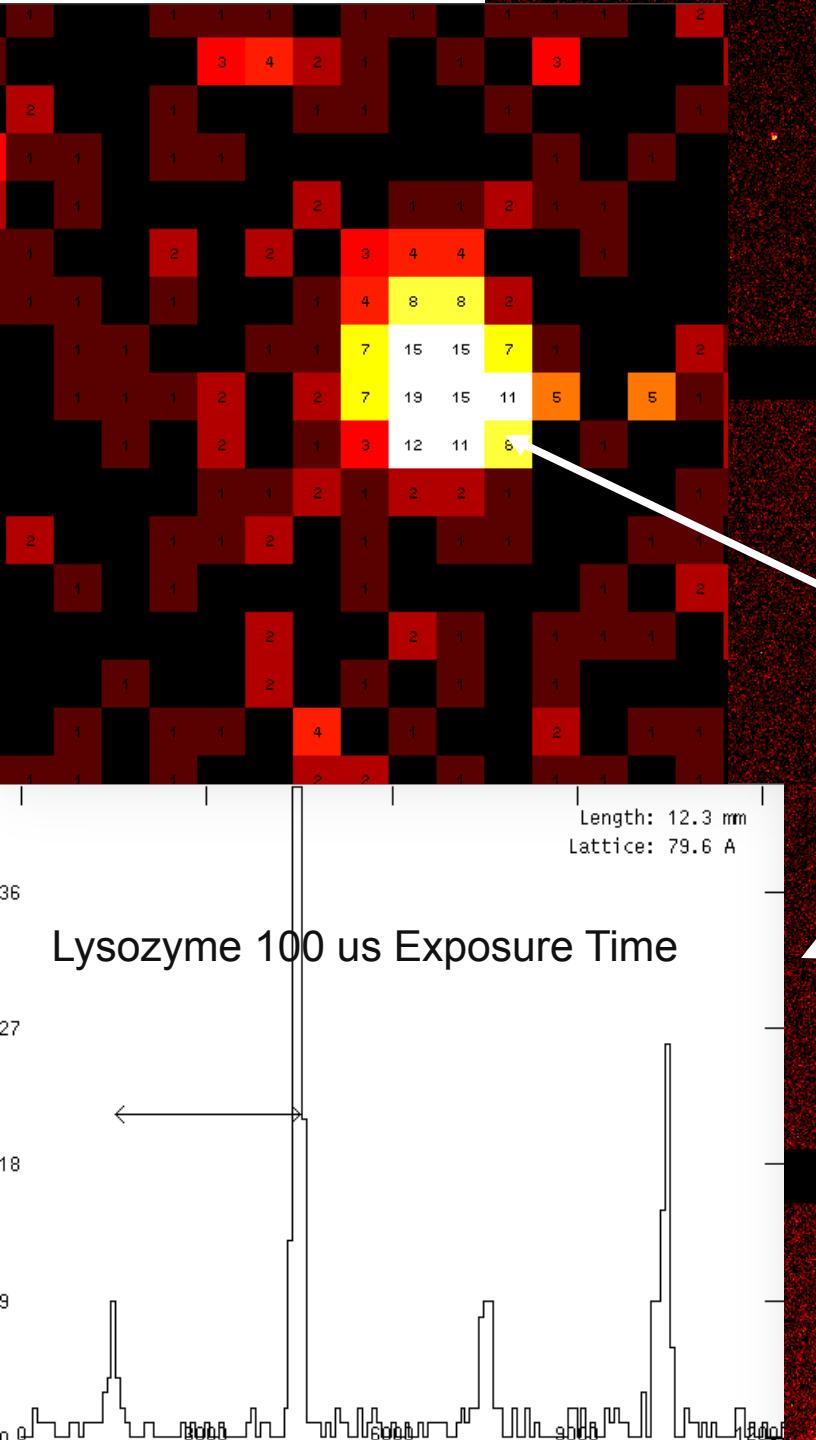


MxCuBE for time-resolved SSX at T-REXX

gleb.bourenkov@embl-hamburg.de



10^{13} ph/sec

Length: 12.3 nm
lattice: 79.6 Å

Lysozyme 100 us Exposure Time

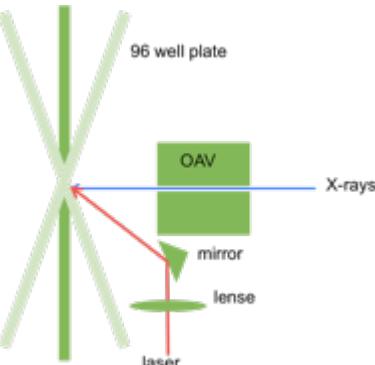
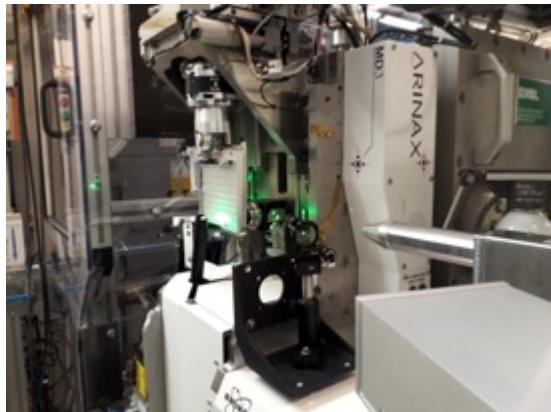
Exposure time = 7.6 μ s
40 PETRAIII bunches

