

PAUL SCHERRER INSTITUT



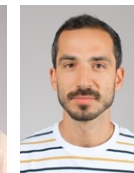
WIR SCHAFFEN WISSEN – HEUTE FÜR MORGEN

Vincent Olieric :: Beamline Scientist :: Paul Scherrer Institut

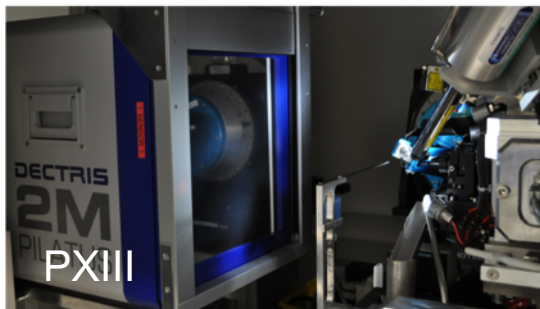
## MX Current Status

Villigen PSI, March 1, 2022

## MX groups @ Photon Science Division

**Meitian Wang****MX application  
group****Katherine  
McAuley****Takashi  
Tomizaki****Vincent  
Olieric****Florian  
Dworkowski****Anuschka  
Pauluhn****John  
Beale****Sylvain  
Aumonier****Michal  
Kepa****MX instrumentation  
group****Wayne  
Glettig****Dominik  
Buntschu****Nathalie  
Meier****Roman  
Schneider****Sonia  
Reber****Tomislav  
Marijolic****MX data  
group****Justyna  
Wojdyla****Kate  
Smith****Ezequiel  
Panepucci****Filip  
Leonarski****Greta  
Assmann****MX sample  
group****May  
Sharpe****Eric  
Plichta****Chia-Ying  
Huang****Deniz  
Eris**

## SLS MX Beamlines



	PXI (X06SA)	PXII (X10SA)	PXIII (X06DA)
Wavelength range [Å]	0.7 - 2.2	0.62 - 2.07	0.71 - 2.07
Source	in-vacuum undulator	in-vacuum undulator	bending magnet
Spectral range [keV]	5.7 - 17.5	6.0 - 20.0	6.0 - 17.5
Flux at 12.4 keV [ph/s]	$> 2 \times 10^{12}$	$> 2 \times 10^{12}$	$5 \times 10^{11}$
Focused spot size $h \times v$ [ $\mu\text{m}^2$ ]	$5 \times 5 (2 \times 1)$ -> $100 \times 100$	$73 \times 16$	$80 \times 45$
Detector	EIGER 16M	EIGER2 16M	PILATUS 2M-F
Frame rates [Hz]	133 750 (4M ROI)	130 500 (4M ROI)	60
Goniometer	multi-axis SmarGon	single-axis	multi-axis PRIGo
Robot & pucks	TELL Unipucks	TELL Unipucks	TELL Unipucks

**Academic** 1000 unique users  
4000 publications  
8000 PDBs

**Industry** 8 beamline partners  
20 regular industry customers

A magnifying glass icon with a yellow handle and a white circular lens, positioned to the left of the first text block.

Automation with TELL

A magnifying glass icon with a yellow handle and a white circular lens, positioned to the left of the second text block.

Unattended data collection

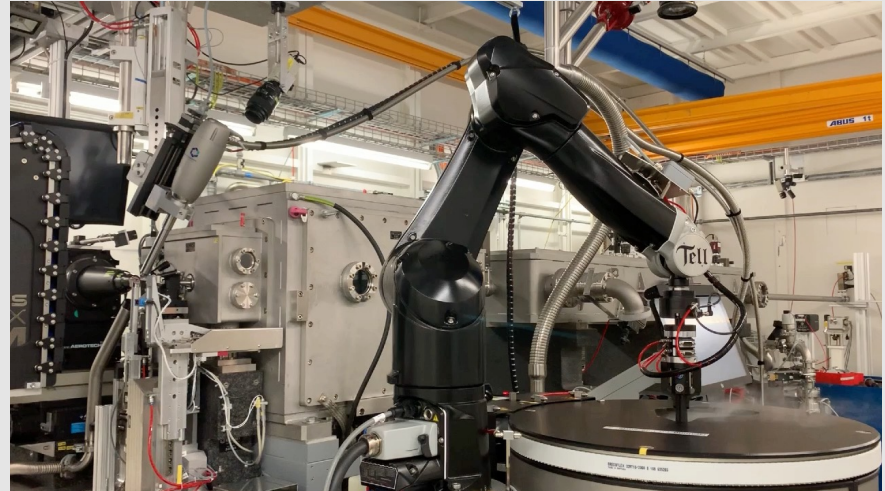
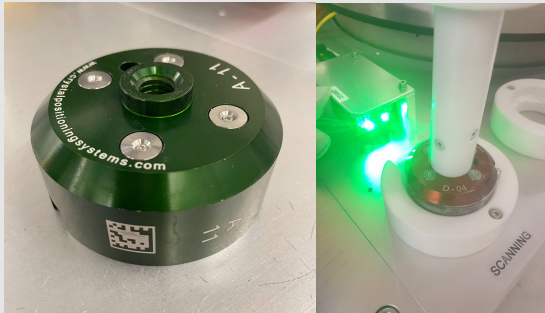
A magnifying glass icon with a yellow handle and a white circular lens, positioned to the left of the third text block.

