

MFX Instrument capabilities for run 23

LCLS Virtual Town Hall

Leland B. Gee/ Lead Instrument Scientist / MFX

January 30th, 2024

MFX Instrument Staff

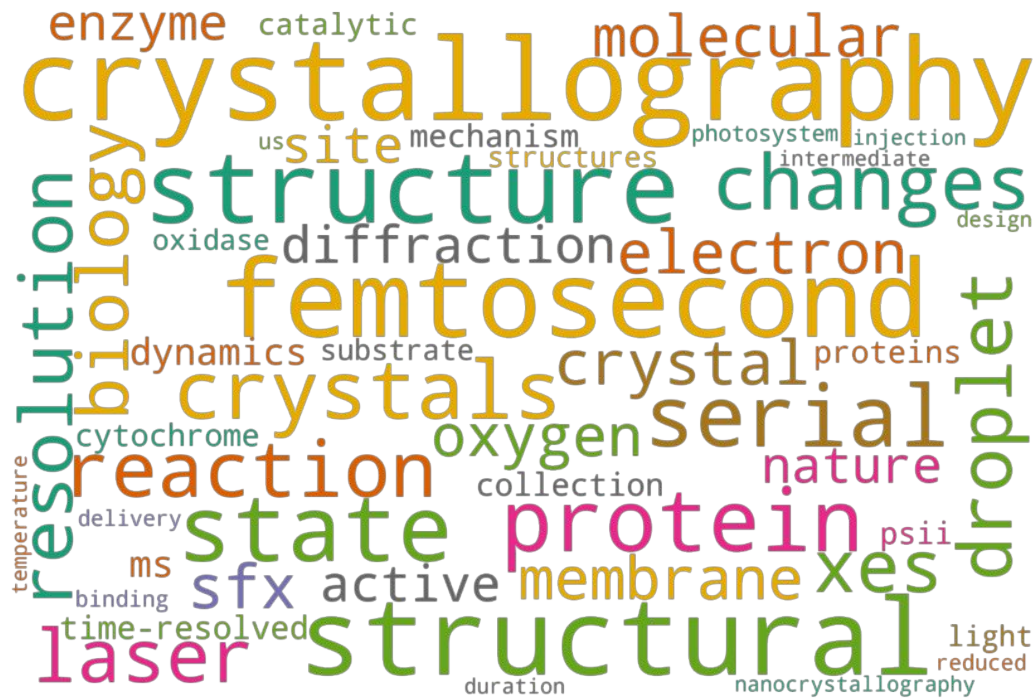
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MFX scientific capabilities

Scientific Applications	Femtosecond Crystallography
	Time-resolved scattering with hard X-rays
Techniques and Scattering Geometry	Macromolecular Crystallography
	Small-molecule Crystallography
	Forward scattering on fixed-mounted samples and in liquid jets
	Small Angle X-ray Scattering
	Wide Angle X-ray Scattering
	X-ray Emission Spectroscopy

What's important to MFX users?

