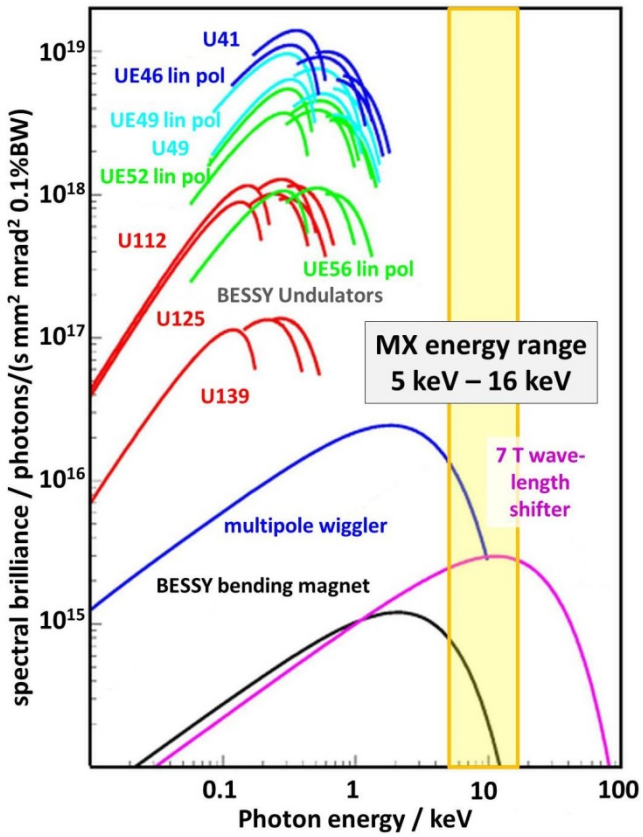
Status of MXCuBE Beamline Control at BESSY II

Michael Hellmig,
on behalf of the HZB-MX group

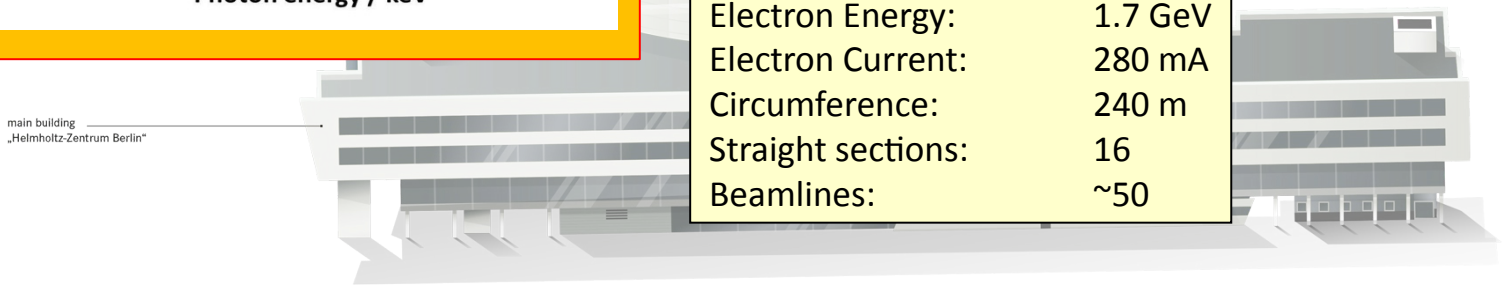
MXCuBE/ISPyB Joint Meeting, 29.10.-31.10.2019,
BESSY II @HZB, Berlin

Photon source BESSY II

Synchrotron sources at BESSY II



7 Tesla wavelength shifter and MX Beamlines



BESSY II ring parameters:

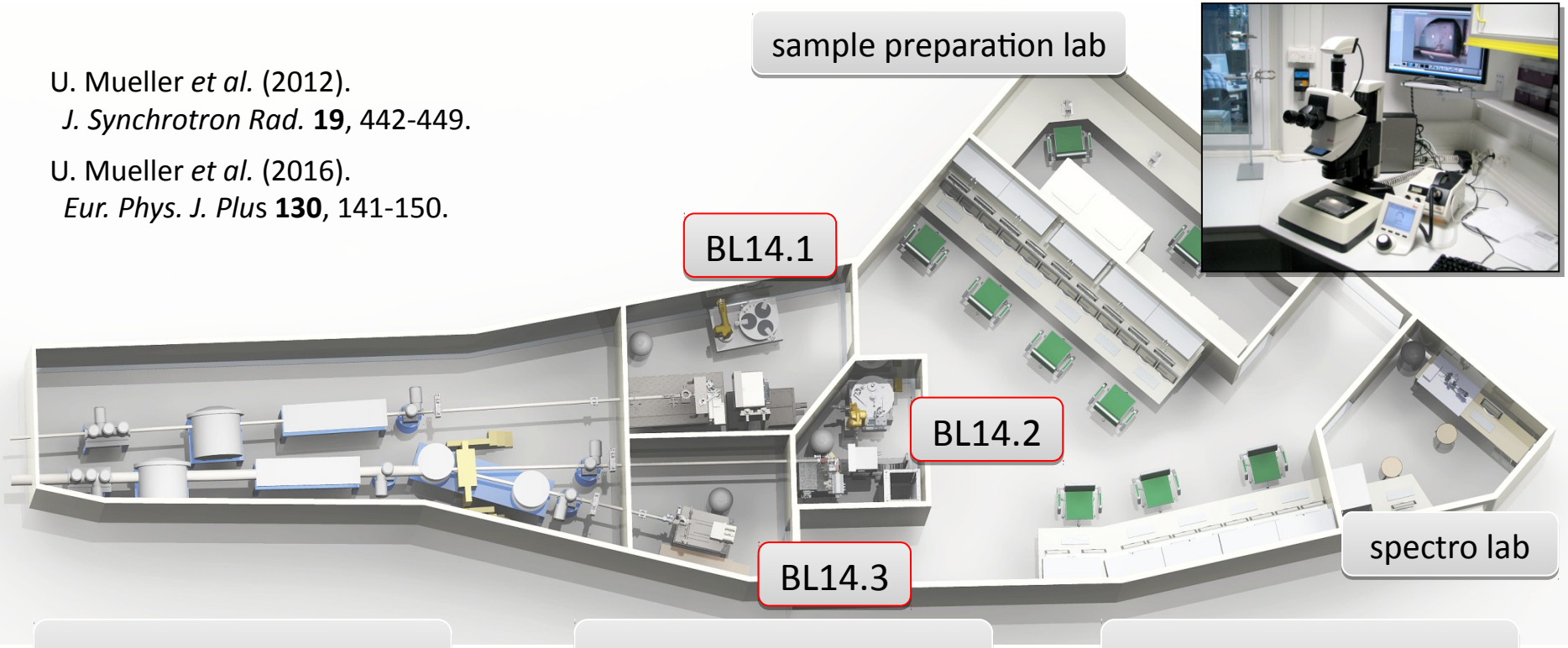
Electron Energy:	1.7 GeV
Electron Current:	280 mA
Circumference:	240 m
Straight sections:	16
Beamlines:	~50