SmarGon on PXI

A magnifying glass icon with a yellow handle and a white circular lens, positioned to the left of the fourth text block.

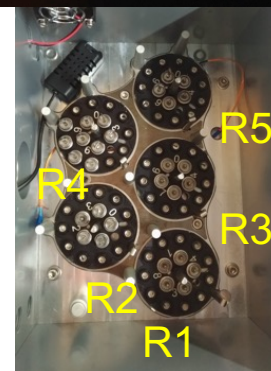
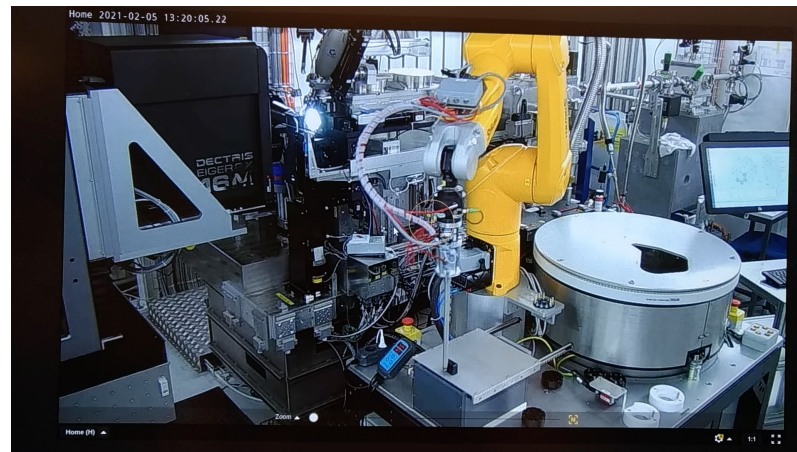
PXIII Upgrade

- TELL robot in operation on all 3 beamlines
- SPINE sample holders and Unipucks
- Puck capacity
  - 30 pucks at PXI and PXII (480 samples)
  - 20 Pucks at PXIII
- Transfer time < 20s
- Puck tracking with barcode reading





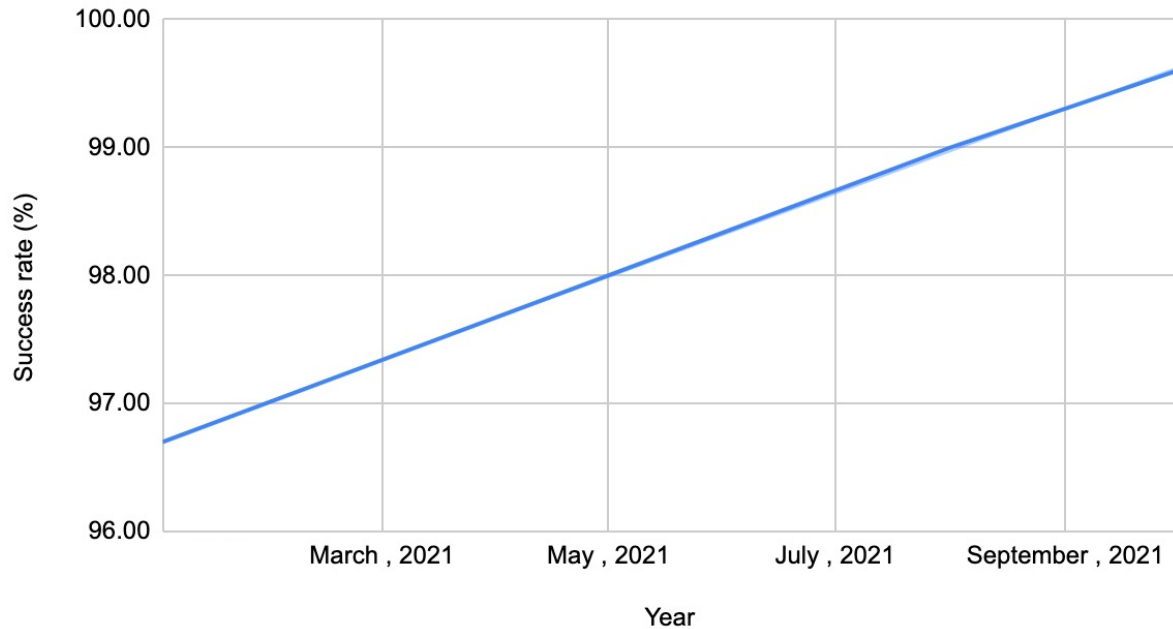
- New “Kraftschluss” gripper with sample detection
- Room temperature setup (at X10SA-PXII)
- Updated sample spreadsheet (V6) for SDU  
<https://www.psi.ch/en/sls/pxiii/sample-changer>



