



MXCuBE Site Report

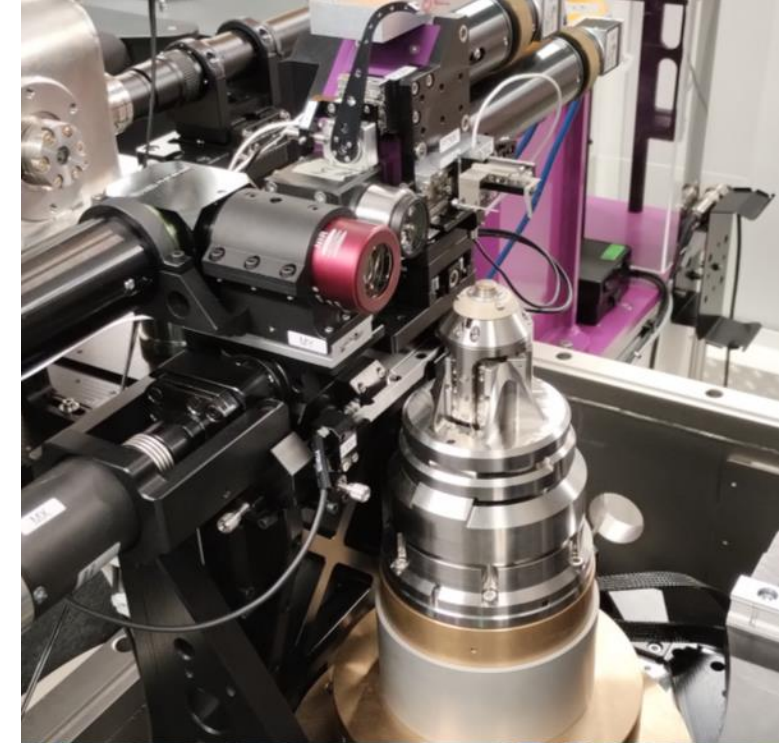
ALBA Synchrotron

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(On behalf of controls Group)*

22.11.2024 – MXCuBE/ISPyB meeting

ALBA MX Beamlines

- 2 beamlines: XALOC in production, XAIRA with expert users
- BL13-XALOC:
 - High-throughput tunable beamline
 - Arinax MiniDiff MD2M; Dectris Pilatus 3X 6M; IRELEC CATS ISARA² sample-changer robot
- BL06-XAIRA:
 - Microfocus beamline
 - In-house diffractometer (Aerotech+Smaract); Dectris Eiger 9M; IRELEC ISARA² sample-changer robot
- Controls software stack:
 - Tango and Sardana, Taurus GUIs
 - LImA for cameras and detectors



MXCuBE Status

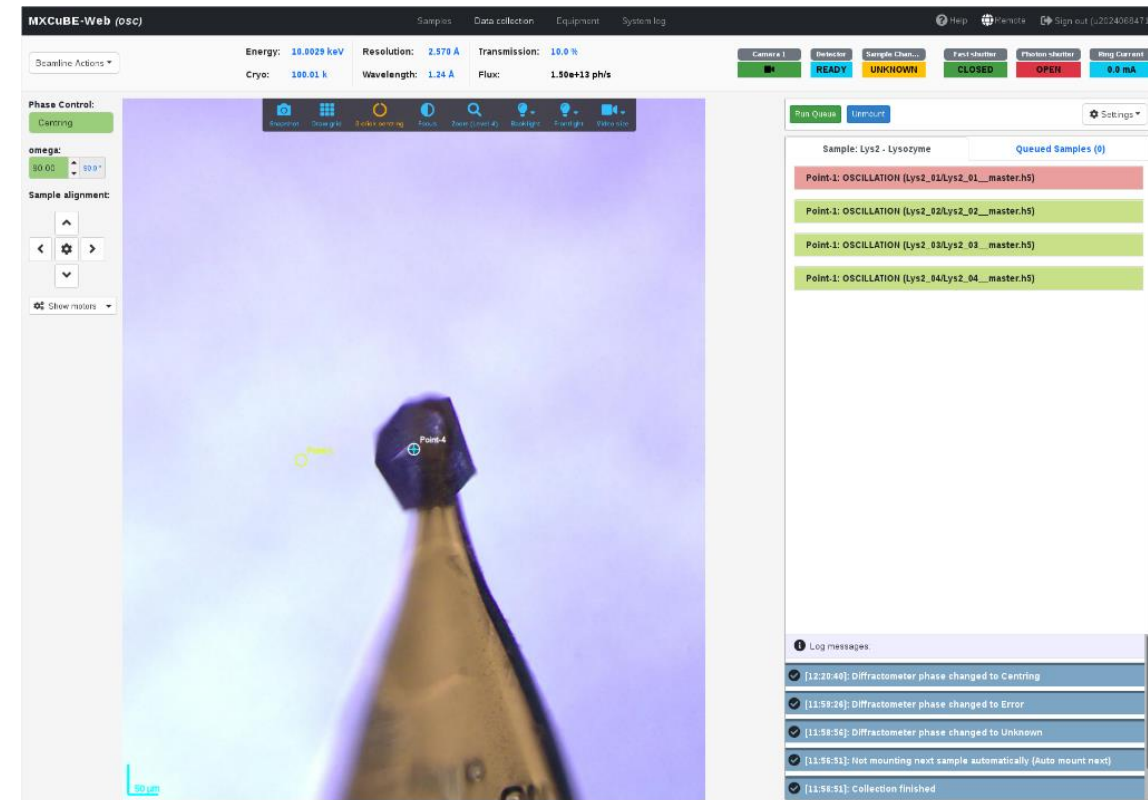
- BL13-XALOC:
 - Python 3.9 Qt5
- BL06-XAIRA:
 - Python 3.10 Web-version, 10-month old mxcubecore
- LIMS:
 - XALOC: ISPyB with EXI
 - XAIRA: ICAT with DataPortal

