PAUL SCHERRER INSTITUT

PSI

Oliver Bunk :: Laboratory for Macromolecules and Bioimaging (LSB) :: Paul Scherrer Institute

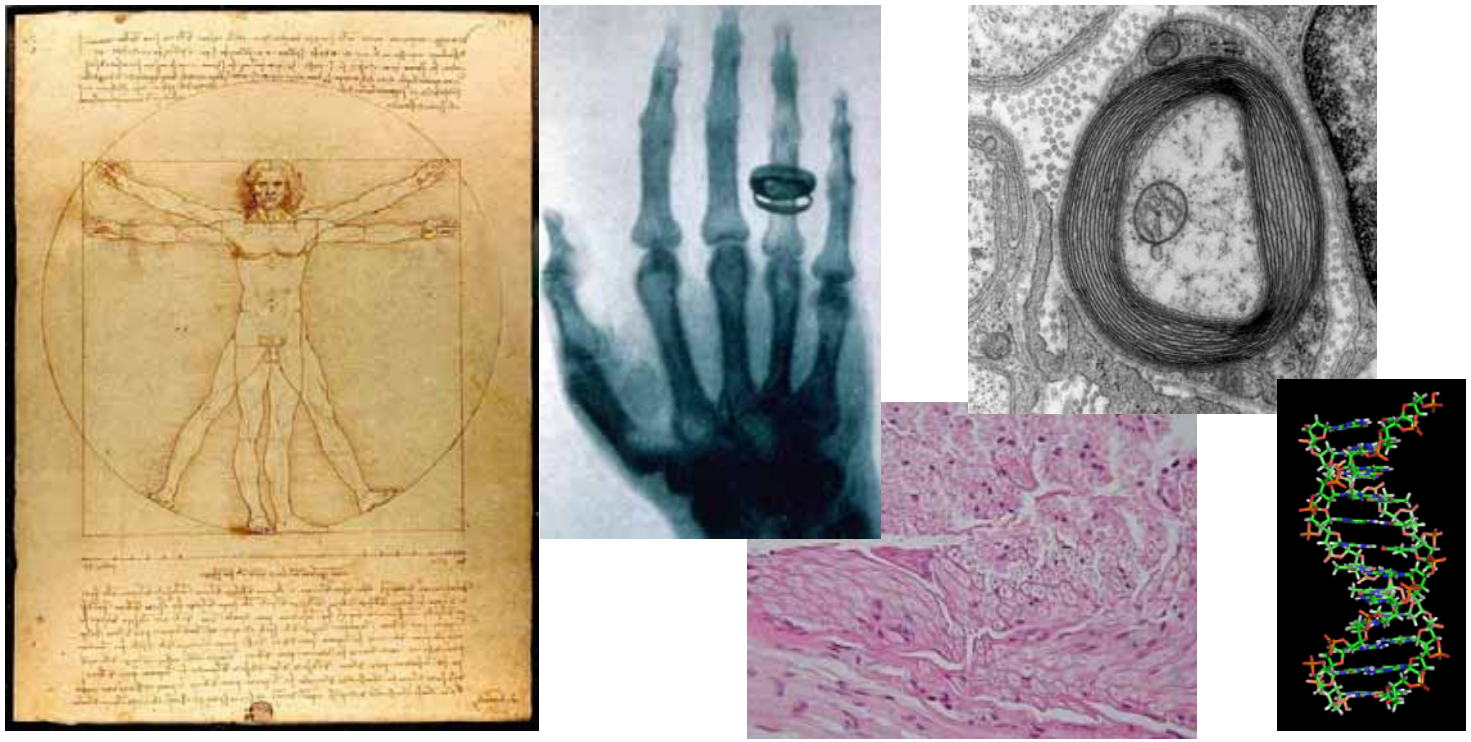
PX I, II, III, S-/I-TOMCAT, cSAXS @ SLS 2.0

Seeing is believing.

Crystallography and imaging in life and materials science at synchrotron radiation facilities

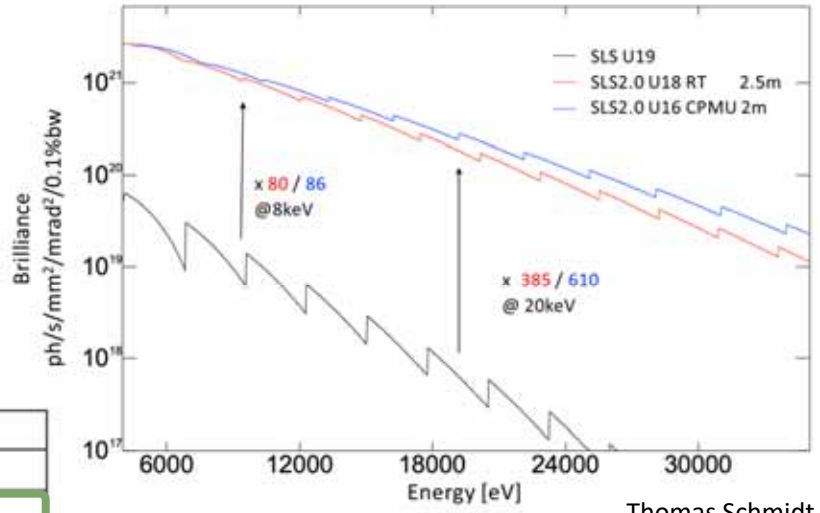
SLS 2.0 upgrade workshop, Feb. 28th 2022

Hierarchically structured materials



(from Wikipedia)