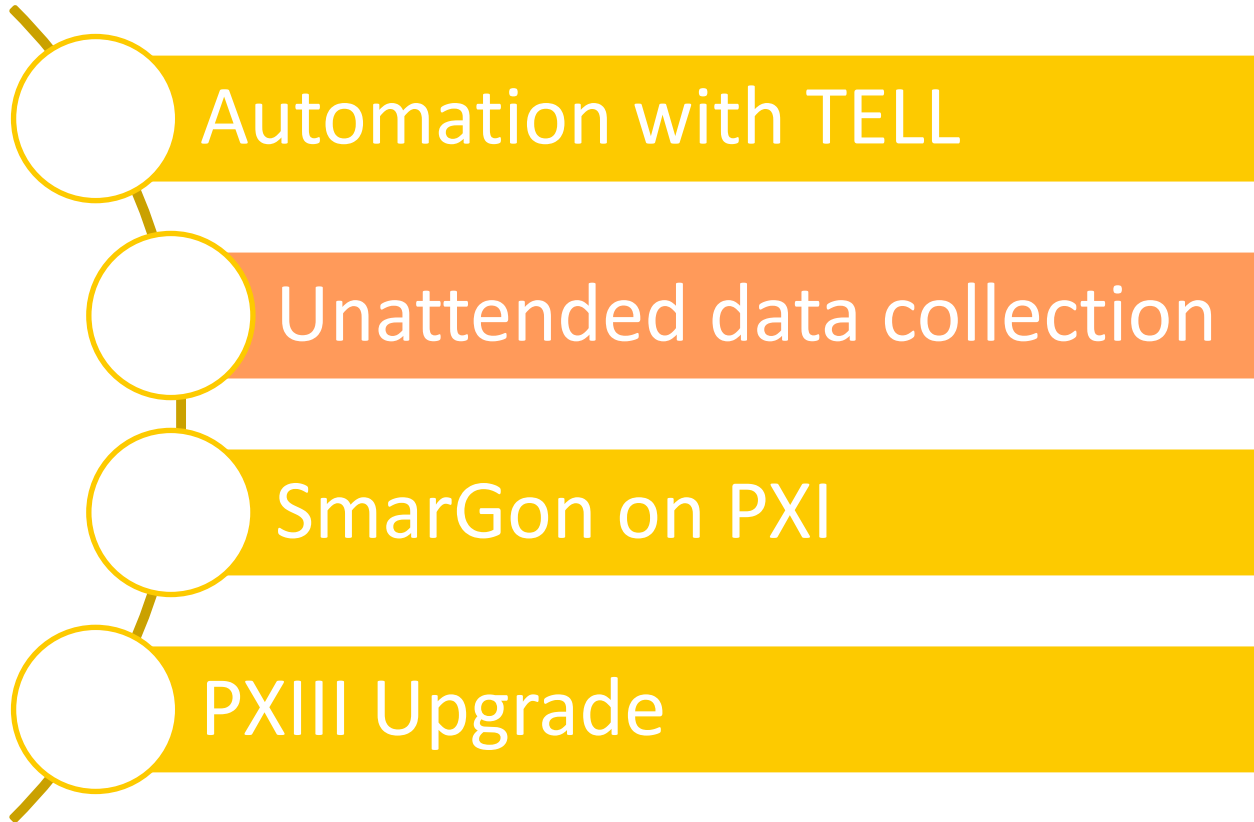
[r]	Data Collection					Automation		Space Group Number [x int]	Cell Parameters [x real number]	Res Cut Key [str]	Res Cut Value [float]	PDB Model [str]
	Oscillation [deg]	Exposure [s]	Total Range [deg]	Transmission [%]	Target Resolution [Å]	Data Collection Type [str]	Processing Pipeline [str]					
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	60	my_lysozyme_model	
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	30	my_lysozyme_model	
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	270	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	360	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	360	20	1.5	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	360	10	2.0	standard	autoproc	89	78 78 60 90 90	cchalf	20	my_lysozyme_model	
0.1	0.02	360	10	2.0	standard	autoproc	89	78 78 60 90 90	is	1.5	my_lysozyme_model	
0.1	0.02	360	10	2.0	standard	autoproc	89	78 78 60 90 90	is	1.5	my_lysozyme_model	
0.1	0.02	360	10	2.0	standard	autoproc	89	78 78 60 90 90	is	2.0	my_lysozyme_model	
0.1	0.02	360	10	2.0	standard	autoproc	89	78 78 60 90 90	is	2.0	my_lysozyme_model	