Cybersecurity

- Mostly “delegated” to our IT Systems Department
- Users connect through NoMachine with their proposal username to the current session of the beamline control machine
 - They have all the permissions of the local account
 - Mouse “battles” with the local-contact during interventions...

Developments Since Last Meeting

- BL13-XALOC:
 - Software “maintenance” to keep up with hardware changes and libraries version updates
 - Upgraded to IRELEC ISARA² sample-changer robot
- BL06-XAIRA:
 - Production-ready!
 - 3-click centring, simple rotation experiment



Developments Since Last Meeting

- BL06-XAIRA:
 - ICAT integration (sessions and simple rotation experiments) and Offline data processing
 - Successful experiments from cristal centring, data collection/upload to ICAT and autoprocessing trigger

The screenshot displays the ALBA Data Portal interface for experiment BL06. The main content area shows the 'Estimated best auto processing' results for a Tetragonal system (P422) with unit cell parameters a=b=93.8 Å and c=93.8 Å. The data collection statistics are as follows:

	Compl.	Res. low	Res. high	Rmerge	I/(I)	cc1/2	ccAno
inner	94.0%	29.0	11.6	6.7	30.9	1.0	-
outer	98.9%	2.7	2.6	82.5	2.2	0.8	-
overall	99.9%	29.0	2.6	12.4	14.4	1.0	-

Below this, a table lists the 'Estimated best auto processing' for various programs and runs, including completion percentages and resolution values.

Overlaid on the interface is a 'Data collection' window showing a Dozor plot. The plot displays the 'Number of spots / Dozor score (*10)' on the y-axis (ranging from 200 to 1000) against the 'Image number' on the x-axis (ranging from 0 to 1800). The plot includes data points for 'Number of spots' (yellow), 'ExecDozor score' (light blue), and 'Visible resolution' (purple). A blue button at the bottom of the plot reads 'Click on the plot to visualize collected images.'

Another window shows a 2D diffraction pattern for '_02_data_000002.h5' with a color scale for 'Resolution (Å)' ranging from 2e+1 to 2e+0.

RNA-dependant RNA polymerase from Foot-and-Mouth Disease Virus
 Courtesy of C. Ferrer (IBMB-CSIC)

Plans For The Next Six Months

- BL13-XALOC:
 - Restart effort on the (stalled) update to MXCuBE-Web
- BL06-XAIRA:
 - X-ray centring
 - Online processing
 - Helical scans
 - Review integration of IRELEC ISARA² sample-changer robot (fix minor bugs, check for missing features)

Acknowledgements

ID, FE and vacuum

- Pep Campmany
- Jordi Marcos
- Raquel Monge

Alignment

- Marta Llonch
- Jon Ladrera

Cryogenics/FEA

- Marcos Quispe
- Yury Nikitin
- Liudmila Nikitina

Workshop

- Jose Ferrer

MIS

- Marc Armenter
- Rodrigo Cabezas

IT

- Pau Carnicer
- Sergi Pusó
- Jordi Salabert

Technicians

- Alex Enrique

Optics and Metrology

- Josep Nicolas
- Igors Sics
- José Luis Frieiro
- Nilson Pereira

Engineering/TBM

- Nahikari González
- Alejandro Crisol
- Antonio Carballado
- Carles Colldelram

Scientists

- Judith Juanhuix
- Damià Garriga
- Isidro Crespo

Infrastructures

- Núria Martí

Electronics

- Bernat Molas
- Alberto Ruz
- Alberto Rubio
- Xevi Serra
- Sergio Astorga
- Electronics Technicians

Controls

- Jose Gabadinho
- Steven Wohl
- Oriol Vallcorba
- Fulvio Becheri
- Albert Ollé

Scientific Data Management

- Albert Castellví
- Emilio Centeno
- Joa Gómez



+ all ALBA Technical and Administrative support staff