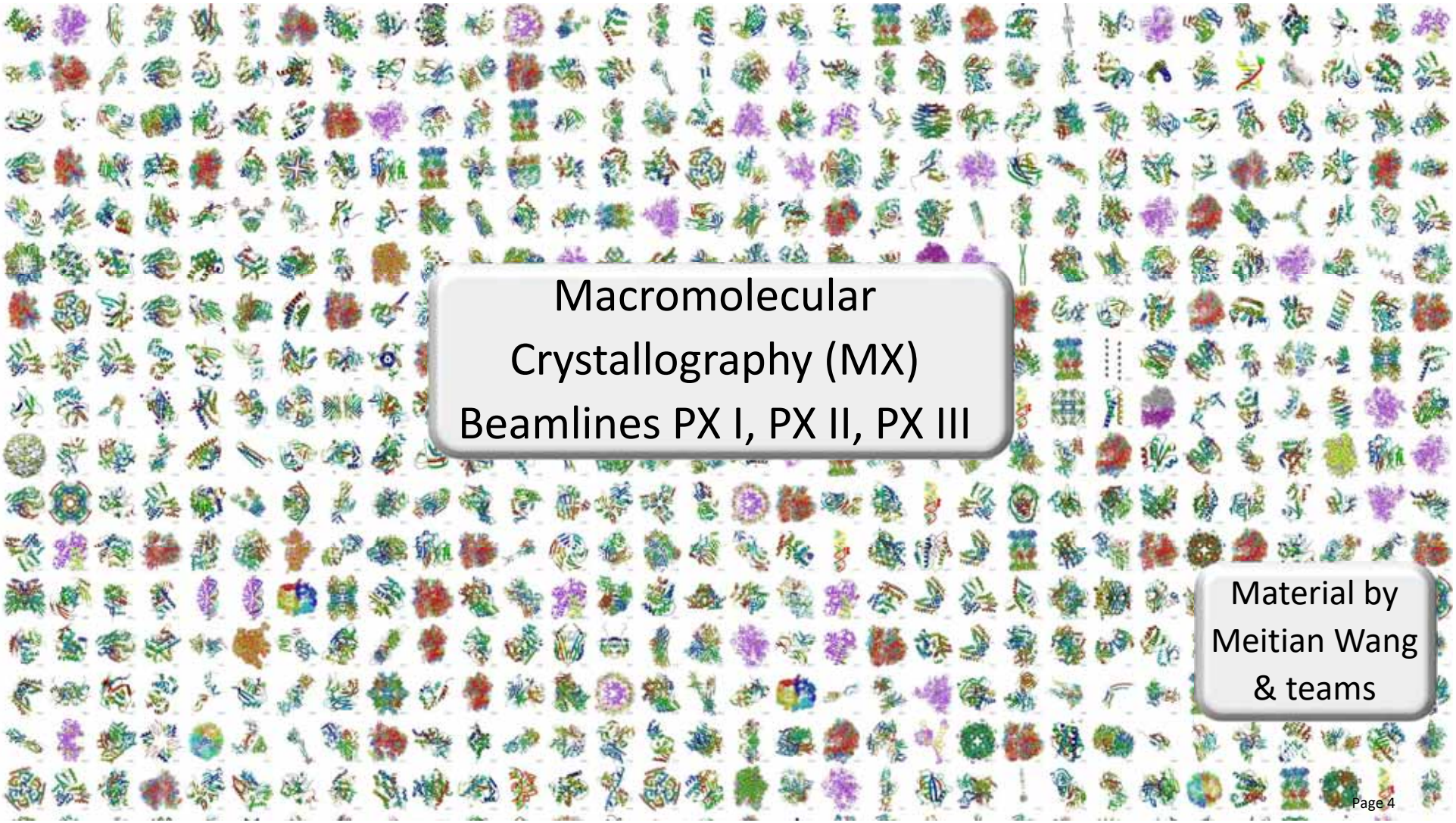
SLS 2.0 is highly benefiting all hard X-ray techniques



Thomas Schmidt, SLS 2.0 beamline CDR advisory committee

	SLS today	**SLS 2.0**
Circumference [m]	288.007'289	288.000'000 → **288.000'222**
Energy [GeV]	2.411	**2.700**
Working point Q_x / Q_y	20.43 / 8.74	**39.37 / 15.22**
Natural chromaticity ξ_x /ξ_y	−67.3 / −21.0	**−99.0 / −33.4**
Emittance [pm.rad]	5630	149 → **157** → 136
Energy spread [10^{-3}]	0.878	1.103 → **1.147** → 1.038
Radiation loss per turn [keV/turn]	549	666 → **689** → 892
Momentum compaction factor [10^{-4}]	+6.04	+1.06 → **+1.04** → +1.04
Horizontal damping partition Jx	1.00	1.85 → **1.82** → 1.64
Damping times [ms]		4.2/7.8/6.8 → **4.1/7.5/6.4** → 3.6/5.8/4.3

Andreas Streun, SLS 2.0 Baseline Lattice, SLS2-SA81-004-14 (1.9.2020)