Count rate limit:
18 events/pixel

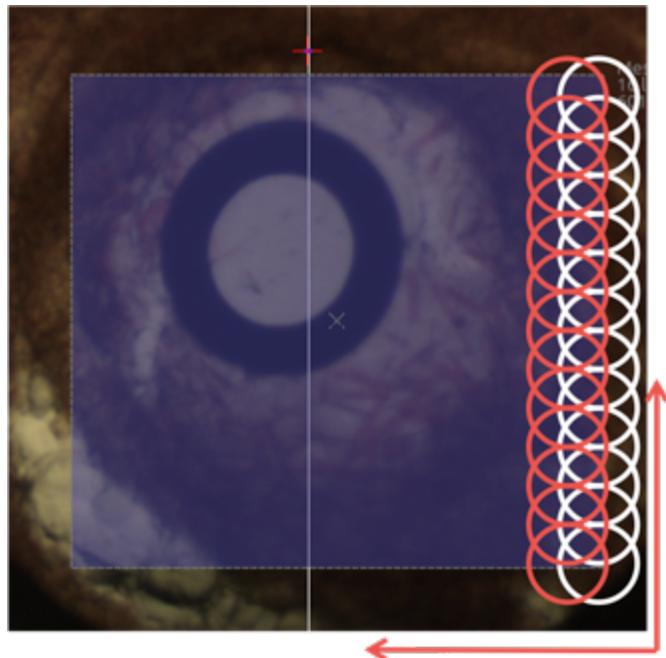
3.07 Å

5.97 Å

Time-resolved SSX by serial helical scans



Laser-flashes delivered at the sample in 96-well plate at a sub-harmonic of the detector framing frequency

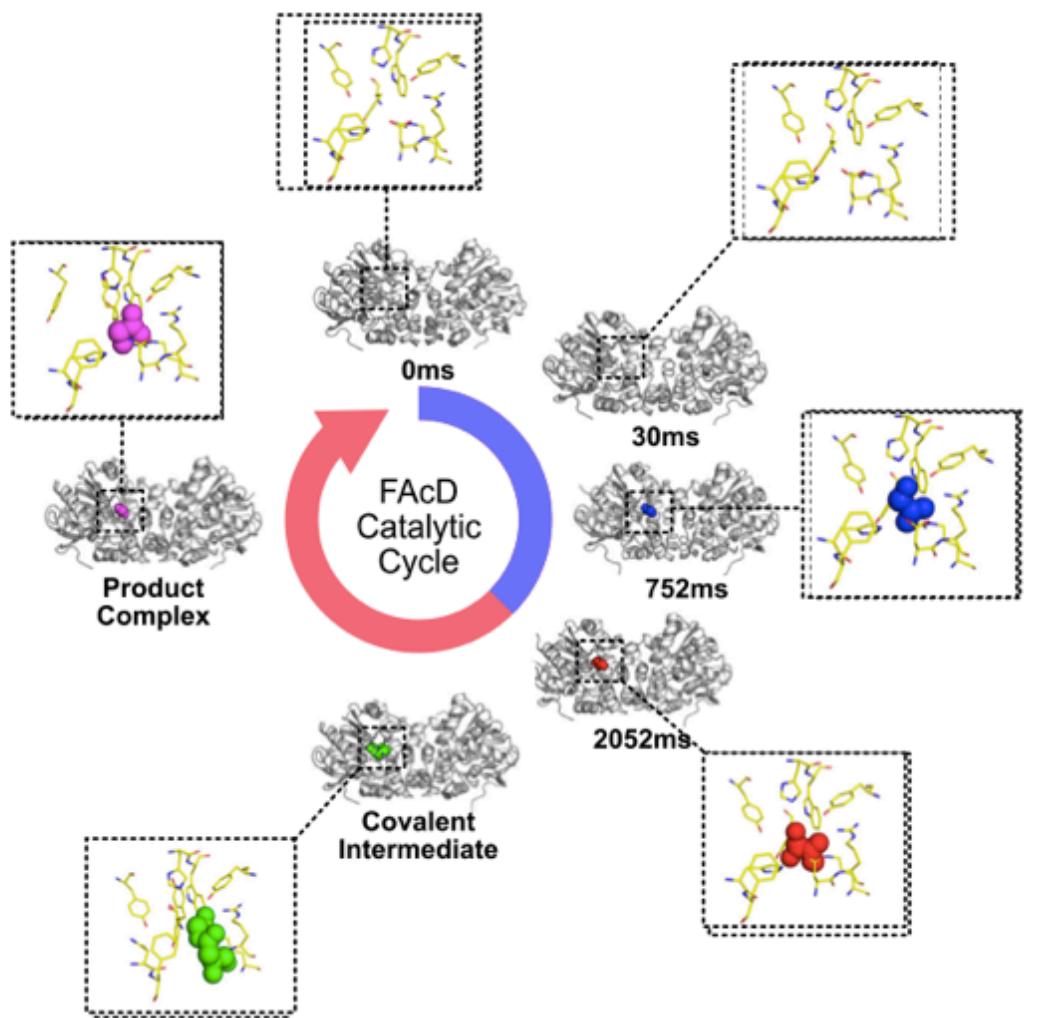


- Laser beam $\odot 50 \mu\text{m}$
- Exposure time 1.3 ms / frame
- Ver. translation 1 $\mu\text{m}/\text{frame}$
- Laser flash at every 30th frame
- Hor. translation 30 $\mu\text{m} / \text{line}$

