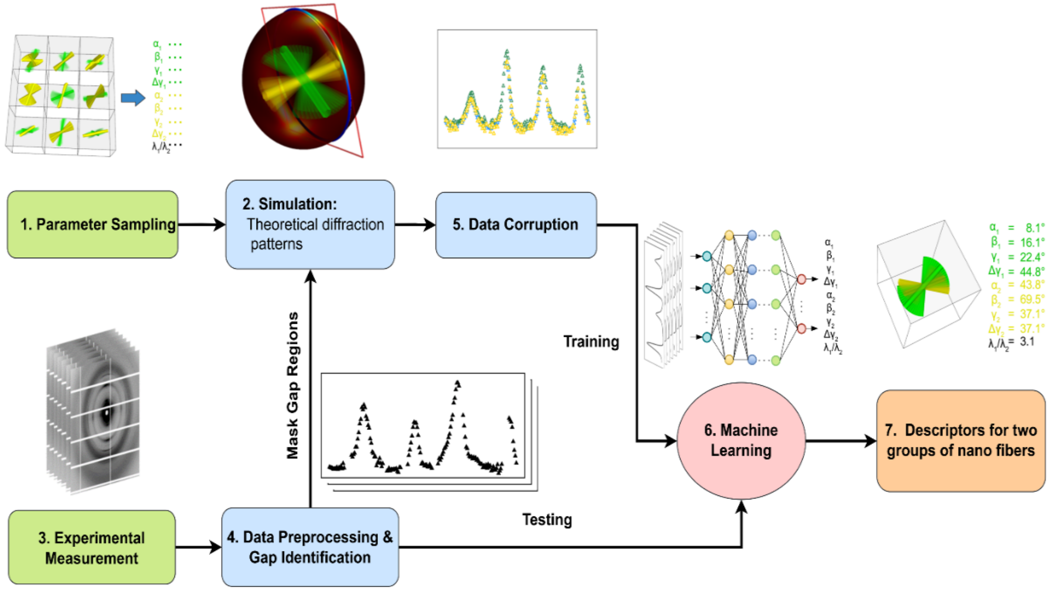
✦Robust across specimens: consistent improvements on highly different biological samples.

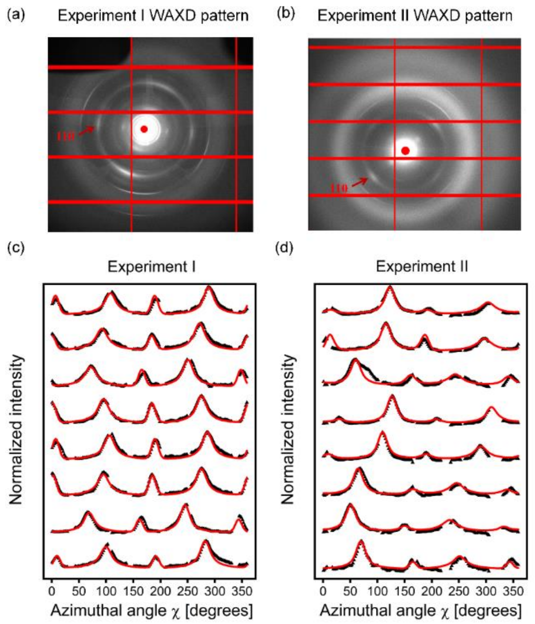
2.3 Diffraction Data Analysis by AI Aiding

Diffraction

Physical knowledge guided machine learning on diffraction data

Training dataset: more than 100,000 samples





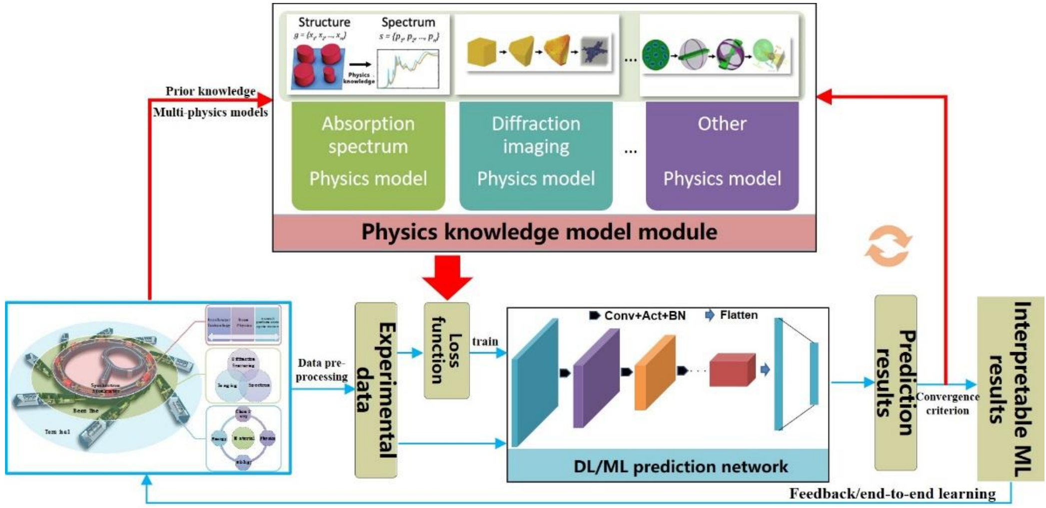
Contribution: Achieve high precision (R^2>0.91) and fast (~10^4 times faster than existing fitting methods) analysis of experimental data, and be able to apply across light sources and beamlines, and lay the foundation for knowledge-driven machine learning analysis.