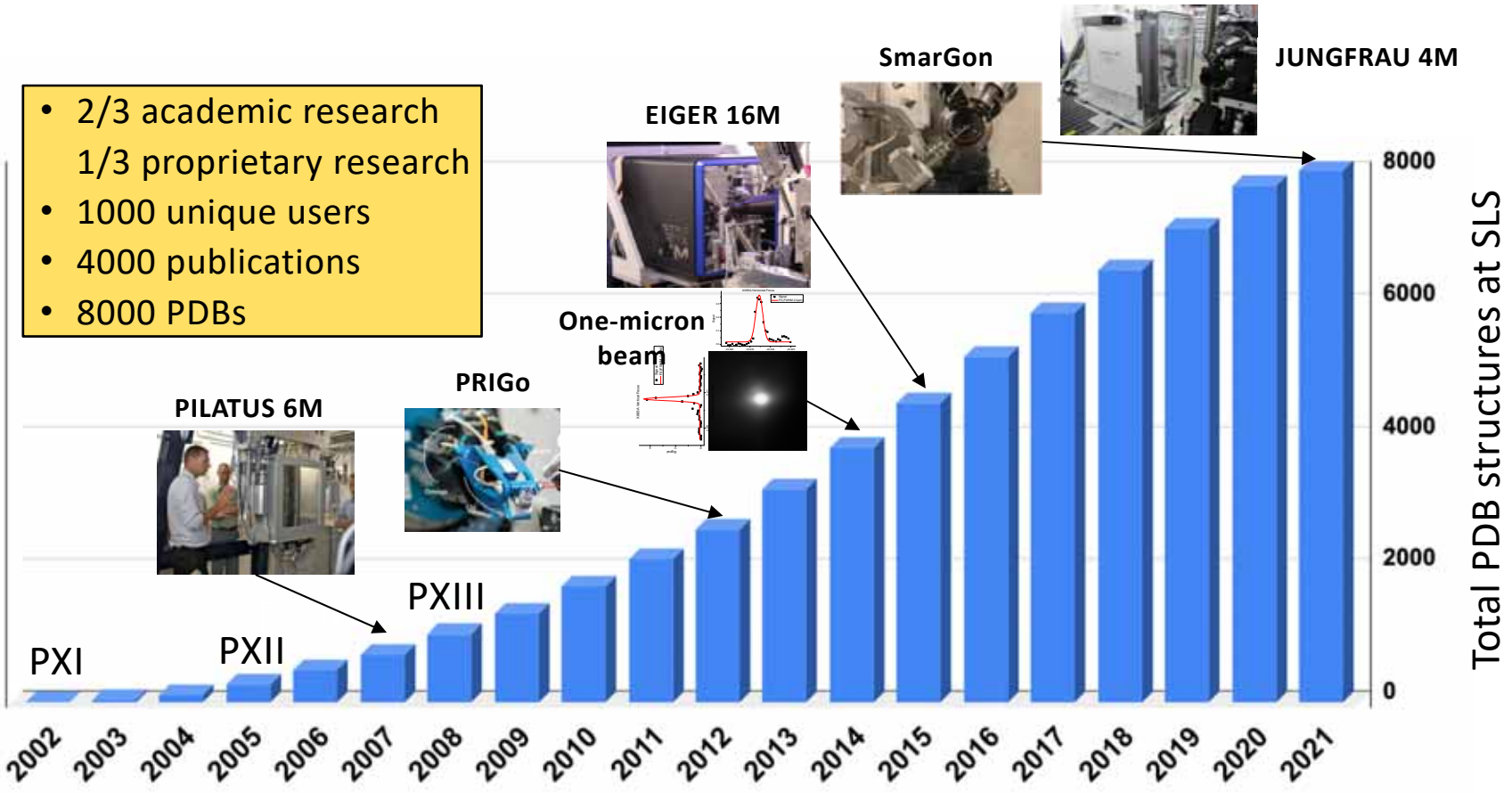


Macromolecular Crystallography (MX) Beamlines PX I, PX II, PX III

Material by Meitian Wang & teams

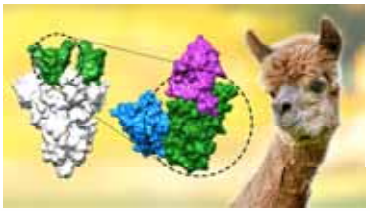
SLS MX Beamlines: 20 years

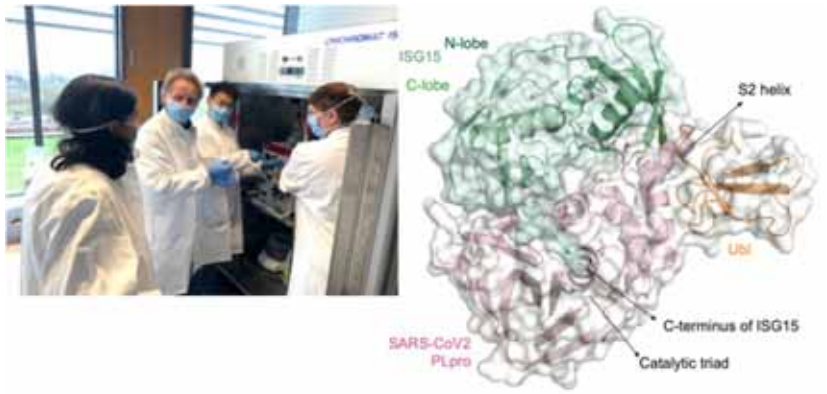
- 2/3 academic research
  1/3 proprietary research
- 1000 unique users
- 4000 publications
- 8000 PDBs



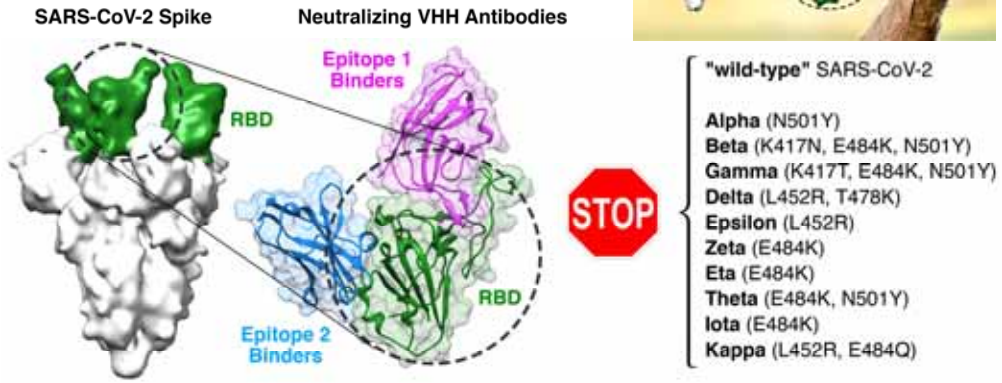
COVID-19, and COVID-19 related research

- Continuous user operation through the pandemic
- 100% remote mode since 2020
- > 50’000 sample mounts in 2021
- SLS Special call for COVID-19 research





Papain-like protease regulates SARS-CoV-2 viral spread and innate immunity.
Ivan Dikic / University Frankfurt, ***Nature*** (2020)
Four months from X-ray data collection to publication



Nanobodies (blue and magenta) bind to the receptor-binding domain (green) of the coronavirus spike protein (grey), thus preventing infection with SARS-CoV-2 and its variants.
Thomas Güttler / MPI for Biophysical Chemistry, ***EMBO J*** (2021)