From Run 22 MFX Proposals



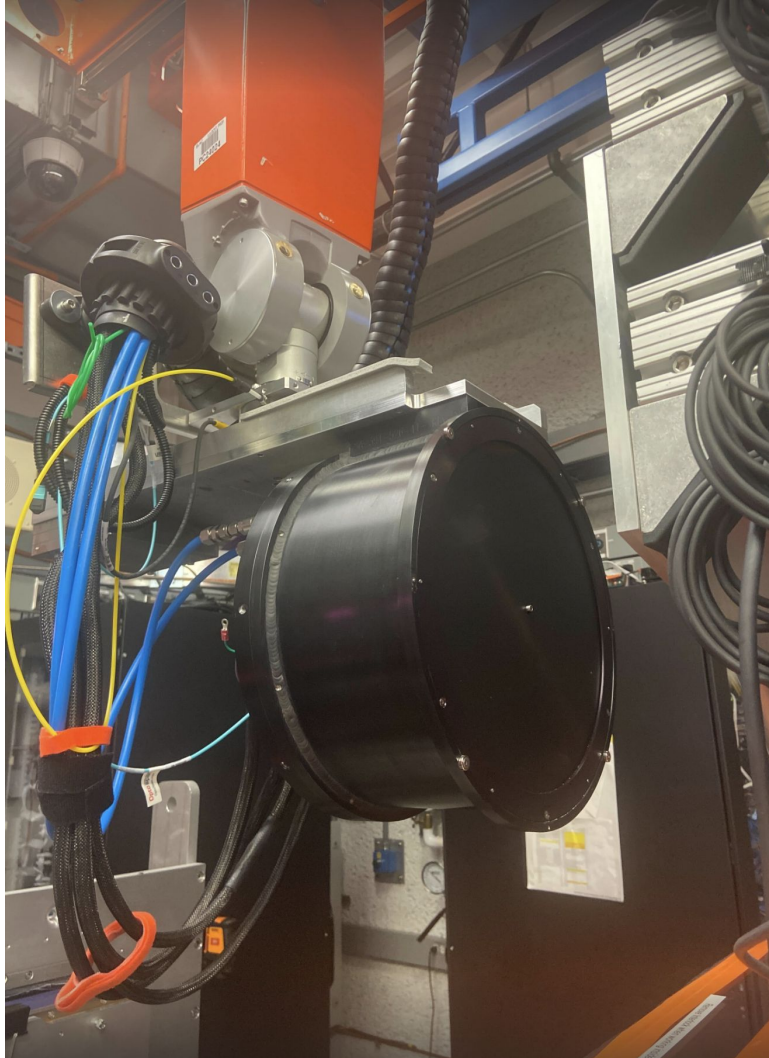
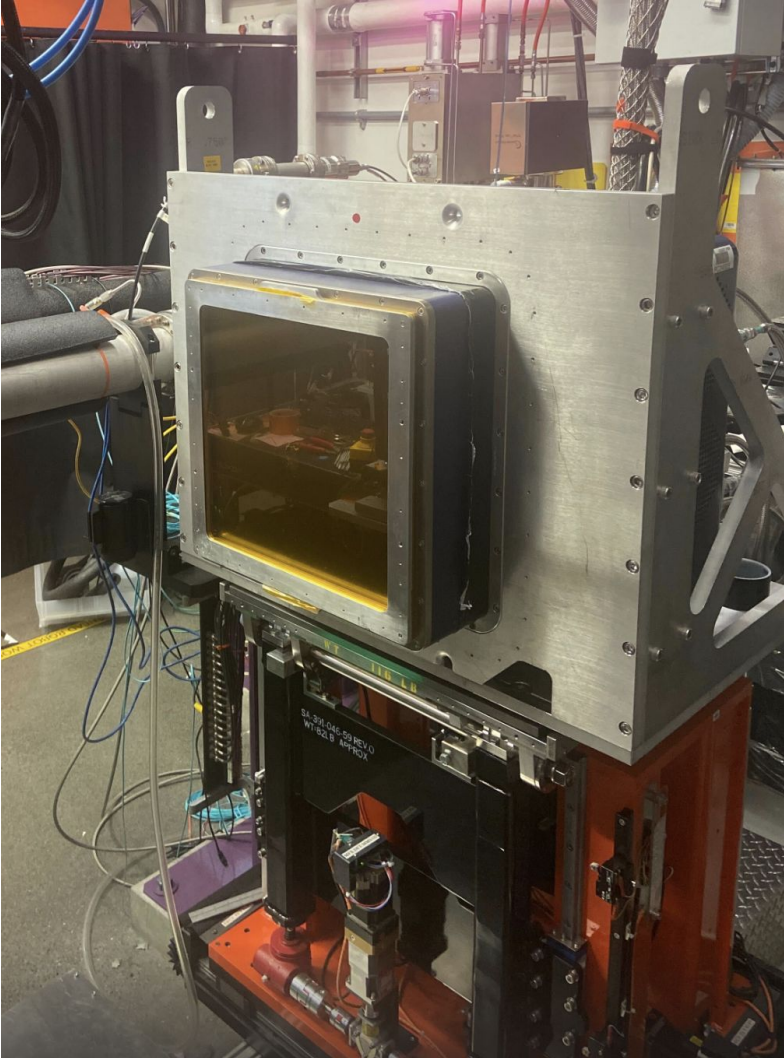
Highlights

- Transient sample conditions:
 - Optical-pump
 - Temperature-jump
 - Gas dosing
 - Chemical mixing
- Multimodal Probes:
 - XES+XRD
- Minimizing sample consumption:
 - Droplet-on-tape (DOT)
 - Droplet-on-demand (DOD)
 - GDVNs