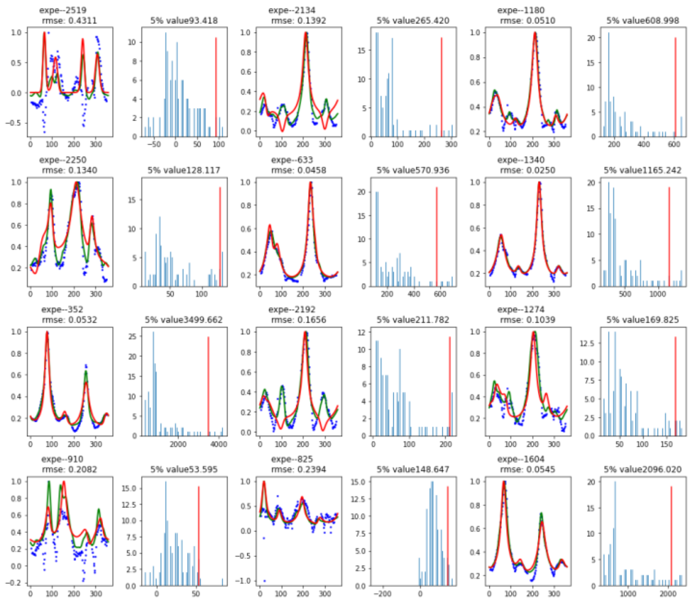
https://github.com/LinaZhaoAIGroup/nanofiber **Minghui Sun, …, Yi Zhang*, Lina Zhao*, *IUCrJ*** 10, 297, **2023.**

2.3 Diffraction Data Analysis by AI Aiding

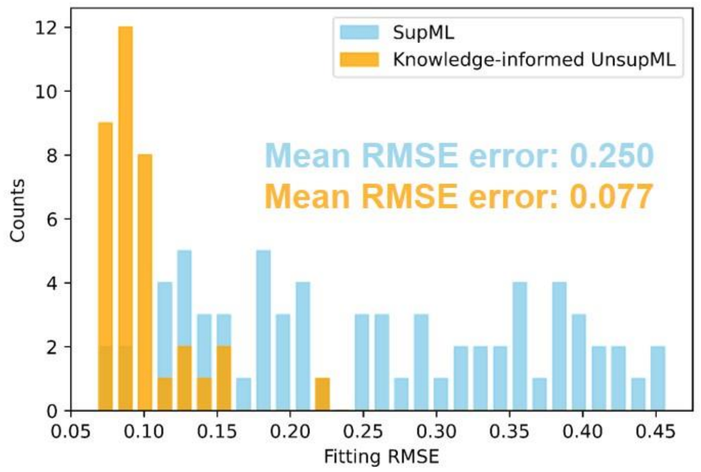
Diffraction

Physical knowledge guided machine learning on diffraction data





physics-driven *vs* data-driven



Contribution:

- ✓ X-ray diffraction knowledge-driven ML method achieves high-precision, self-supervised, interpretable analysis
- ✓ It makes online data analysis come true without tagging.