# TELL gripper

## *Incremental improvement*



- Essential during COVID time (100% remote)
- Essential for unattended data collection





# Unattended data collection

## *Smart Digital User (SDU)*

- **SDU**

- Sample mounting with TELL
- Automatic loop centering with ALC
- X-ray crystal centering (grid scans)
- Automatic data collection (parameters from spreadsheet)
- Automatic data processing

Demo by Kate at 3:35 pm

- Available at all beamlines
- Possible to combine SDU and manual data collection within a shift

# Software infrastructure

## User-driven data collection

DA+ server

Viewer

DA+ GUI

TELL GUI

Tracker

The image displays three main software components:

- DA+ GUI:** A graphical interface for controlling the DA+ server. It features a central 3D model of a crystal, a sidebar with various settings (e.g., Data Collection, Beam Transmission), and a bottom section with a status bar and a table of experimental data.
- Tracker:** A software interface showing a circular detector layout with red spots representing data points. It includes a data table with columns for 'Page', 'Status', and 'Count'.
- DA+ server:** A terminal window showing command-line output, likely representing the server's log or configuration files.

# Software infrastructure

## Automated data collection

DA+ server

Smart  
Digital User

ALC



Viewer

TELL GUI

Tracker

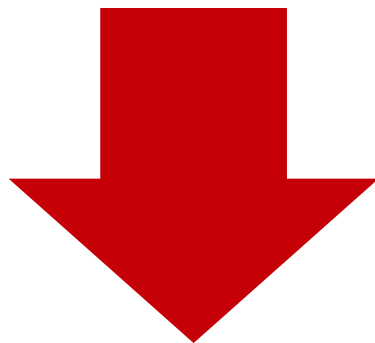
Safety	Mount	ALC	DIR	Center	DAQ	Dewar	Loc.	Puck ID	Sample #
121	AS	AS	AS	AS	AS	AS	AS	CPS-5497	12
122	AS	AS	AS	AS	AS	AS	AS	CPS-5497	14
123	AS	AS	AS	AS	AS	AS	AS	CPS-5497	16
124	AS	AS	AS	AS	AS	AS	AS	CPS-5499	3
125	AS	AS	AS	AS	AS	AS	AS	CPS-5499	5
126	AS	AS	AS	AS	AS	AS	AS	CPS-5499	8
127	AS	AS	AS	AS	AS	AS	AS	CPS-5499	10
128	AS	AS	AS	AS	AS	AS	AS	CPS-5499	12
129	AS	AS	AS	AS	AS	AS	AS	CPS-5499	14
130	AS	AS	AS	AS	AS	AS	AS	CPS-5501	6
131	AS	AS	AS	AS	AS	AS	AS	CPS-5501	7
132	AS	AS	AS	AS	AS	AS	AS	CPS-5501	9
133	AS	AS	AS	AS	AS	AS	AS	CPS-5501	10
134	AS	AS	AS	AS	AS	AS	AS	CPS-5501	11
135	AS	AS	AS	AS	AS	AS	AS	CPS-5501	12
136	AS	AS	AS	AS	AS	AS	AS	CPS-5502	15
137	AS	AS	AS	AS	AS	AS	AS	CPS-5502	16
138	AS	AS	AS	AS	AS	AS	AS	CPS-5103	3
139	AS	AS	AS	AS	AS	AS	AS	CPS-5106	1
140	AS	AS	AS	AS	AS	AS	AS	CPS-5106	2
141	AS	AS	AS	AS	AS	AS	AS	CPS-5106	3
142	AS	AS	AS	AS	AS	AS	AS	CPS-5106	4
143	AS	AS	AS	AS	AS	AS	AS	CPS-5106	5
144	AS	AS	AS	AS	AS	AS	AS	CPS-5125	2
145	AS	AS	AS	AS	AS	AS	AS	CPS-5125	3
146	AS	AS	AS	AS	AS	AS	AS	CPS-5125	5
147	AS	AS	AS	AS	AS	AS	AS	CPS-5125	6
148	AS	AS	AS	AS	AS	AS	AS	CPS-5125	8
149	AS	AS	AS	AS	AS	AS	AS	CPS-5125	10
150	AS	AS	AS	AS	AS	AS	AS	CPS-5125	11