Positioning MX on the international landscape

https://www.epfl.ch/labs/lbem/instruments/

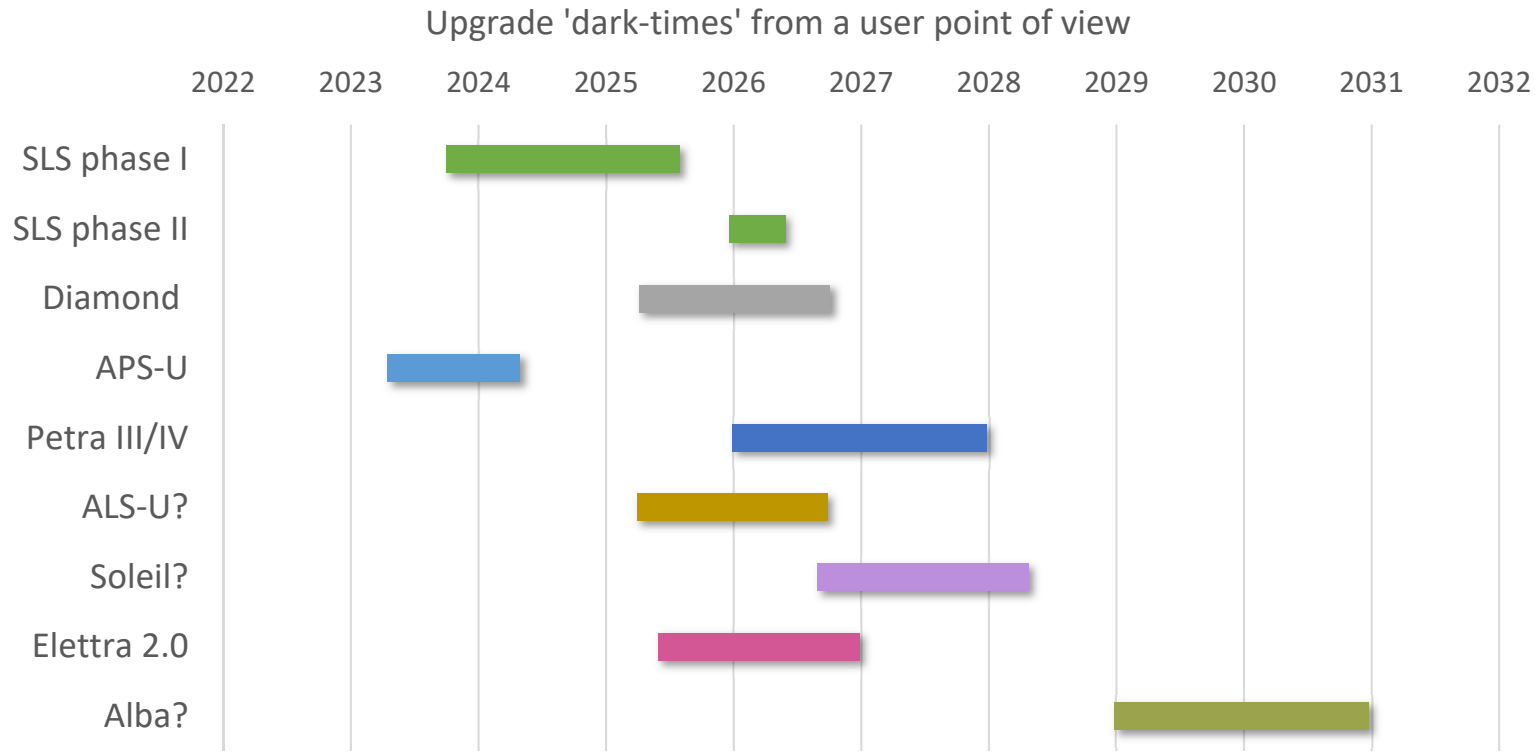
PX I beamline at the SLS (PSI).

Rules of thumb:

- Ribosome Nobel Prize would be based on cryo EM data nowadays.
- The phase problem is solved.
- **MX excels at high spatial and time resolution in combination with high throughput.**