HZB-MX BEAMLINES OVERVIEW

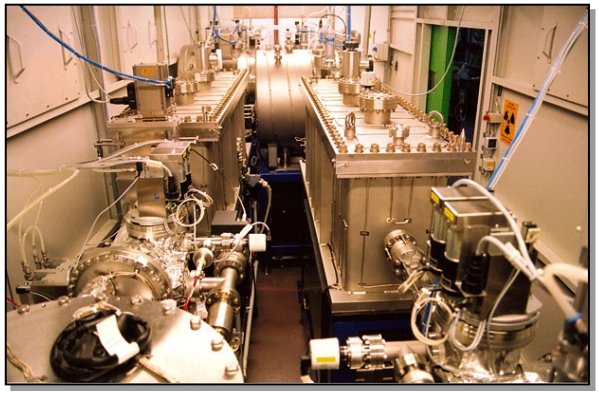
HZB Helmholtz Zentrum Berlin

U. Mueller *et al.* (2012).
J. Synchrotron Rad. **19**, 442-449.

U. Mueller *et al.* (2016).
Eur. Phys. J. Plus **130**, 141-150.



optics hutch



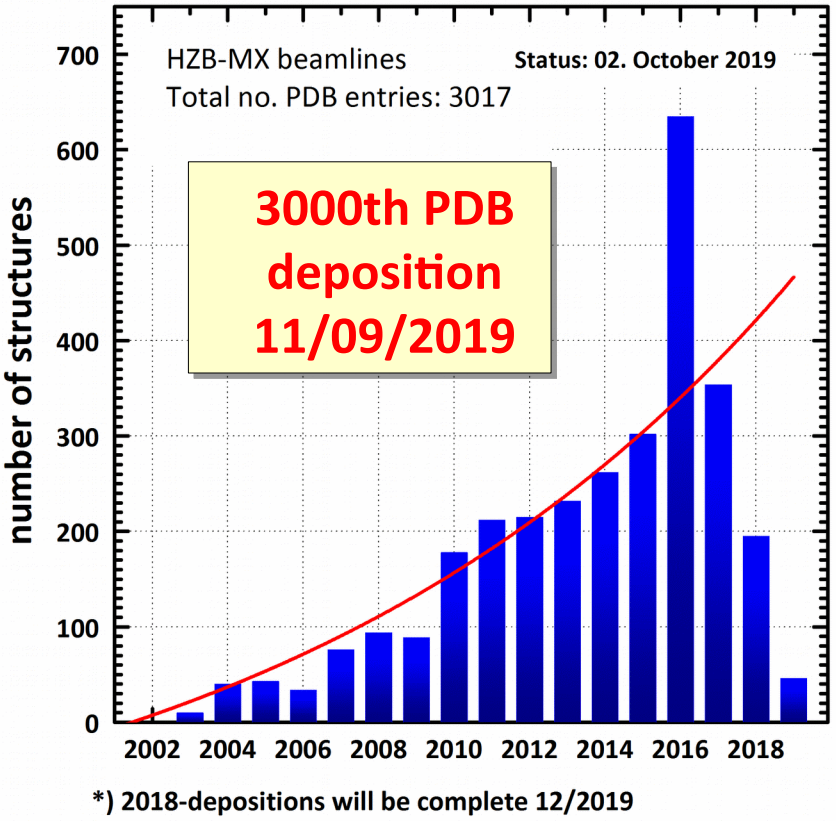
experimental hutches

user control room

HZB-MX USER COMMUNITY 2019

More than 80 groups
from 15 countries

source: biosync.sbkb.org



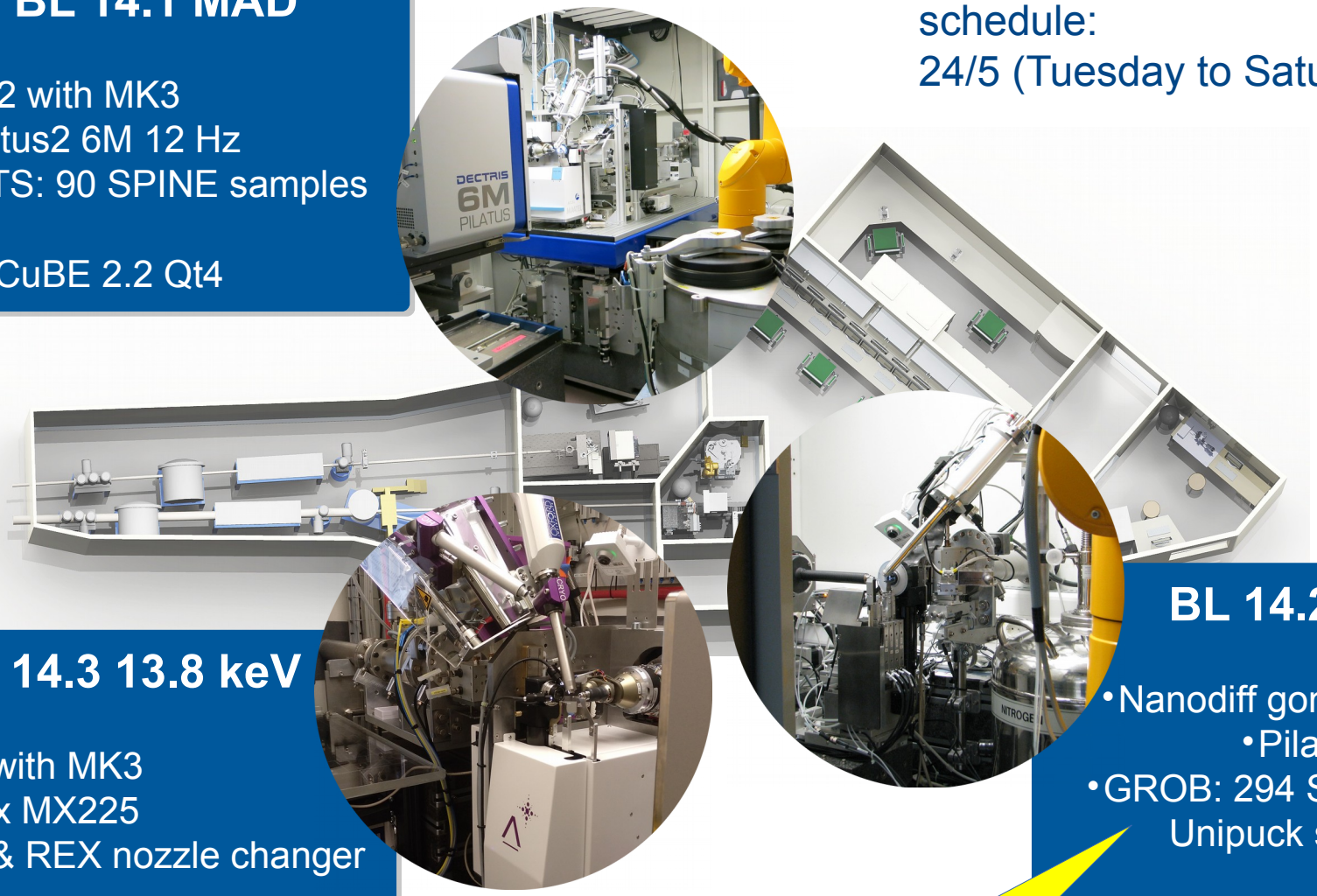
MX experimental floor at BESSY II

BL 14.1 MAD

- MD2 with MK3
- Pilatus2 6M 12 Hz
- CATS: 90 SPINE samples

- MXCuBE 2.2 Qt4

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



BL 14.3 13.8 keV

- MD2S with MK3