# Unattended data collection

## *Smart Digital User (SDU)*

- Throughput
  - PXI 18-20 samples per hour -> max 140 samples per shift
  - PXIII 10-11 samples per hour -> max 80 samples per shift
- Nearly all FFCS campaign samples measured with SDU
- Close to **7,000** SDU samples up to the end of 2021

# When to try automated data collection?



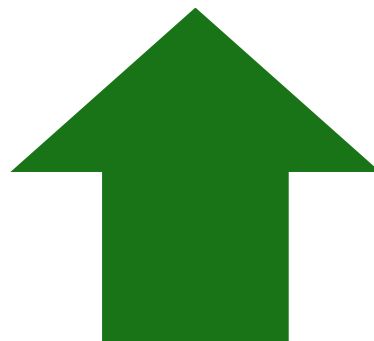
## Don't use SDU if....

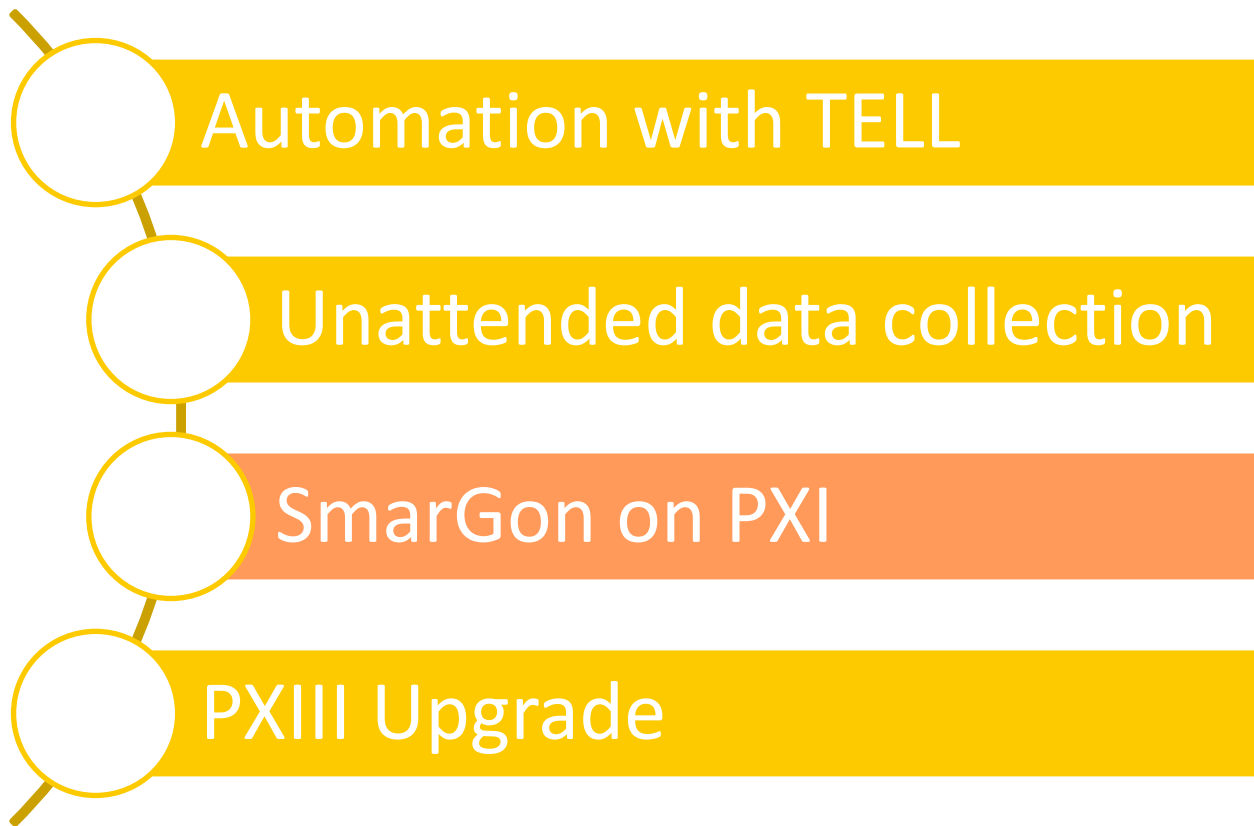
- Pathological crystals, multi-crystal
- Non-standard experiments (e.g., serial, anomalous, RT)



