Status of MXCuBE Beamline Control at BESSY II

Michael Hellmig,
on behalf of the HZB-MX group

MXCuBE/ISPyB Joint Meeting, 29.10.-31.10.2019,
BESSY II @HVB, Berlin
Photon source BESSY II

**BESSY II ring parameters:**
- Electron Energy: 1.7 GeV
- Electron Current: 280 mA
- Circumference: 240 m
- Straight sections: 16
- Beamlines: ~50

**Synchrotron sources at BESSY II**

- Photon energy range: 5 keV – 16 keV
- 7 Tesla wavelength shifter and MX Beamlines

![Image of BESSY II synchrotron](image-url)

More than 80 groups from 15 countries

source: biosync.sbkb.org

3000th PDB deposition 11/09/2019

HZB-MX beamlines
Total no. PDB entries: 3017

*) 2018-depositions will be complete 12/2019
MX experimental floor at BESSY II

**BL 14.1 MAD**
- MD2 with MK3
- Pilatus2 6M 12 Hz
- CATS: 90 SPINE samples
- MXCuBE 2.2 Qt4

**BL 14.3 13.8 keV**
- MD2S with MK3
- Rayonix MX225
- HClab & REX nozzle changer
- MXCuBE 2.2 Qt4

**BL 14.2 MAD**
- Nanodiff goniometer
  - Pilatus3 2M
- GROB: 294 SPINE & Unipuck samples
- MXCuBE 2.2 Qt4

- standard user operation schedule: 24/5 (Tuesday to Saturday)

**User Operation**
- back in operation
- user operation
MX beamline 14.1

- detector upgrade planned for 2020
  - existing detector installed 01/2013
    - manufacturer support ended
    - no issues with detector head
    - detector control computer: Ubuntu 10.04 LTS
  - replacement of Pilatus2 6M with current model Pilatus3 6M (S or X)
    - PPU for fast online data analysis

- re-use existing detector at BL14.3
  - replace Rayonix CCD detector
  - enable shutterless data acquisition
  - ~3 times faster data collection

- CATS Uni-puck upgrade under evaluation
  - SPINE and Uni-puck support
  - shorter exchange time with Uni-puck double gripper
• upgrade of beam-shaping devices in progress
  • unreliable operation
  • slow
  • on-call service intervention

• new setup by Smaract
  • larger travel range
  • transparent control-system integration with Tango DS
  • to be installed 12/2019
MXCUBE-HClab integration

- integration in progress
  - HClabGroupQueueEntry
  - HClabQueueEntry
  - HClabDataCollectionQueueEntry

BL 14.3 13.8 keV

TO-DO:
- HClab status widget
- online analysis: DISTL.Spotfinder/Dozor

Oleg Kornelsen
Bachelor student
MXCuBE 2.2 Qt4 experiment-control software at all three HZB-MX beamlines

Diffractometers:
- Arinax MD2
- Arinax MD2S
- DESY Nanodiff

Sample-transfer robots:
- Irelec CATS
- NatX-ray GROB

Detectors:
- Dectris Pilatus2 6M
- Dectris Pilatus3 2M
- Rayonix MX225

Auxiliary devices:
- Wago I/O controller
- Amptek X-123SDD

Control systems:
- EPICS
- Tango
- Exporter
- SPEC
MXCuBE: status and future plans

**current status:**
- MXCuBE 2.2 Qt4 running on all three HZB-MX beamlines

**current issues:**
- resources mostly spend on testing, maintenance, trouble shooting
- commissioning/testing time at the beamline strongly limited
- outdated MXCuBE control computer at the beamline
  - Debian 7, **32-bit**

**short- and mid-term plans:**
- modernization of MXCuBE control computer
  - Debian 9/10, 64-bit
  - Anaconda/Miniconda development environment
- offline MXCuBE update:
  - unified HZB-specific HardwareObjects „branch“
  - HardwareRepository → branch 2.3.0 → master
  - MXCuBE2 → GitHub master branch
- complete integration of HClab into MXCuBE software setup
  - HCLab brick
  - analysis
Workflow of crystallographic fragment screening

1. Library selection
2. Crystal treatment and cryo-cooling
3. Data collection
4. Identification of hit fragments

FragMAX webapp: collaboration MAX IV and HZB:
- Auto-refinement Pipeline
- PanDDA
- XDSAPP

Gustavo Lima (MAX IV), Jan Wollenhaupt (HZB)
**XtalTool:**
- All-in-One sample holder
- *in situ* method
- Crystallize on sample holder
- Use as a lid
- Data collection at beamline with magnetic base
- Developed by C. Feiler, patent
- Distributed by Jena Bioscience

X-ray transparent Kapton film with 5 µm pores

Transparent removable COC film

Feiler et al., (2019) *J. Vis. Exp.* (149), e59722
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The MXCuBE collaboration

Industrial partners:

Thank you for your attention.

Questions?