- Rayonix MX225
- HClab & REX nozzle changer

- MXCuBE 2.2 Qt4

user operation

BL 14.2 MAD

- Nanodiff goniometer
- Pilatus3 2M
- GROB: 294 SPINE & Unipuck samples

- MXCuBE 2.2 Qt4

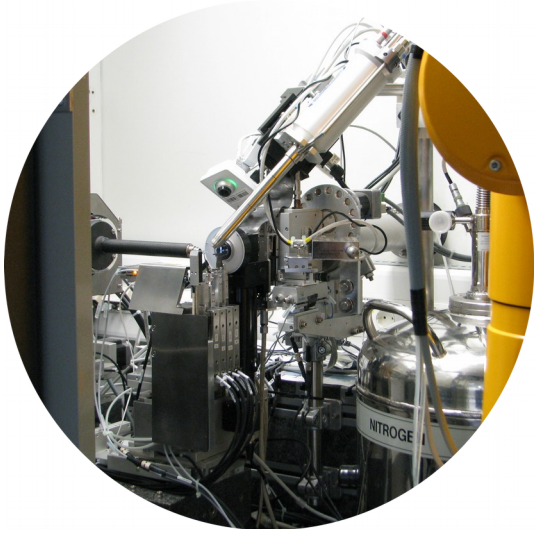
back in operation

MX beamline 14.1

BL 14.1 MAD

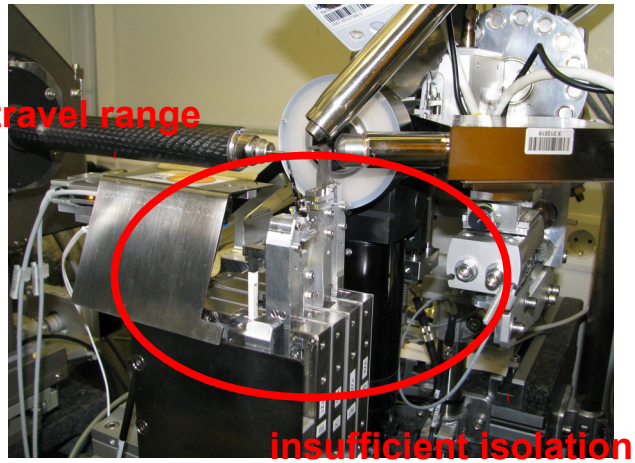
- detector upgrade planned for 2020
  - existing detector installed 01/2013
    - manufacturer support ended
    - no issues with detector head
    - detector control computer: Ubuntu 10.04 LTS
  - replacement of Pilatus2 6M with current model Pilatus3 6M (S or X)
    - PPU for fast online data analysis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