## Do use it if.....

- Single crystals
- Fragment-based approach





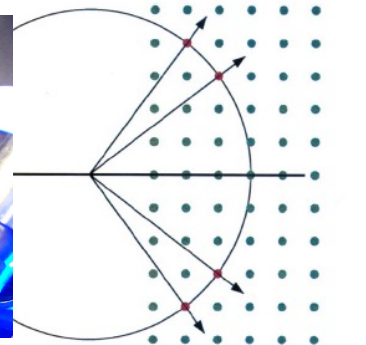
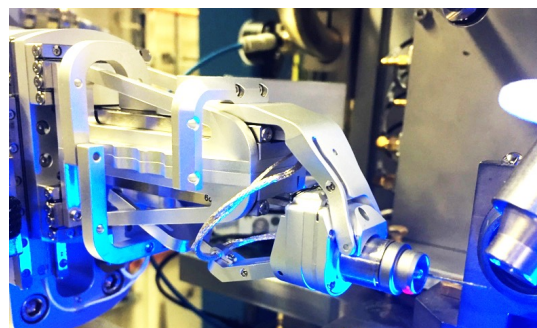
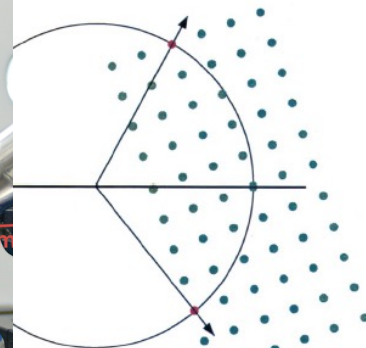
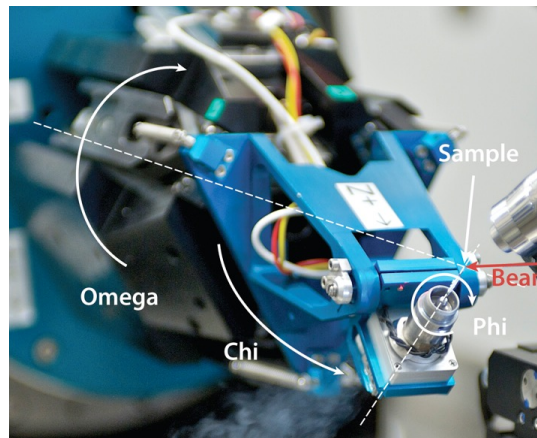


# Multi-Axis Goniometry

*From PRIGo to SmarGon*

- Allows re-orientation of your crystals
- Useful for:
  - Chemical crystallography
  - Low symmetry space-groups
  - Crystals with a large unit cell axis
  - Phasing experiments