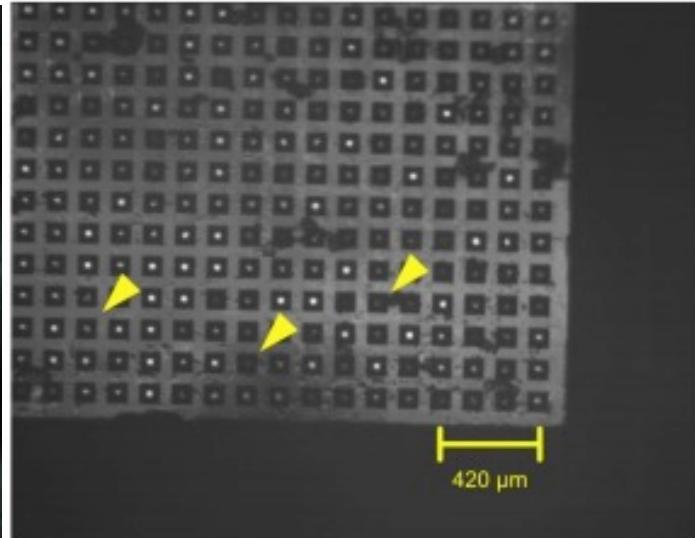
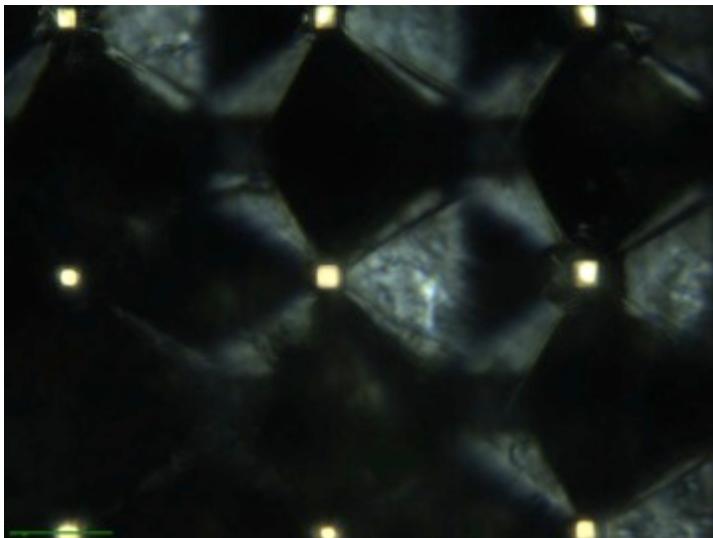
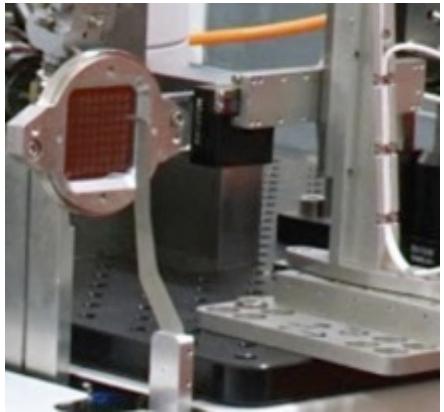
== 30 time points \times 1.3 ms

**10⁶ frames in 3 hours wall clock
~30% hit rate**

Time series: *linear vs logarithmic*



Si chips for sample delivery

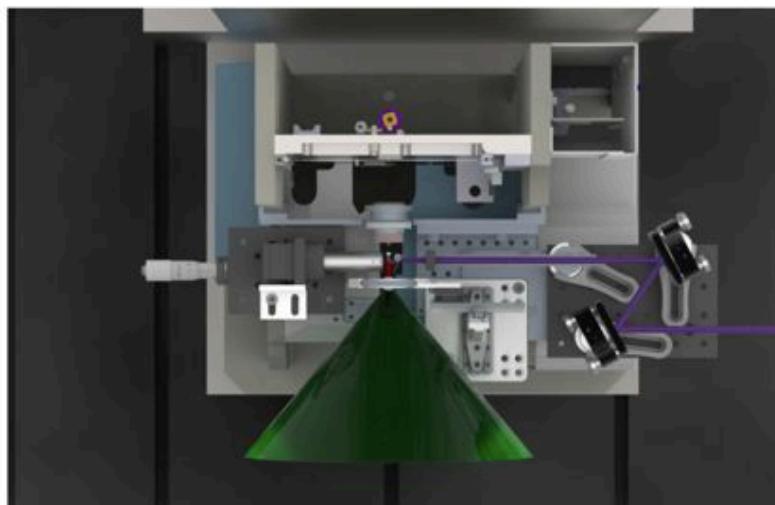
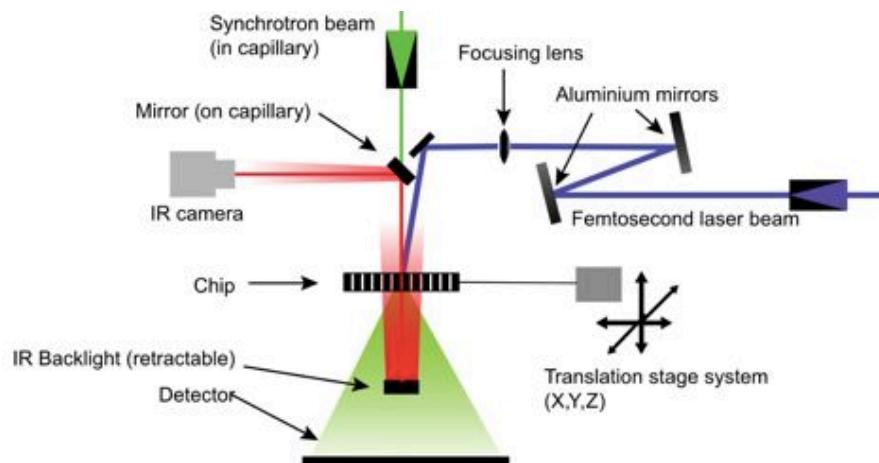


Zarrine-Asfar et al. (2012) Acta Cryst. D
Sherrell et al. (2015) J Synch. Rad.

- 20000-25000 compartments
- 120-150 μm pitch
- 25 Hz re-positioning

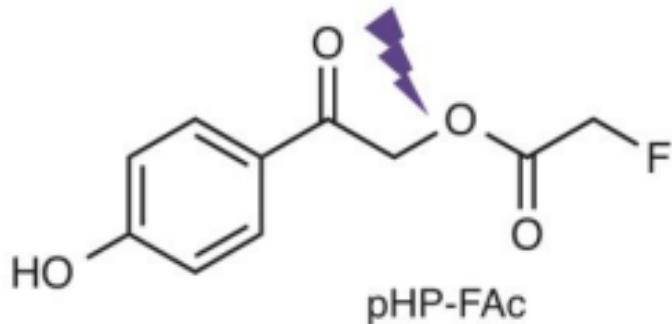
Eike Schulz, Pedram Mehrabi, Rike Müller-Werkmeister, Dwayne Miller,
MPISDM Hamburg

Un-caging experiments at P14.EH1

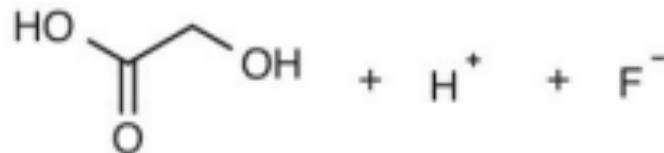
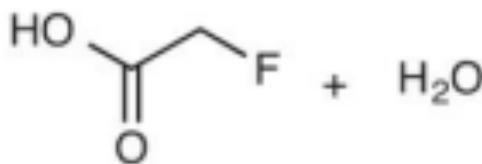