MX beamline 14.2

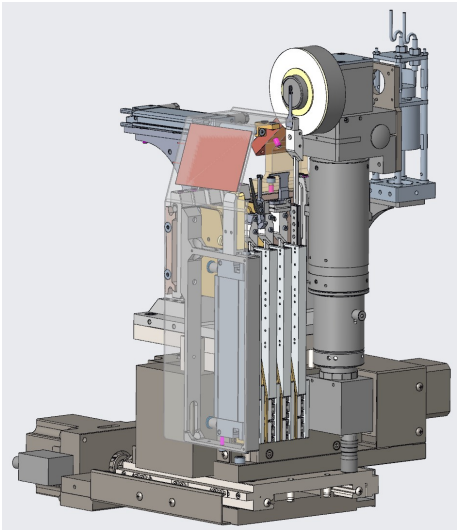


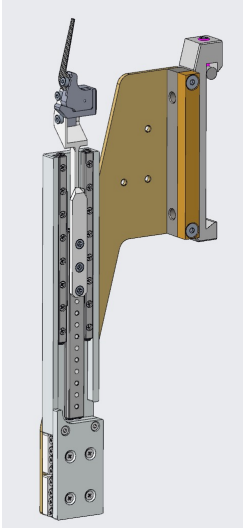
BL 14.2 MAD

- 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

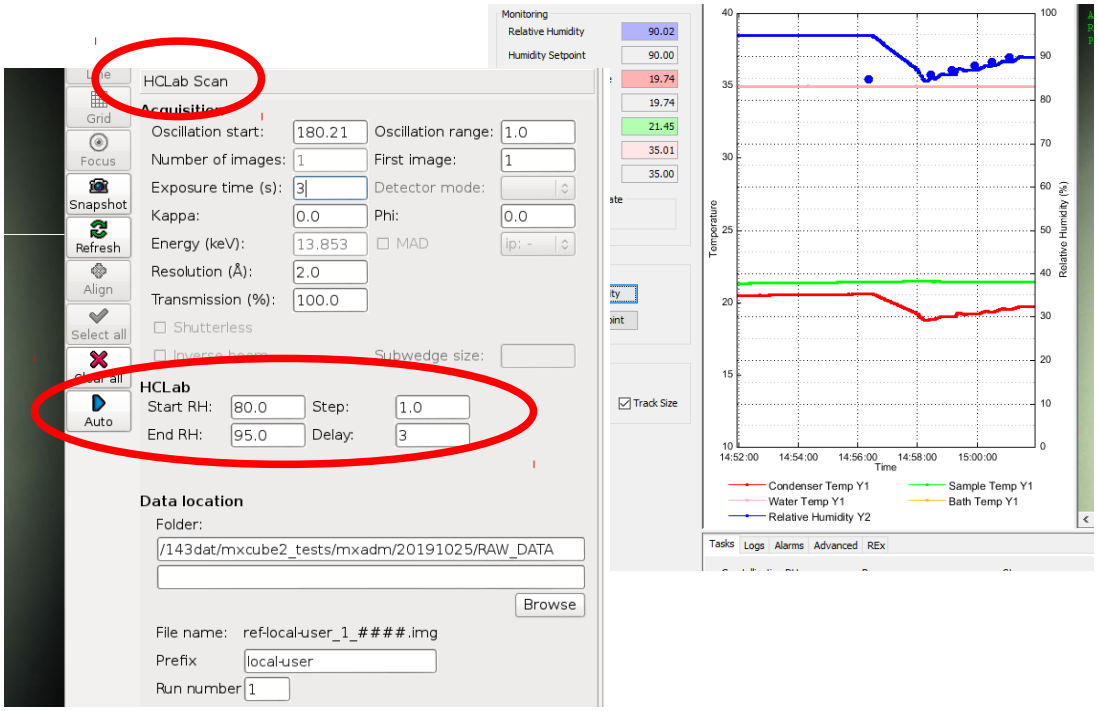