*PRIGo at X06DA-PXIII*

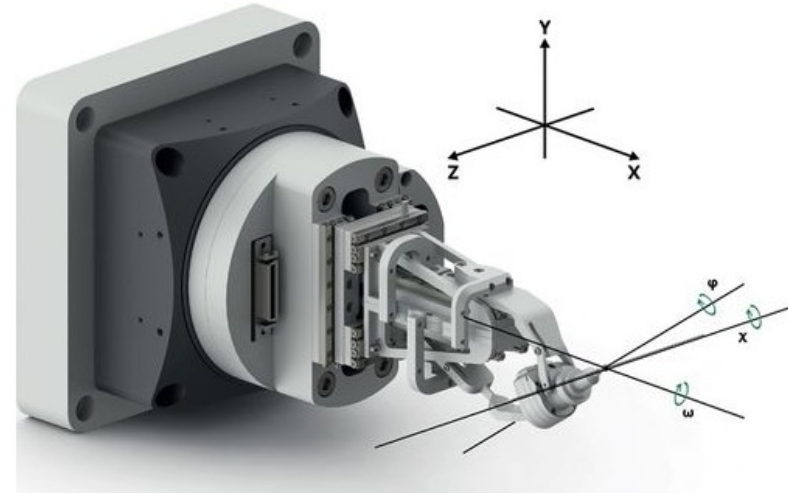


*SmarGon at X06SA-PXI*

# SmarGon-MCS2 at PXI

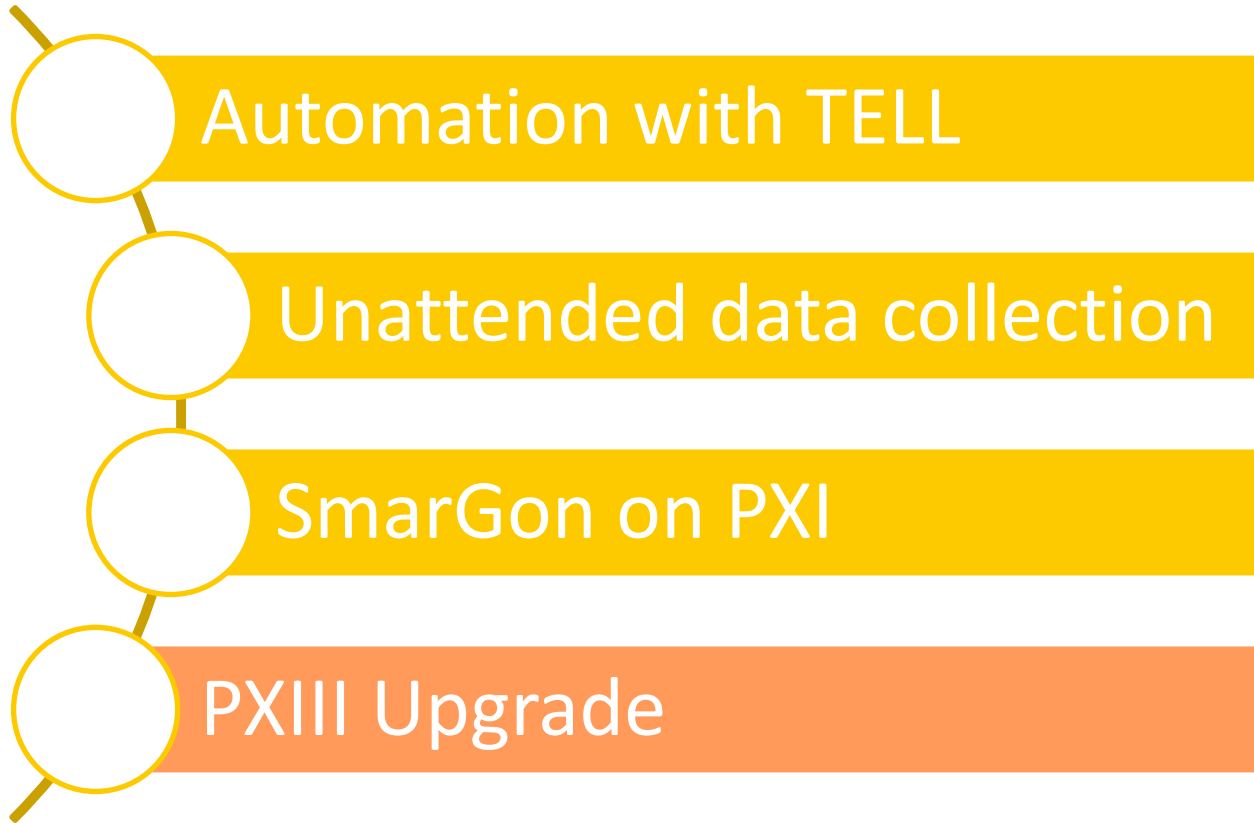
- Installed permanently at PXI since Jan. 2022
- Planned installation on PXII in Aug. 2022

Demo by Zac at 4pm



## SmarGon-MCS2 (in-house) vs. other SmarGons

- Control System changed from PowerPMAC to MCS2 (Smaract Controller)
- New Encoder with distance coded reference marks (initializing position requires only small motions -> probe can stay in cryo-stream)
- Faster encoder read out (allows to apply force on the SmarGon without losing its position -> better tolerance to sample changer kicks)
- Slightly optimized mechanics