The MFX User Experience



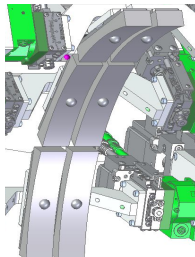
MFX Detectors



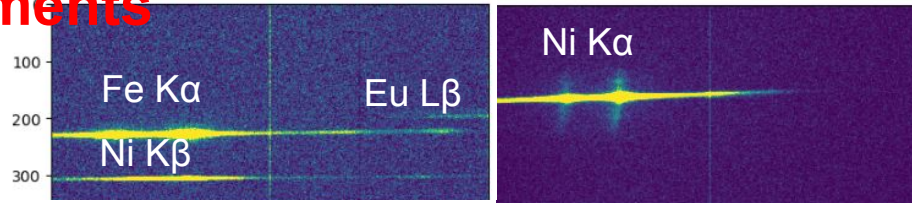
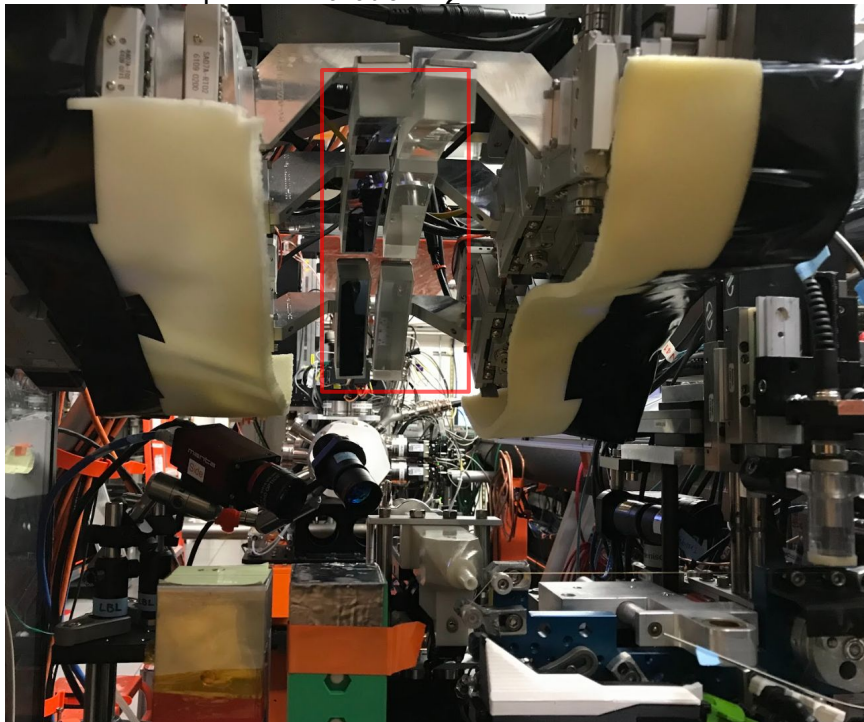
- Rayonix on the mover
- ePix10k-2M and other smaller detectors on the robot arm
- ePix100
- Jungfrau 0.5M and 1M

XES: 6-crystal multi-line Spectrometer @ MFX

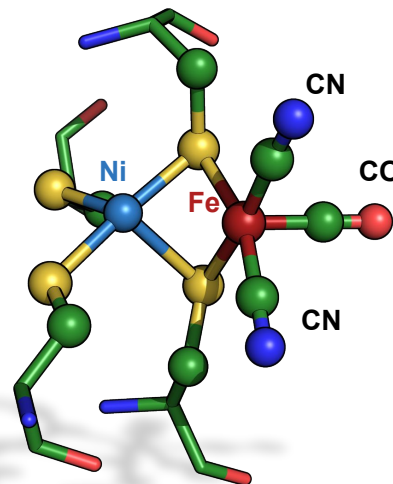
XES flexibility and improving alignments