https://alphafold.ebi.ac.uk/

Dark-times from a user point of view



MX Team @ SLS

Meitian Wang

MX application group

Katherine McAuley

Takashi Tomizaki

Florian Dworkowski

Anuschka Pauluhn

Sylvain Aumonier

Vincent Olieric

John Beale

MX instrumentation group

Wayne Glettig

Dominik Buntschu

Nathalie Meier

Roman Schneider

Sonia Reber

Tomislav Marijolovic

MX data group

Justyna Wojdyla

Kate Smith

Ezequiel Panepucci

Filip Leonarski

Greta Assmann

MX sample group

May Sharpe

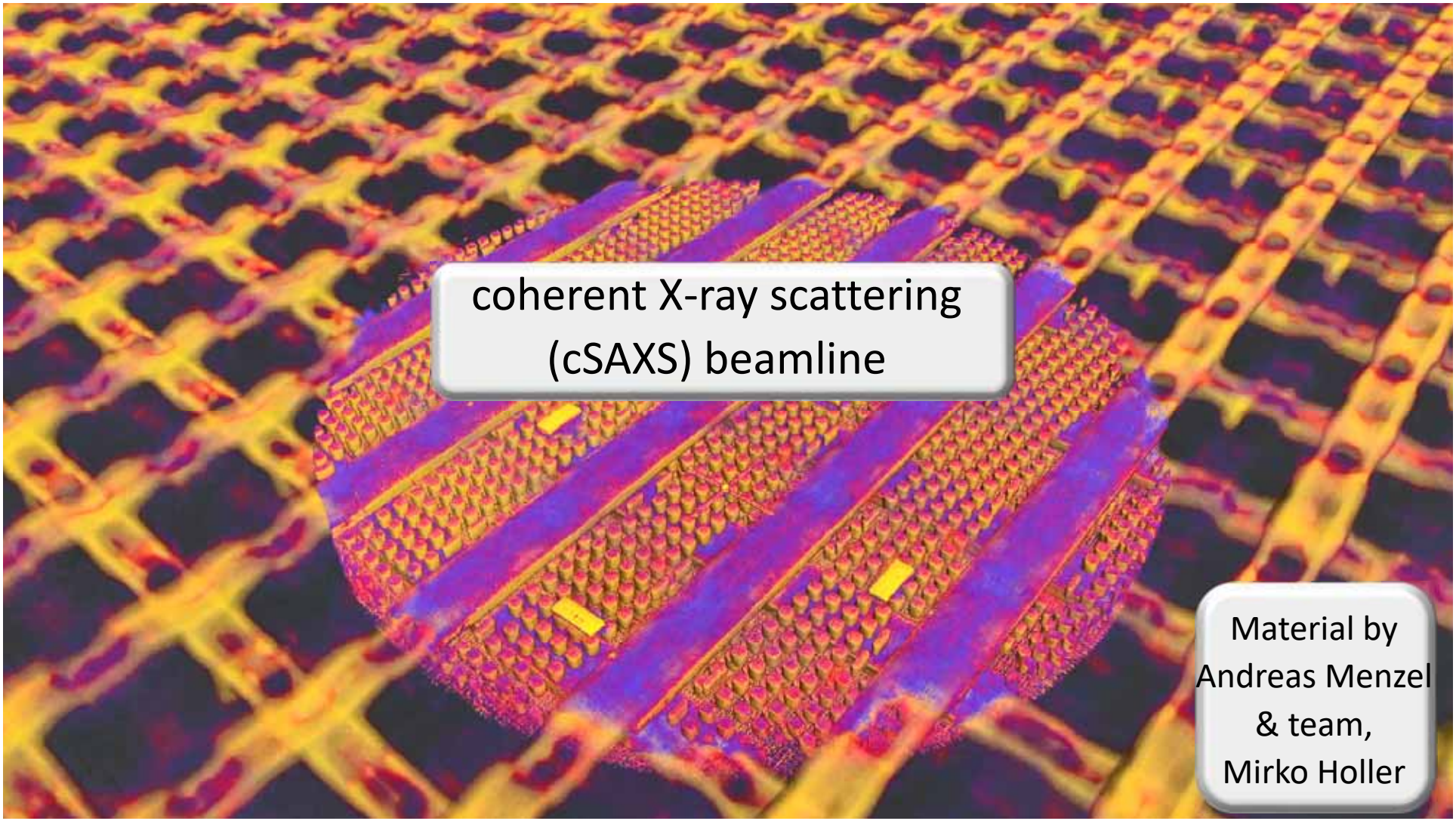
Eric Plichta

Chia-Ying Huang

Deniz Eris

X-ray imaging
Beamlines cSAXS,
S-TOMCAT, I-TOMCAT

Nick Veasey, 1971 California Bug (May 2015)


coherent X-ray scattering
(cSAXS) beamline
Material by
Andreas Menzel
& team,
Mirko Holler

Main Activities at cSAXS

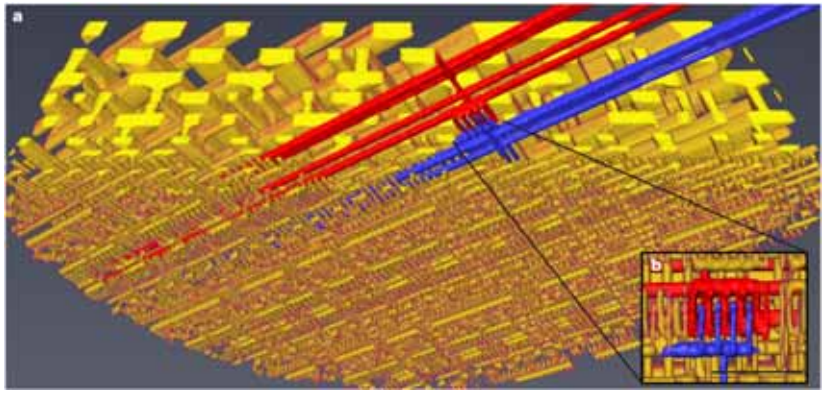
High-Resolution Imaging
Ptychography

LETTER

doi:10.1038/nature21698

High-resolution non-destructive three-dimensional imaging of integrated circuits

Mirko Holler[1], Manuel Guizar-Sicairos[2], Esther H. R. Tsai[1], Roberto Dinapoli[1], Elisabeth Müller[1], Oliver Bunk[1], Jörg Raabe[2] & Gabriel Aeppli[1,2,3]



Holler *et al.,* Nature **543**, 402 (2017)

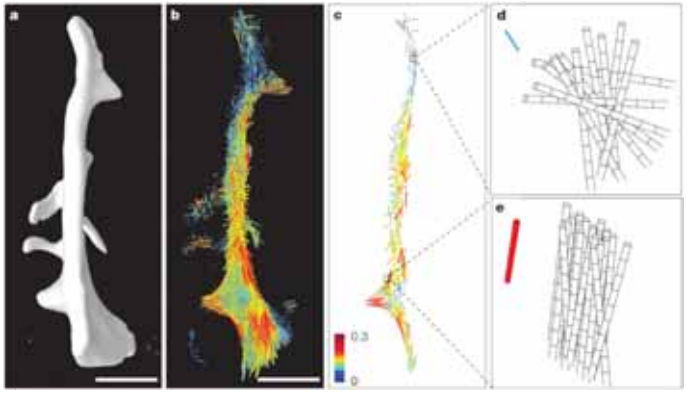
SAXS Imaging, Tomography,
and other High-Brilliance Applications

LETTER

doi:10.1038/nature16056

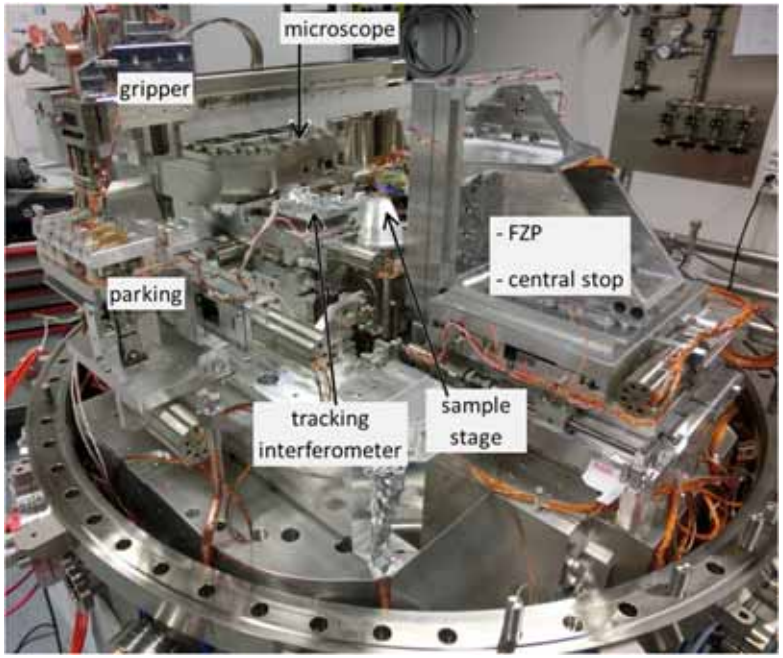
Nanostructure surveys of macroscopic specimens by small-angle scattering tensor tomography