MXCUBE-HClab integration

BL 14.3 13.8 keV

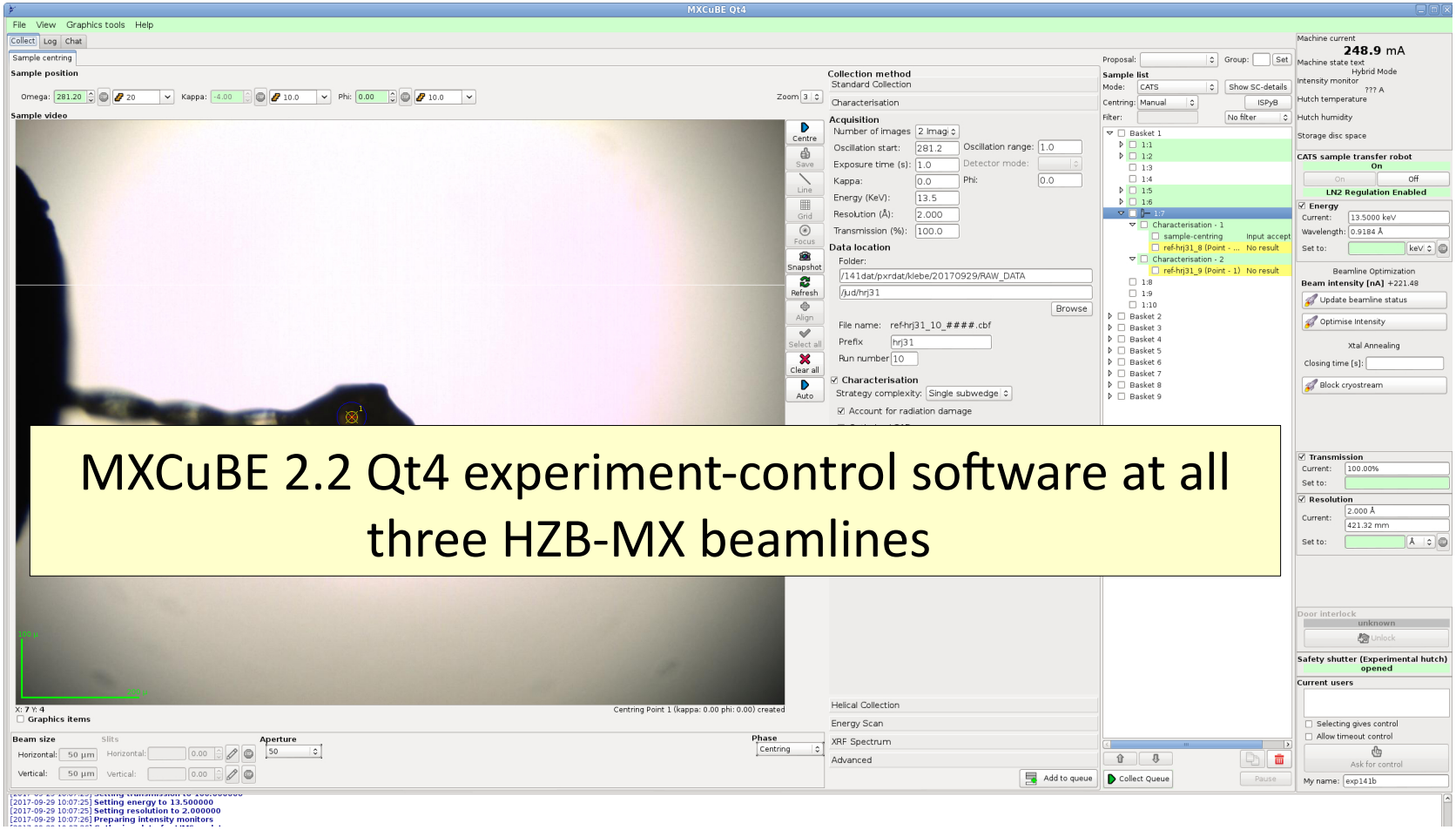
- integration in progress
  - HCLabGroupQueueEntry
    - HCLabQueueEntry
    - HCLabDataCollectionQueueEntry