Crystal set 1 Variable Crystal set 2



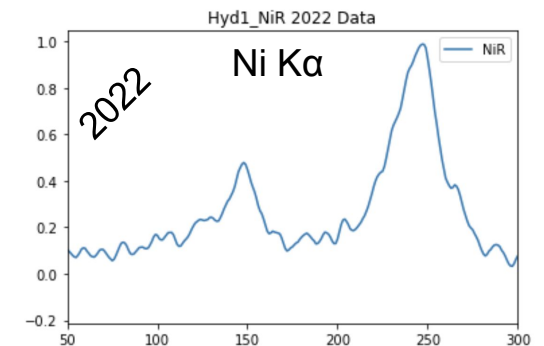
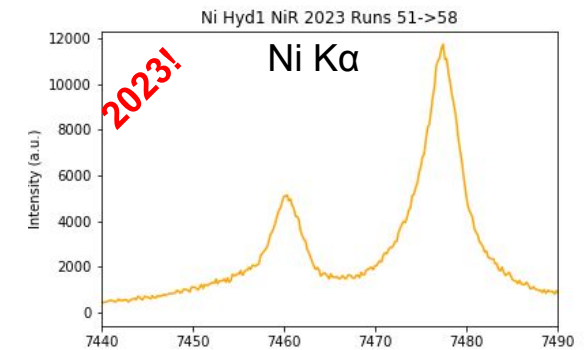
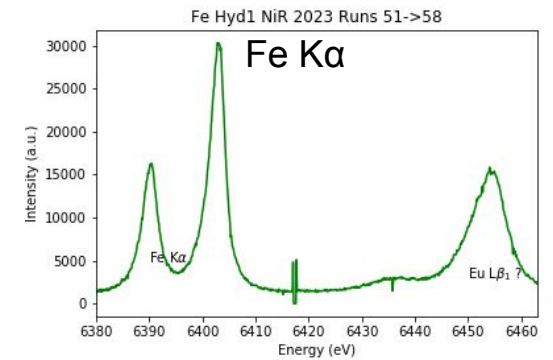
4 XES lines simultaneously!