Eike Schulz, Pedram Mehrabi, Rike Müller-Werkmeister, Dwayne Miller,
MPISDM Hamburg

Fluoroacetate dehalogenase substrate un-caging



Pump: 340 nm 45 nJ / 100x100 μm^2
4-15 ms X-ray exposures
20000 frames x 4 time delays in 1 hour
>3.5K diffraction images per time delay
Resolution 1.8 Å

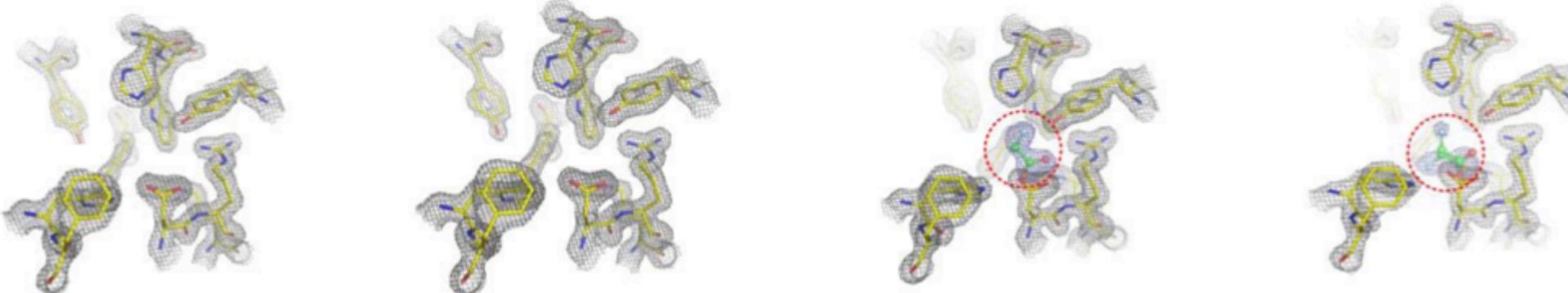


0MS

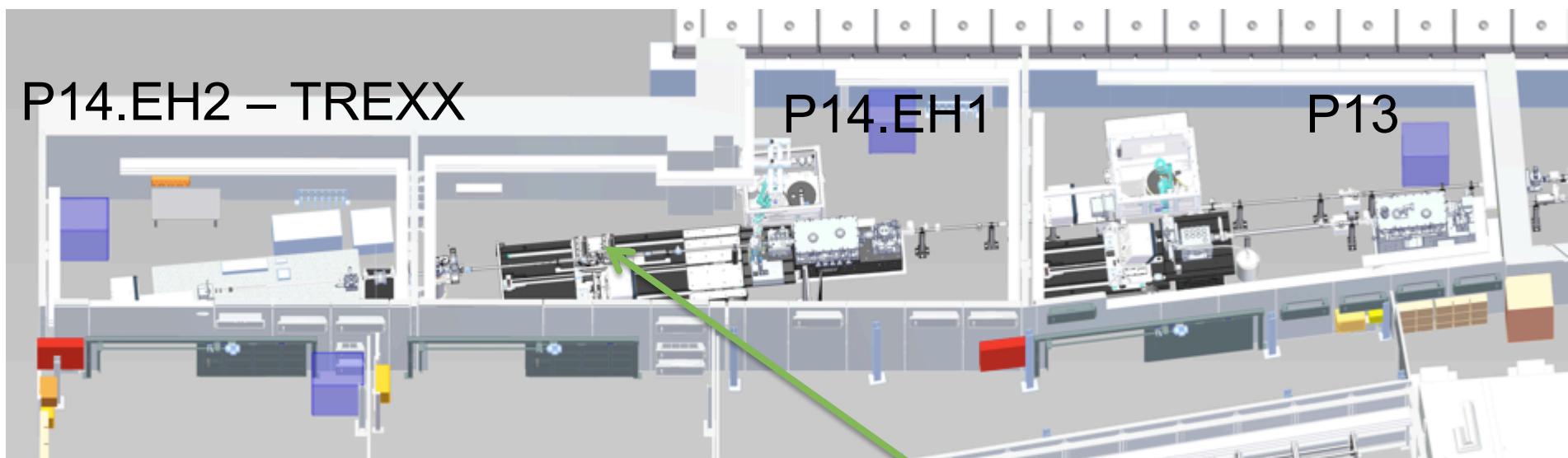
30MS

752MS

2052MS



Dedicated P14 end station for time-resolved MX

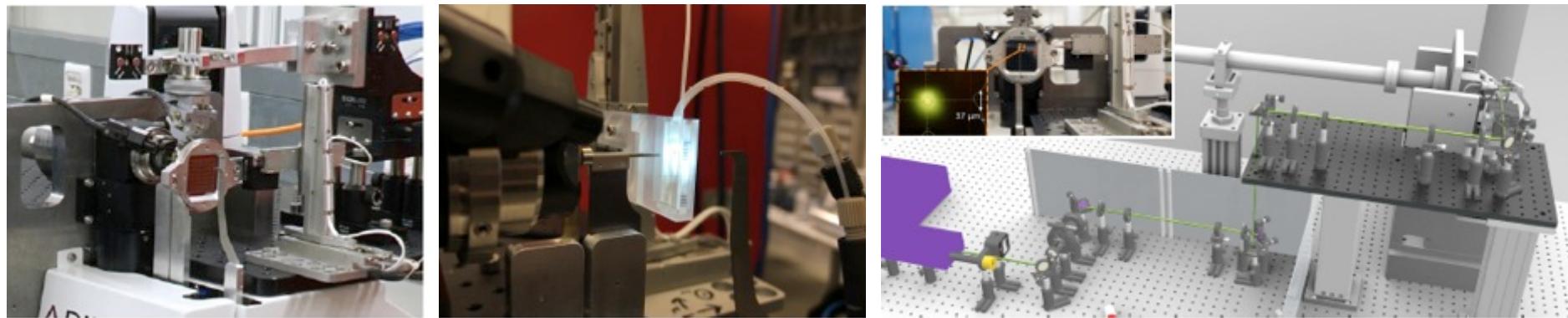
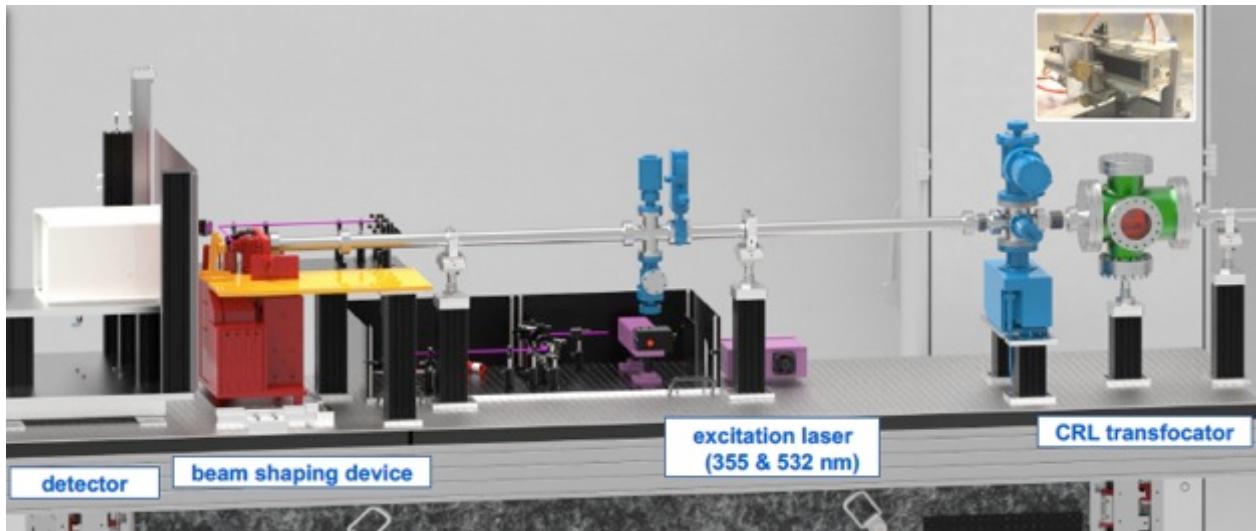


- In operation since 10/2018
- EH1/EH2 switch in 1 hour
- 66 shifts scheduled for 2019
- 1-day allocations



beam transport

TREXX Instrumentation



MXCuBE @ TREXX : data acquisition

Collect Log
Sample centring

Front light: 0.29 Back light: 2.00

Zoom: 100% 200% 500%

Scans: catalase_chip1_532nm_1

Acquisition

Number of triggers: 25600 Images per trigger: 20
Number of images: 512000
Exposure time (s): 0.0014 Detector mode: 0
Energy (keV): 12.6799
Resolution (Å): 1.844
Transmission (%): 100

Data location

Folder: /mnt/beegfs/PE2/2018/11264_206/dvorzettzen/20181025/Raw_DATA/
/catalase_chip1_532nm
File name: catalase_chip1_532nm_1_#####.cbf.gz