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

Oleg Kornelsen
Bachelor student

MXCuBE2 Qt4 @HZB-MX



MXCuBE 2.2 Qt4 experiment-control software at all three HZB-MX beamlines

Diffractometers:	Sample-transfer robots:	Detectors:	Auxiliary devices:	Control systems:
Arinax MD2 Arinax MD2S DESY Nanodiff	Irelec CATS NatX-ray GROB	Dectris Pilatus2 6M Dectris Pilatus3 2M Rayonix MX225	Wago I/O controller Amptek X-123SDD	EPICS, Tango, Exporter, SPEC

MXCuBE: status and future plans

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

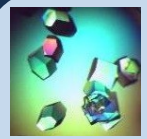
- current issues:
  - resources mostly spend on testing, maintenance, trouble shooting
  - commissioning/testing time at the beamline strongly limited
  - outdated MXCuBE control computer at the beamline
    - Debian 7, **32-bit**

- 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

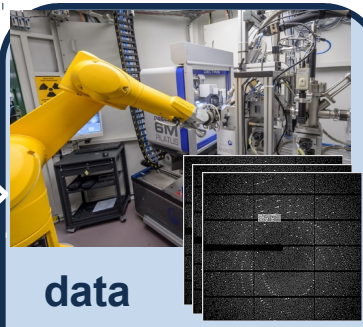
Workflow of crystallographic fragment screening

HZB Helmholtz Zentrum Berlin

library selection



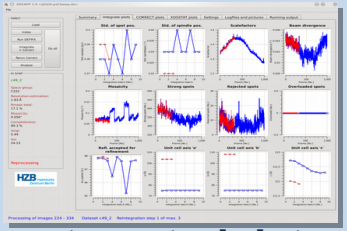
crystal treatment and cryo-cooling



data collection

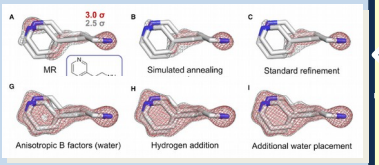
FragMAX webapp: collaboration MAX IV and HZB:

XDSAPP



automated data processing

auto-refinement Pipeline



and PanDDA

identification of hit fragments

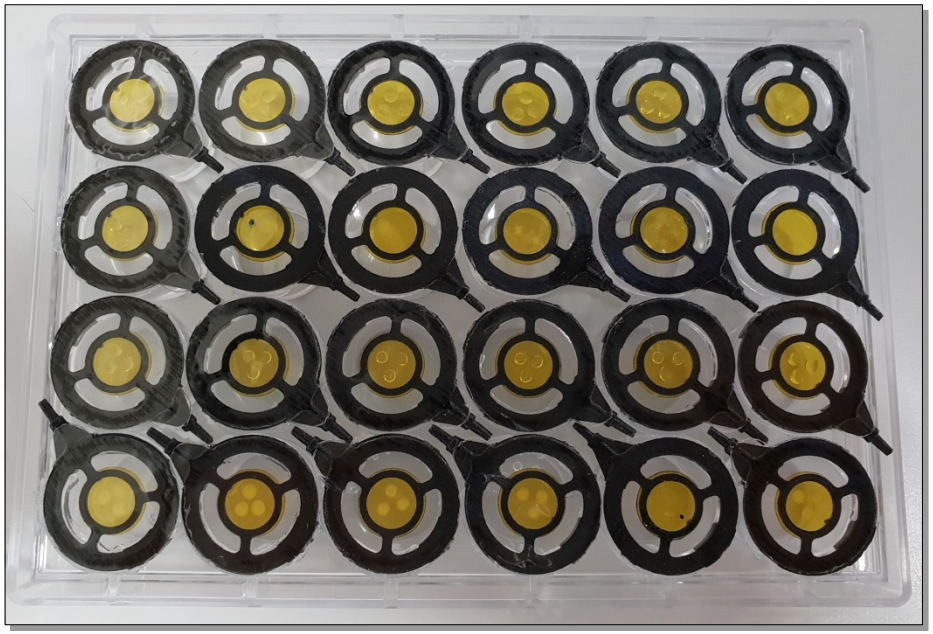
Gustavo Lima (MAX IV), Jan Wollenhaupt (HZB)

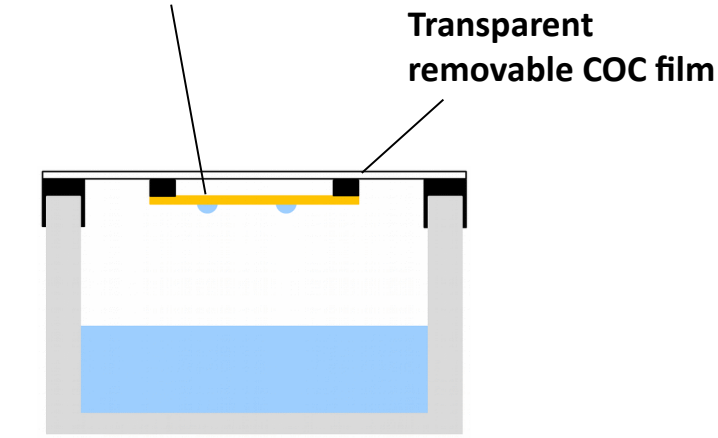
XTALTOOL

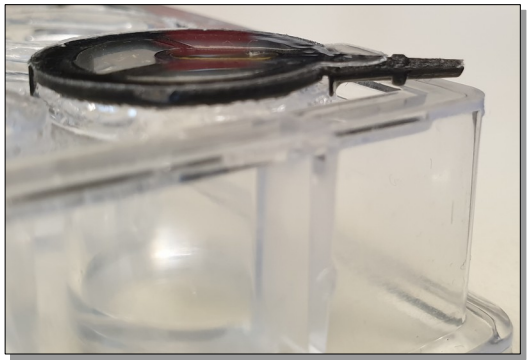
HZB Helmholtz Zentrum Berlin

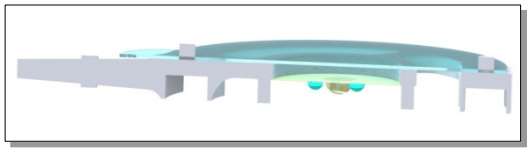
XtalTool:

- 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









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

Acknowledgements

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Michael Steffien
Helena Taberman
Jan Wollenhaupt

The MXCuBE collaboration

Industrial partners:

Thank you for your attention.

Questions?