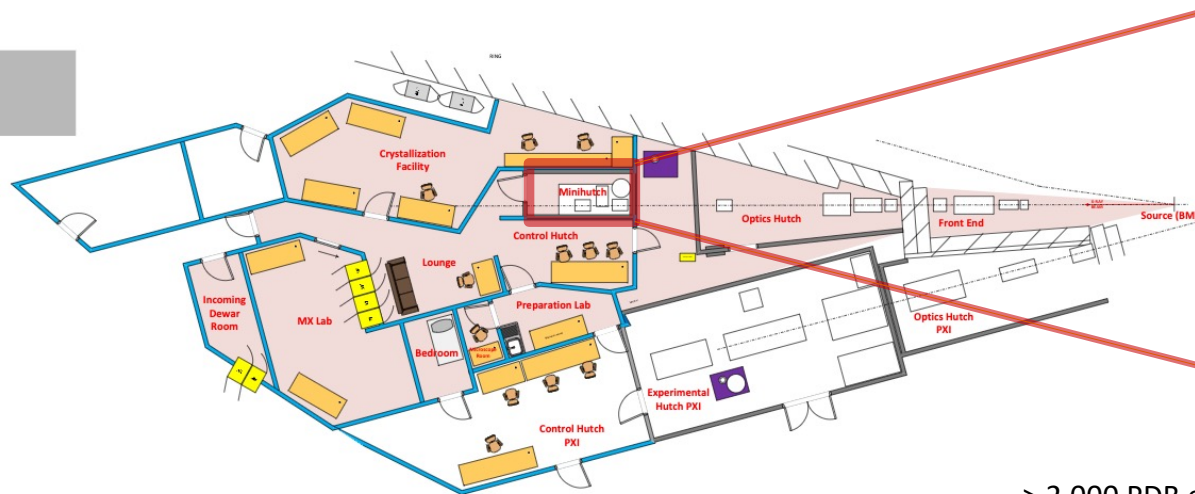




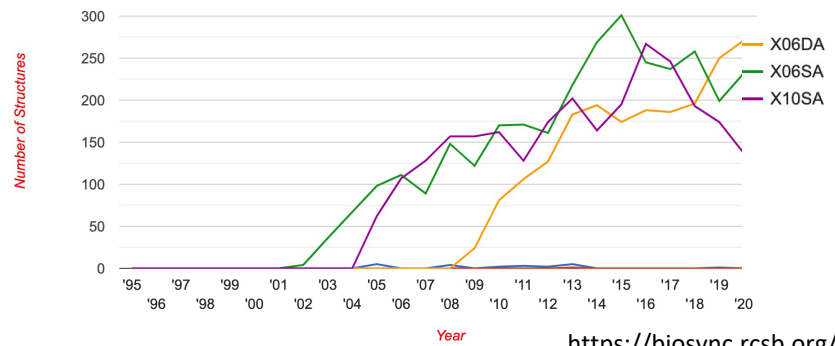
# Xo6DA-PXIII 1.5 Upgrade (before SLS 2.0)

- PXIII will close mid-April 2022 for a major upgrade
- Active proposals will be transferred to PXI (and PXII)
- Next proposal call (deadline April 15) -> X06SA-PXI
  
- Specifications after upgrade
  - 10 um beam size
  - $10^{12}$  ph/s
  - New detector
  
- What changes?
  - New KB Mirrors
  - Upgraded monochromator
  - New hutch
  - Larger end-station (similar to PXI and PXII)

# Xo6DA-PXIII mini-hutch (2007-2022)



> 2,000 PDB entries @ X06DA-PXIII



<https://biosync.rcsb.org/>

## Layout of Xo6SA-PXI and Xo6DA-PXIII after 1.5 upgrade





# Xo6DA-PXIII 1.5 upgrade

## Timeline and planning

	2022				2023				2024				2025				2026					
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4		
PXI	User operation								Upgrade phase I								Upgrade phase II		User operation			
PXII	User operation								Complete upgrade								User operation		User operation			
PXIII	User oper.	Upgrade phase I		User operation		Upgrade phase II								User operation		User operation						

- PXIII pre-upgrade as a testbed for new technology



SLS 2.0 machine upgrade



Pilot users



Second "dark period" for sources and beamlines



**Meitian Wang**

## MX application group



**Katherine McAuley**



**Takashi Tomizaki**



**Vincent Olieric**



**Florian Dworkowski**



**Anuschka Pauluhn**



**John Beale**



**Sylvain Aumonier**



**Michal Kepa**

## MX instrumentation group



**Wayne Glettig**



**Dominik Buntschu**



**Nathalie Meier**



**Roman Schneider**



**Sonia Reber**



**Tomislav Marijolic**

## MX data group



**Justyna Wojdyla**



**Kate Smith**



**Ezequiel Panepucci**



**Filip Leonarski**



**Greta Assmann**

## MX sample group



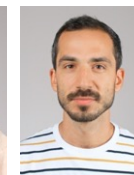
**May Sharpe**



**Eric Plichta**



**Chia-Ying Huang**



**Deniz Eris**

**Users and partners**