Prefix: lase_chip1_532nm
Run number: 1
 Compress data

Processing

No. residues: 200 Space group: P1
Unit cell:
a: 0 b: 0 c: 0
e: 0 f: 0 g: 0
 Run processing after collection
 Run Dozor

ISPyB proposal: mslv0026 - Proposal
Sample tree: Manually mounted
Mode: Manually mounted
Sampler: ISPyB
Centring: Manual 3-click
Filter: No filter

Machine current: 89.3 mA
Machine state: Beamline - Experiments
Front End: Opened
Hutch temperature and humidity: 23.5°C, 23.8%
Disk space: Total: 728.9GB Free: 203.0GB (27%)
Energy: Current: 12.6799 keV Wavelength: 0.9778 Å
Status: Set to: 12.6799 keV Center beam after energy change
Transmission: Current: 100.00 % Set to: 100.00 %
Detector distance: Current: 1.844 Å Set to: 1.844 Å mm
Beamstop distance: Current: 6.00 mm Set to: 6.00 mm

Door interlock: Locked (interlock disabled) Unlock

Safety shutter: in Open Close

Fast shutter: Opened Open Close

Image tracking: tracking Enable Adv. image tracking

Detector status: Frame rate: 331 Hz Exposing
Temperature: 26.1°
Humidity: 2.3%

X: 1198 Y: 1003 Beam size: Horizontal: 15.0 µm Aperture: CRL_eh1 Beam positioning: Manual Set: 0.003

Vertical: 15.0 µm Position: Out Set: 0.003

Phase: PhaseCollection

Heat map:

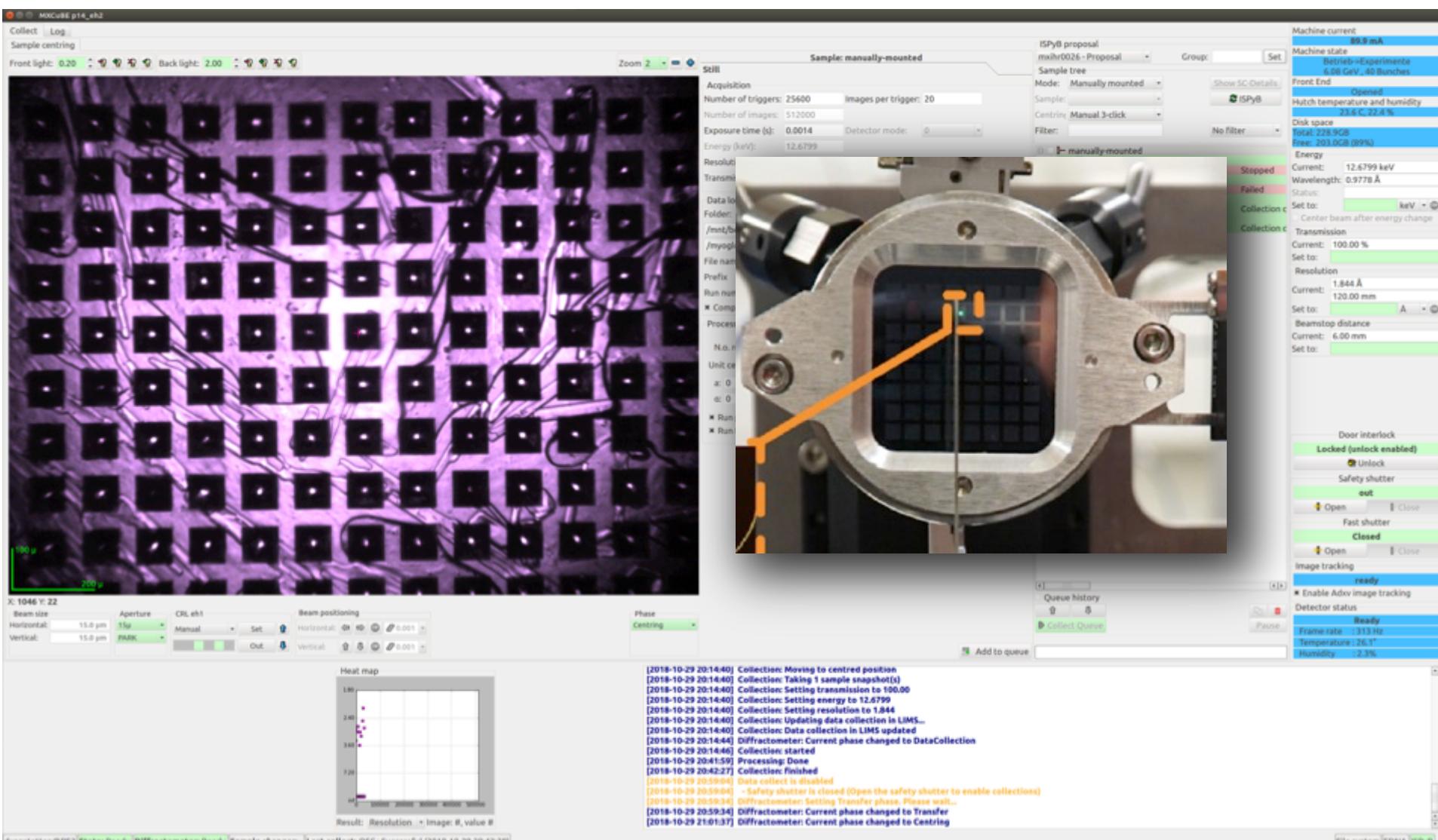
Result: Resolution = Image: 8, value: 8

[2018-10-29 17:35:16] Collection: Preparing to collect
[2018-10-29 17:35:16] Collection: Storing data collection in LIMS
[2018-10-29 17:35:17] Collection: Creating directories for raw images and processing files
[2018-10-29 17:35:17] Collection: Getting sample info from parameters
[2018-10-29 17:35:17] Collection: Starting sample info in LIMS
[2018-10-29 17:35:17] Collection: Moving to centred position
[2018-10-29 17:35:17] Collection: Taking 1 sample snapshot(s)
[2018-10-29 17:35:17] Collection: Setting transmission to 100.00
[2018-10-29 17:35:17] Collection: Setting energy to 12.6799
[2018-10-29 17:35:17] Collection: Setting resolution to 1.844
[2018-10-29 17:35:17] Collection: Updating data collection in LIMS...
[2018-10-29 17:35:17] Collection: Data collection in LIMS updated
[2018-10-29 17:35:18] Detector: Energy change in progress. Please wait...

[2018-10-29 17:35:40] Collection: started

Bvorzettzen@PE2 State: Queue running Diffractometer: Ready Sample changer: Last collect: File system: EDNA ISPyB

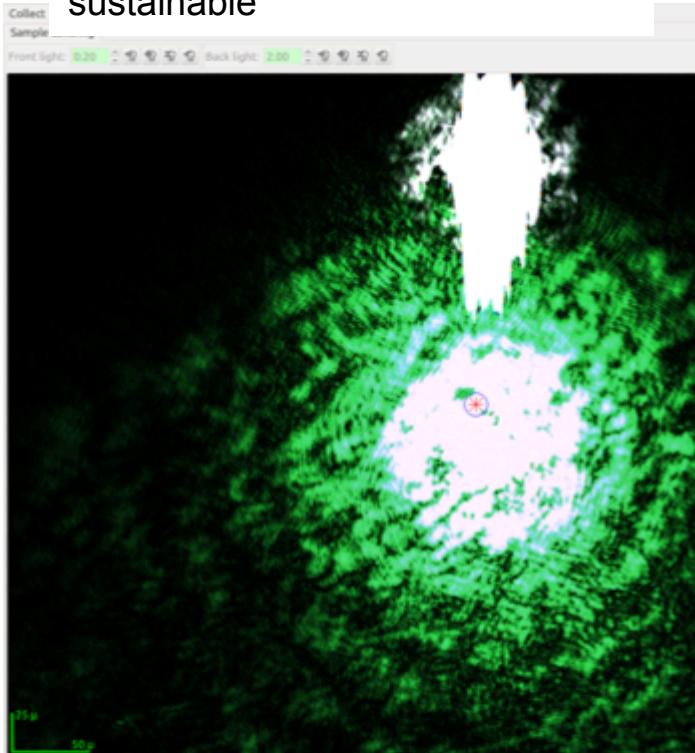
MXCuBE at TREXX : chip centering in IR light (Arinax OAV)



Currently not connected to the chip scanner motors

MXCuBE @ TREXX : data acquisition

Up to 1024000 frames in 35 min
on average 494 fps
sustainable



catalase_chip1_532nm_1

Still

Acquisition

Number of triggers: 25600 Images per trigger: 20

Number of images: 512000

Exposure time (s): 0.0014 Detector mode: 0

Energy (keV): 12.6799

Resolution (Å): 1.844

Transmission (%): 100

Data location

Folder: /mnt/beegfs/PE2/2018/11264_206/dvonstetten/20181029/RAW_DATA /catalase_chip1_532nm