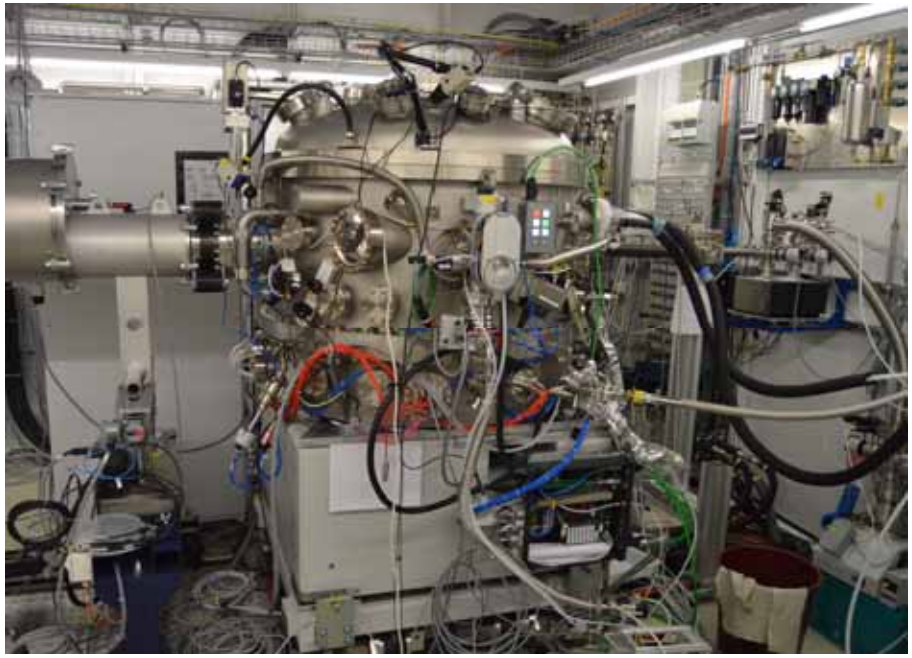
Marianne Liebi[1], Marios Georgiadis[2], Andreas Menzel[3], Philipp Schneider[4], Joachim Kohlbrecher[5], Oliver Bunk[1] & Manuel Guizar-Sicairos[1]



Liebi *et al.,* Nature **527**, 349 (2015)

Unique instrumentation for ptychographic tomography under cryo conditions

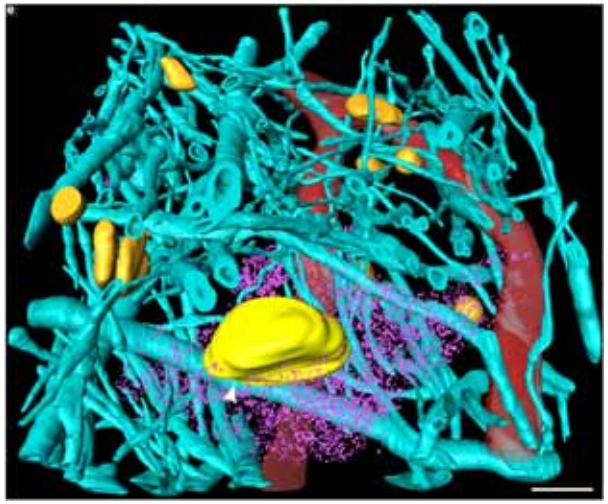




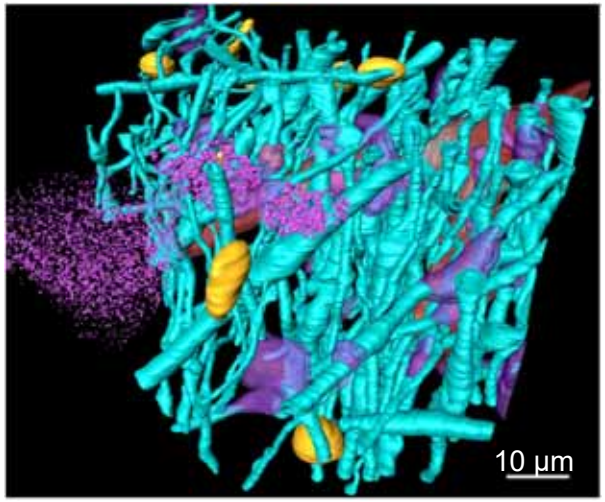
OMNY: Ptychographic nano-tomography for samples under cryo conditions.

Mirko Holler et al., Rev. Sci. Instrum. 83, 073703 (2012). DOI: 10.1063/1.4737624
Mirko Holler and Jörg Raabe, Opt. Eng. 54, 054101 (2015). DOI: 10.1117/1.OE.54.5.054101
Mirko Holler et al., Rev. Sci. Instrum. 89, 043706 (2018). DOI: 10.1063/1.5020247

Human brain tissue



5 specimens imaged from a healthy individual as control



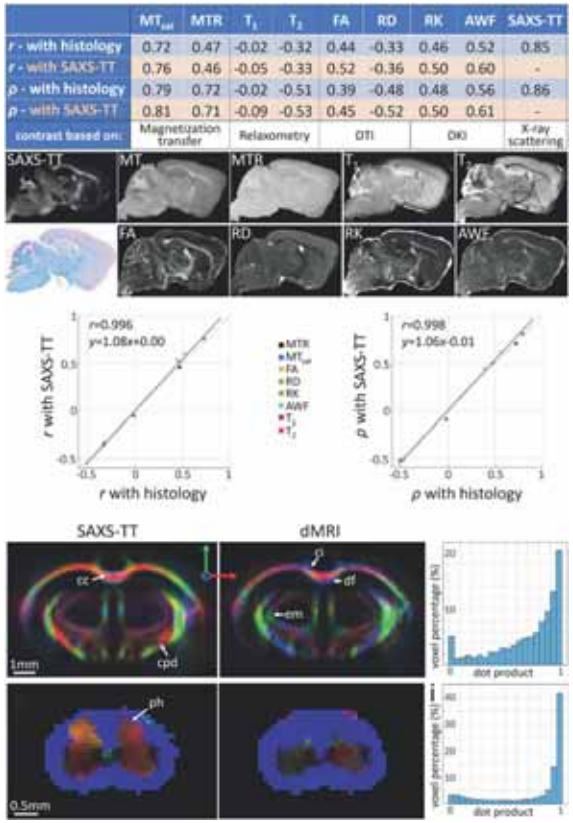
4 specimens imaged from a Parkinson-affected individual