[NiFe]-hydrogenase

6-Crystal Spectrometer

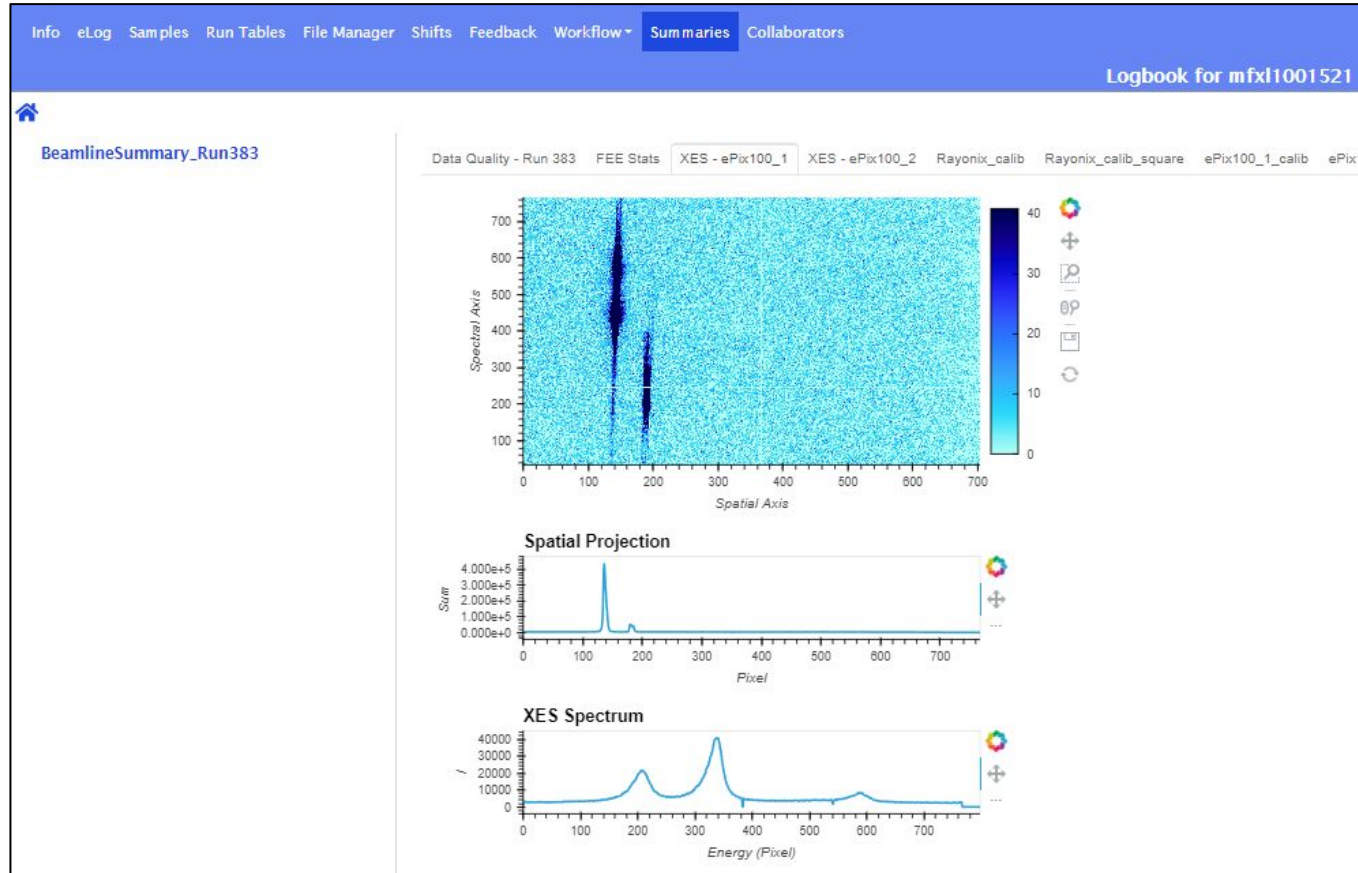
Suboptimal:
2 spectrometer geometry



Commissioned August 2023 (X-10016-Gee)

Near-time feedback from Spectroscopy

Spectral feedback within minutes of data collection



- XES data reduction performed directly from elog interface.
- Near-time spectroscopic feedback for collected data.
- Next steps: data aggregation.

Removing the barriers to entry for spectroscopy at MFX (and other hutches).

Newer Capabilities at MFX

fs Ti:Sapphire optical pump laser

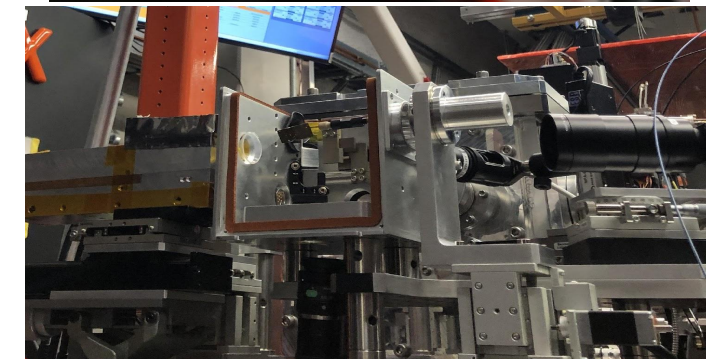
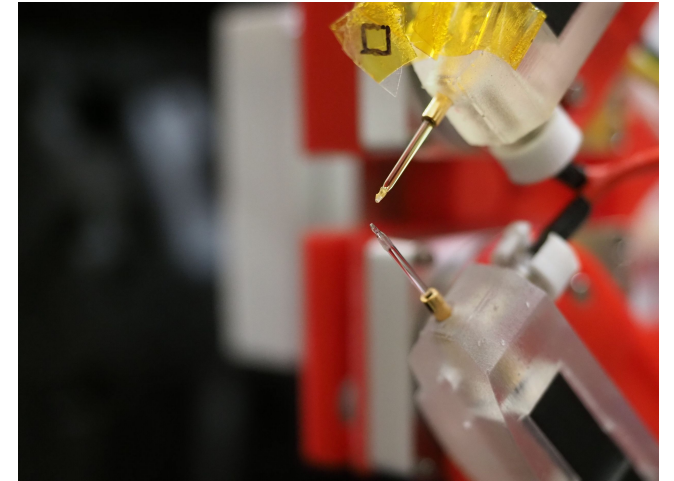
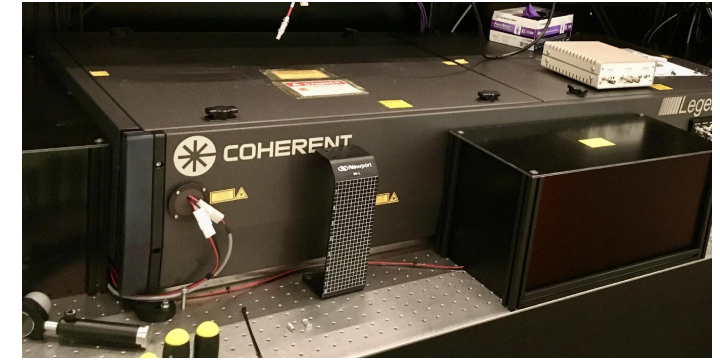
- Fundamental (800 nm) or 2nd harmonic, ~ 50 fs pulse
- Beam delivered to the sample collinearly with X-rays
- TOPAS-Prime OPA capable of 480-2400 nm

Droplet-on-demand (DOD)

- Initial demonstrations with optical-pump & XRD/XES probe (January 2024) works well for single drops.
- Ongoing efforts to mix droplets and monitor subsequent reaction kinetics with X-rays.