File name: catalase_chip1_532nm_1 #####.cbf.gz [Browse](#)

Prefix: lase_chip1_532nm

Run number: 1

Compress data

Processing

N.o. residues: 200 Space group: [▼](#)

Unit cell:

a: 0 b: 0 c: 0

a: 0 β: 0 γ: 0

Run processing after collection

Run Dozor

Please wait... [2018-10-29 17:35:40] Collection started

Machine

Machine current: 89.3 mA

Machine state: Ready

Berries ->Experiment: 6.0 GeV, 40 Bunches

Front End: Opened

Hutch temperature and humidity: 23.5°C, 23.8%

Disk space: Total: 726.9GB Free: 203.0GB (29%)

Energy: Current: 12.6799 keV Wavelength: 0.9778 Å Status: Set to: 12.6799 keV

463786/512

Center beam after energy change: 1.844 Å

Transmission: Current: 100.00 %

Set to: 100.00 %

Detector distance: Current: 1.844 Å mm

Set to: 120.00 mm

Beamstop distance: Current: 6.00 mm

Set to: 6.00 mm

Door interlock

Locked (interlock disabled) [Unlock](#)

Safety shutter

in [Open](#) [Close](#)

Fast shutter

Opened [Open](#) [Close](#)

Image tracking

tracking [Enable Adv. image tracking](#)

Detector status

Frame rate: 331 Hz Exposing

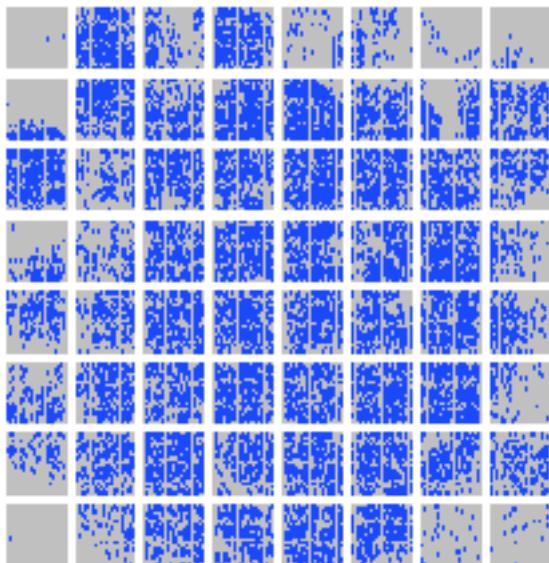
Temperature: 26.1°

Humidity: 2.3%

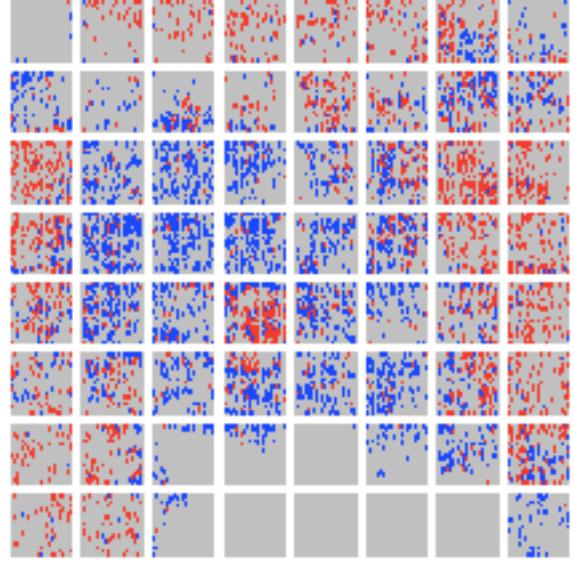
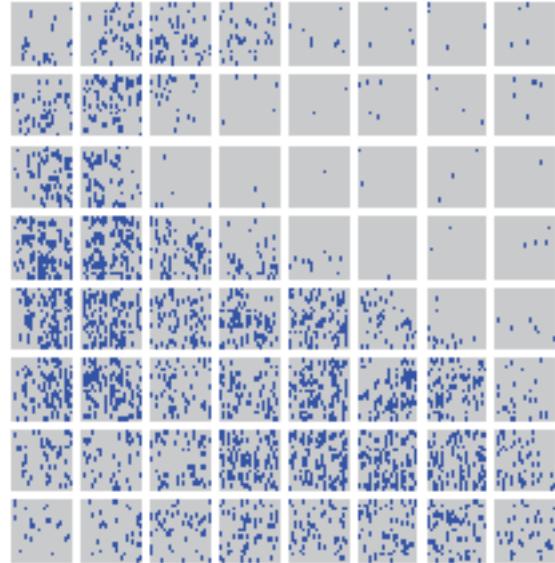
[Pause](#) [Resume](#)