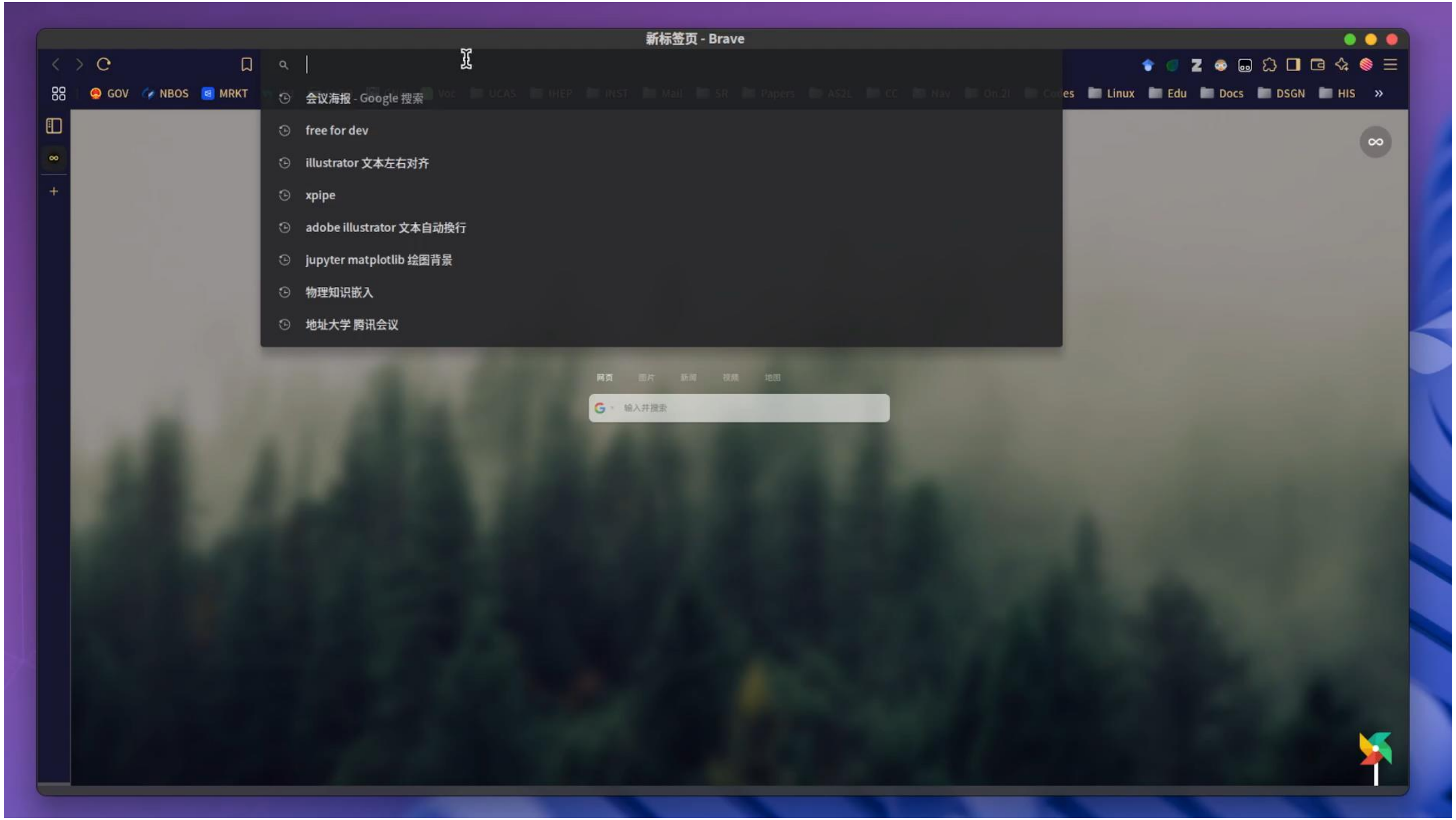
Qingmeng Li, …, Lina Zhao*, *Manuscript* 2025.

3. Deployment of AI Aided Data Analysis

Intelligence Photon Brain (IPSBrain)

3. Deployment of AI Aided Data Analysis

IPSBrain: www.ipsbrain.com **IPSBrain will connect to Mamba**

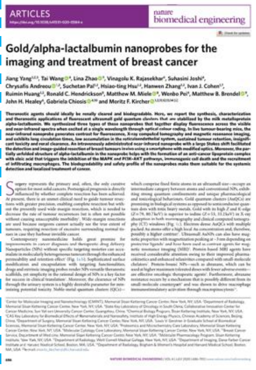


4. Promotion and Application

IPSBrain Promotion

- 2024.8： Release
- Online Training 1000+ People
- Face-to-face Training 200 + People

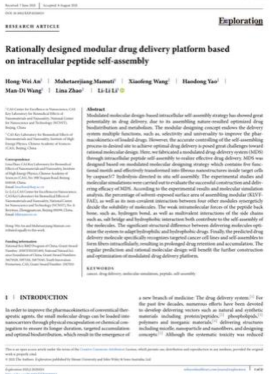
Supporting users' research achievement


ARTICLES
nature biomedical engineering
Gold/alpha-lactalbumin nanoprobes for the imaging and treatment of breast cancer

Nature Biomedical Engineering 2020, 4, 686


nature COMMUNICATIONS
ARTICLE
A bioactivated in vivo assembly nanotechnology fabricated NIR probe for small pancreatic tumor intraoperative imaging

Nature Communications 2022, 13, 418


RESEARCH ARTICLE
Exploration
Rationally designed modular drug delivery platform based on intracellular peptide self-assembly

Exploration 2021, 1, 20210153


Nano Today
A comparison of Remdesivir versus gold cluster in COVID-19 animal model: A better therapeutic outcome of gold cluster

Nano Today 2022, 44, 101468


Nano Today
Polyvinylpyrrolidone functionalization induces deformable structure of graphene oxide nanosheets for lung-targeting delivery

Nano Today 2021, 38, 101151


Nano Today
Polyvinylpyrrolidone functionalization induces deformable structure of graphene oxide nanosheets for lung-targeting delivery

Nano Today 2021, 37, 101079


Acta Pharmaceutica Sinica B
ORIGINAL ARTICLE
Acrylamide fragment inhibitors that induce unprecedented conformational distortions in enterovirus 71 3C and SARS-CoV-2 main protease

Acta Pharmaceutica Sinica B 2022, 12, 3924

Thank you for your attention

Thank all collaborators for their support!

Thank all colleagues and students for their help!

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