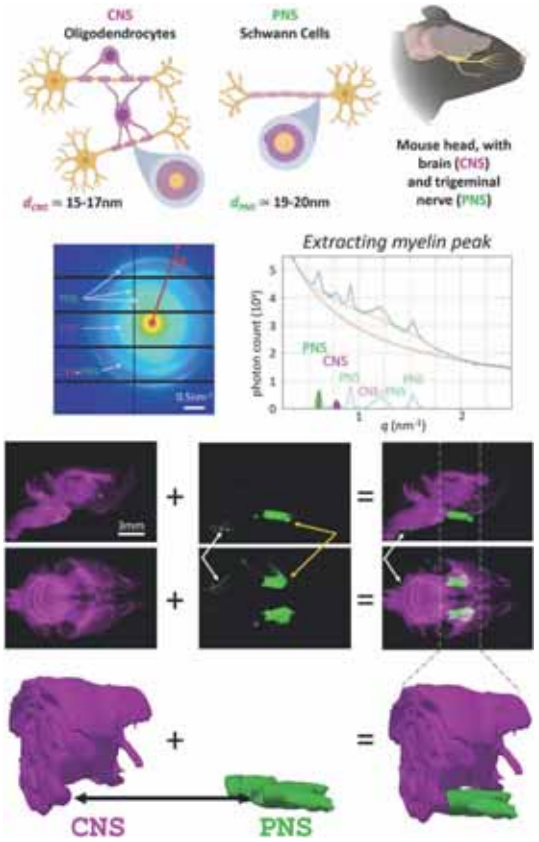
Myelinated axons
Swellings along axons
Cell nuclei
Neuromelanin-containing organelles
Blood vessels
Blood cells

H.T. Tran *et al.*, Front. Neurosci. **14**, 570019 (2020)

SAS TT complementing established techniques for instance, in neuroscience

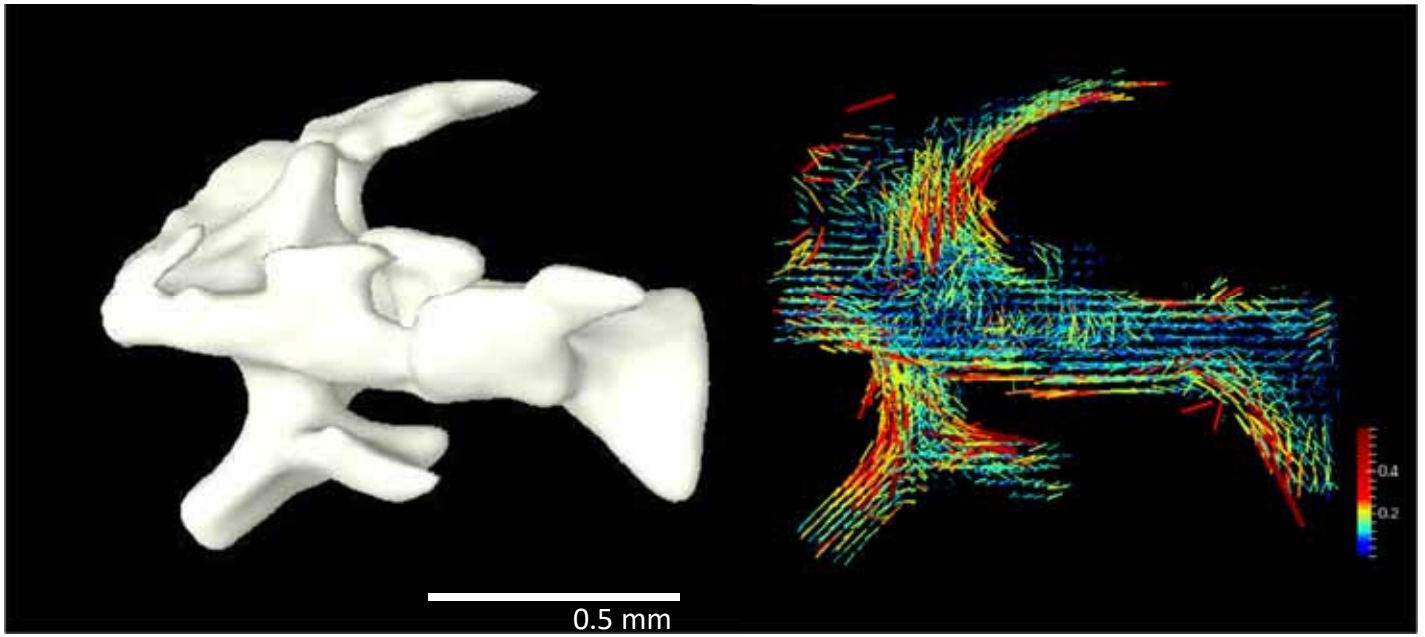
	MT_{sat}	MTR	T_1	T_2	FA	RD	RK	AWF	SAXS-TT
r - with histology	0.72	0.47	-0.02	-0.32	0.44	-0.33	0.46	0.52	0.85
r - with SAXS-TT	0.76	0.46	-0.05	-0.33	0.52	-0.36	0.50	0.60	-
ρ - with histology	0.79	0.72	-0.02	-0.51	0.39	-0.48	0.48	0.56	0.86
ρ - with SAXS-TT	0.81	0.71	-0.09	-0.53	0.45	-0.52	0.50	0.61	-
contrast based on:	Magnetization transfer		Relaxometry		DTI		DKI		X-ray scattering





Marios Georgiadis *et al.*, Nature Comm. **12**, 2941 (2021)

Scanning SAXS in 3D (SAS TT): Trabecular bone from human vertebra



Marianne Liebi *et al.*, Nature **527**, 349 (2015).
Marianne Liebi *et al.*, Acta Cryst. **A74**, 12 (2018).