Liquid Jet Endstation (LJE)

- He environment compatible with spectroscopy and forward scattering
- Horizontal sample delivery

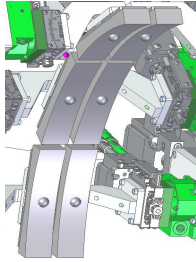


Complex Sample Delivery Methods

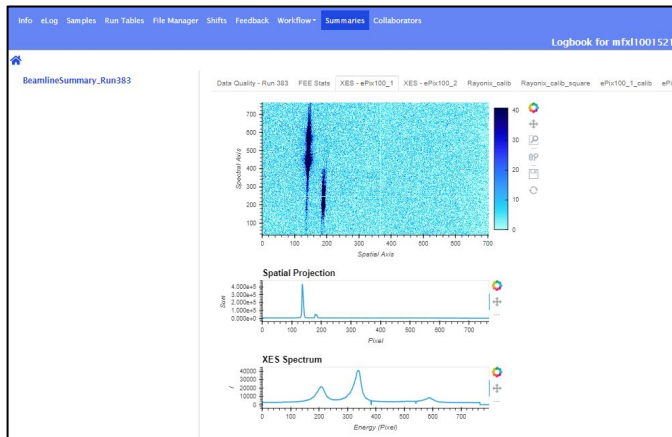
Injection Method	Fastest mixing time (approximate; ms)	Sample consumption (approximate; $\mu\text{L}/\text{min}$)	Reactant Consumption (approximate; $\mu\text{L}/\text{min}$)
Hydrodynamic focus	<~1 ms	<50 $\mu\text{L}/\text{min}$	<150 $\mu\text{L}/\text{min}$
Electrokinetic focus	<~10 ms	<20 $\mu\text{L}/\text{min}$	<20 $\mu\text{L}/\text{min}$
Droplet on Tape	<~10 ms	<20 $\mu\text{L}/\text{min}$	<20 $\mu\text{L}/\text{min}$
Colliding Drops (early user-assisted commissioning)	submillisecond*	<5 $\mu\text{L}/\text{min}$	<5 $\mu\text{L}/\text{min}$

Questions/Discussion?

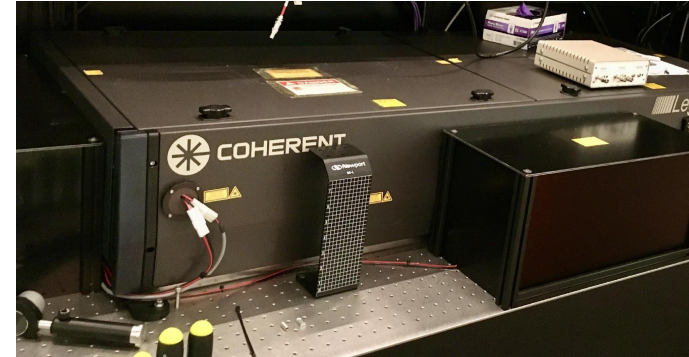
6-Crystal XES Spectrometer



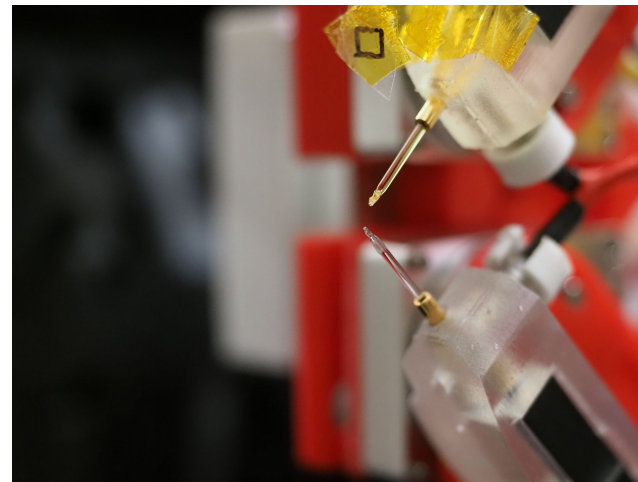
Rapid XES Analysis



New Coherent Astrella fs Laser



Droplet-on-demand



Horizontal Liquid Jet