File system: EDNA ISPyB

Hit maps



DOZOR
real time
chip coverage

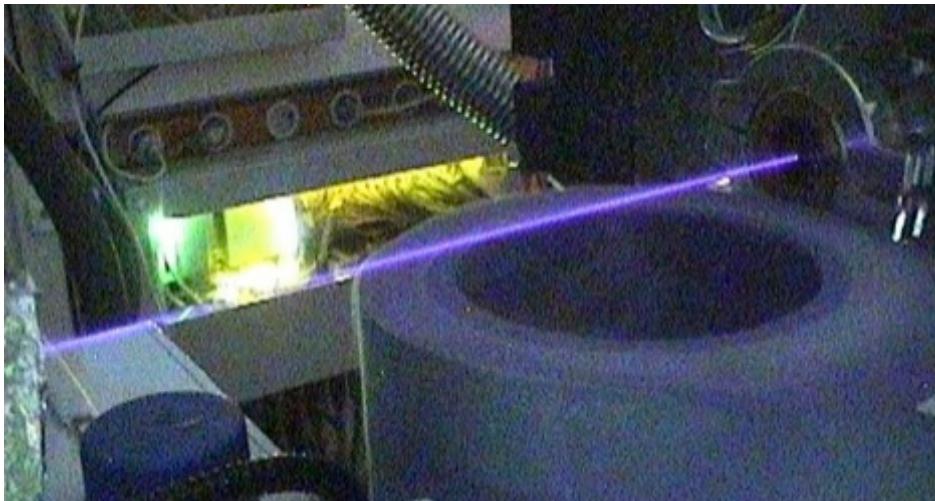


CRYSTFEL
post processing
different unit cells

On going

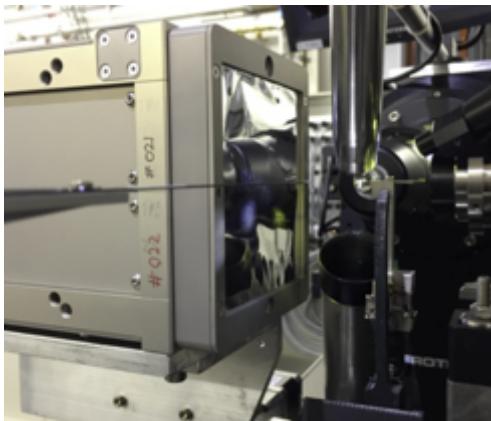
- Chip scanner device server
- Scan trajectory and triggers definition in MXCuBE
- On line auto-processing with
 - EDNA CRYSTFEL plugin
 - EDNA nXDS plugin

Future



Ionized air glow , 4×10^{14} photon/second $\Delta E/E=1.5\%$
with Double SiW multilayer @ P12/PETRAIII
S. Fiedler, EMBL-Hamburg Instrumentation group

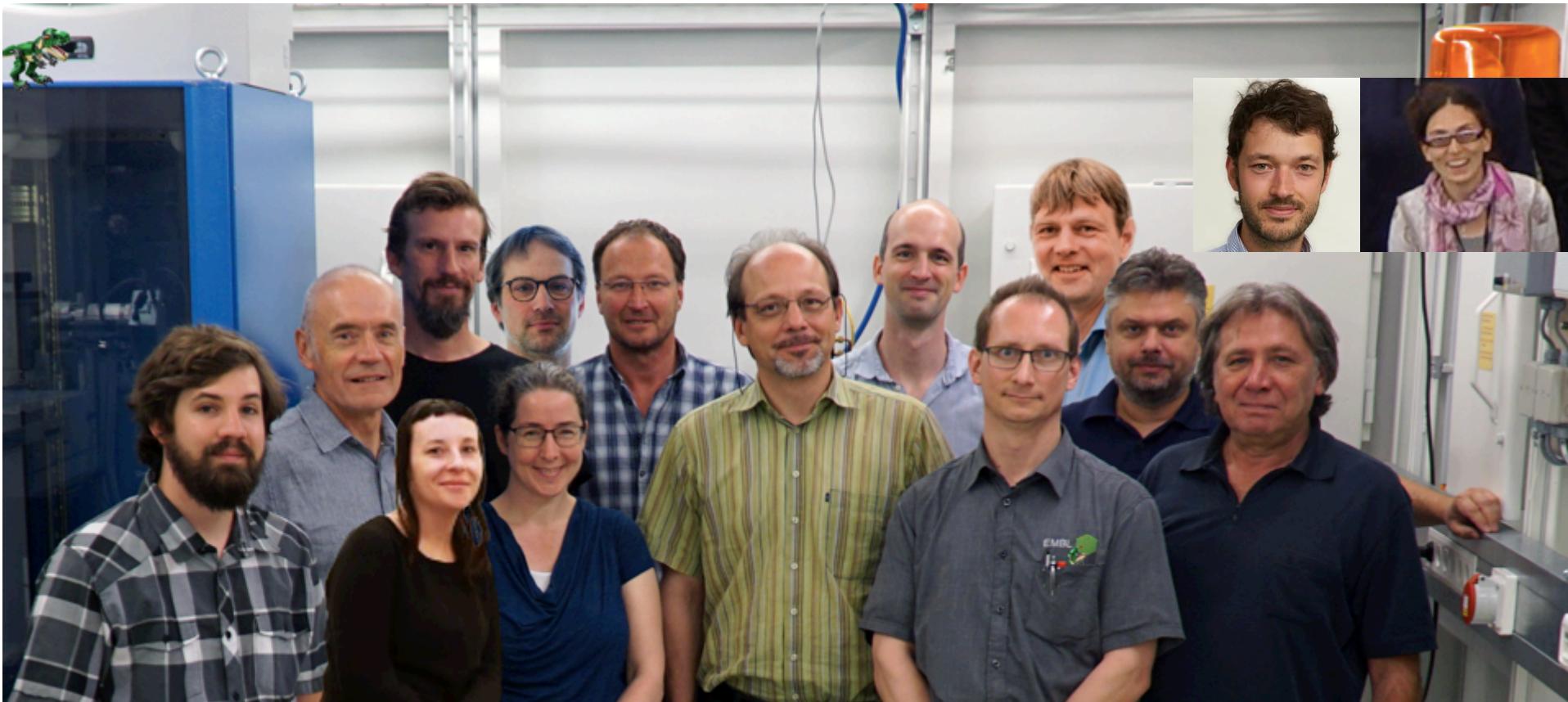
- 100 fold increase in flux with broad energy bandwidth optics
- 150 ps single-bunch exposures will become feasible



JUNGFRAU Detector at SLS

- Integrating pixel-array detectors

Acknowledgements



Michael Agthe¹, David von Stetten², Gleb Bourenkov², Maxim Polikarpov², Sam Horrell¹, Briony A. Yorke¹, Godfrey S. Beddard³, Marina Nikolova², Ivars Karpics², Thomas Gehrmann², Jochen Meyer², Uwe Ristau², Stefan Fiedler², Diana C.F. Monteiro¹, Martin Trebbin⁴, Pedram Mehrabi⁵, Elke-Christian Schulz⁵, Friedjof Tellkamp⁵, Dwayne R. Miller^{5,6}, Nils Huse¹, Arwen R. Pearson¹, and Thomas R. Schneider²

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⁴ University at Buffalo, Buffalo (USA); ⁵ Max Planck Institute for Structure and Dynamics of Matter, Hamburg (Germany); ⁶ University of Toronto, Toronto, (Canada)