The Coherent X-Ray Scattering Group

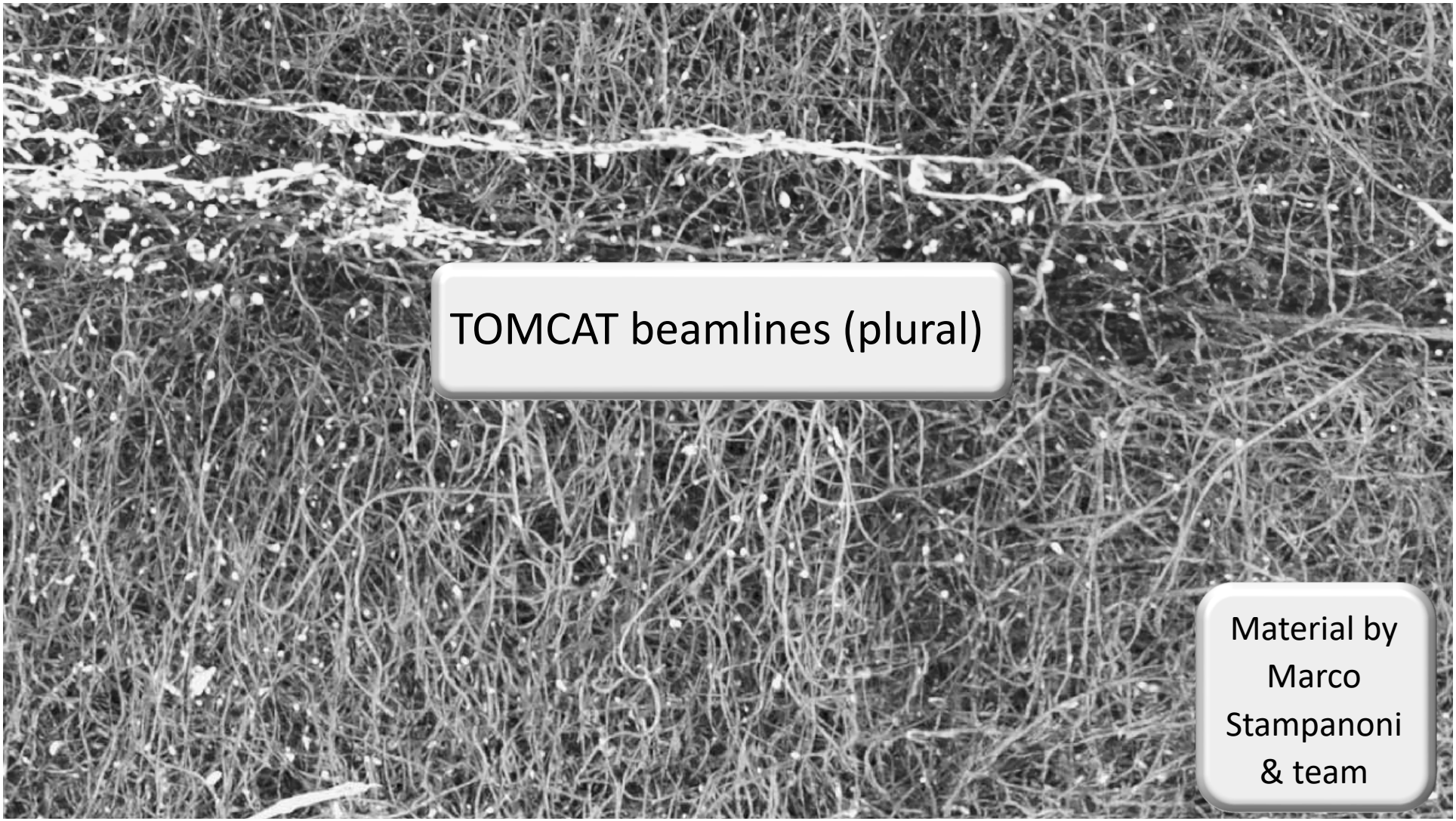
Ana Diaz | **Andreas** Menzel | **Christian** Appel | **Irene** Rodriguez-Fernandez | **Johannes** Ihli | **Manuel** Guizar-Sicairos | **Nicholas** Williams Phillips | **Xavier** Donath | **Zirui** Gao

Mirko Holler
Tomas Aidukas

Benedikt Rösner

Bernd Schmitt
Lars Erik Fröjd
…

Alun Ashton
Markus Janousch
Klaus Wakonig
…


TOMCAT beamlines (plural)
Material by Marco Stampanoni & team

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Needs for **In-situ :: In-vivo :: Operando**

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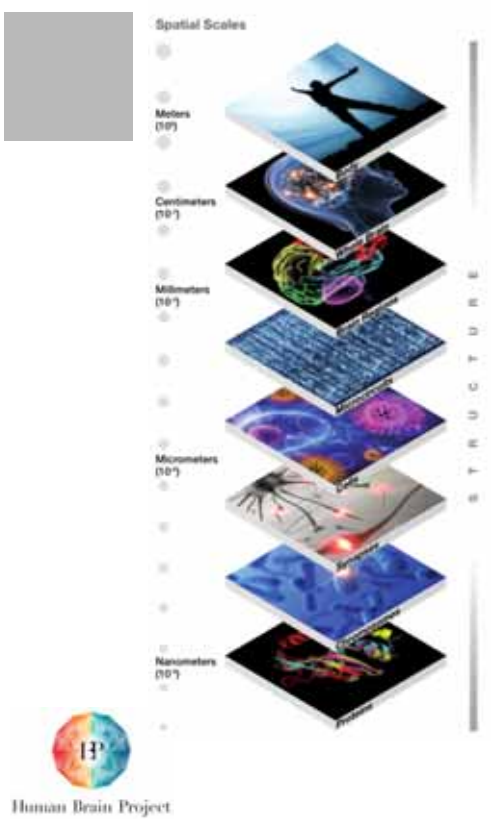
PSI

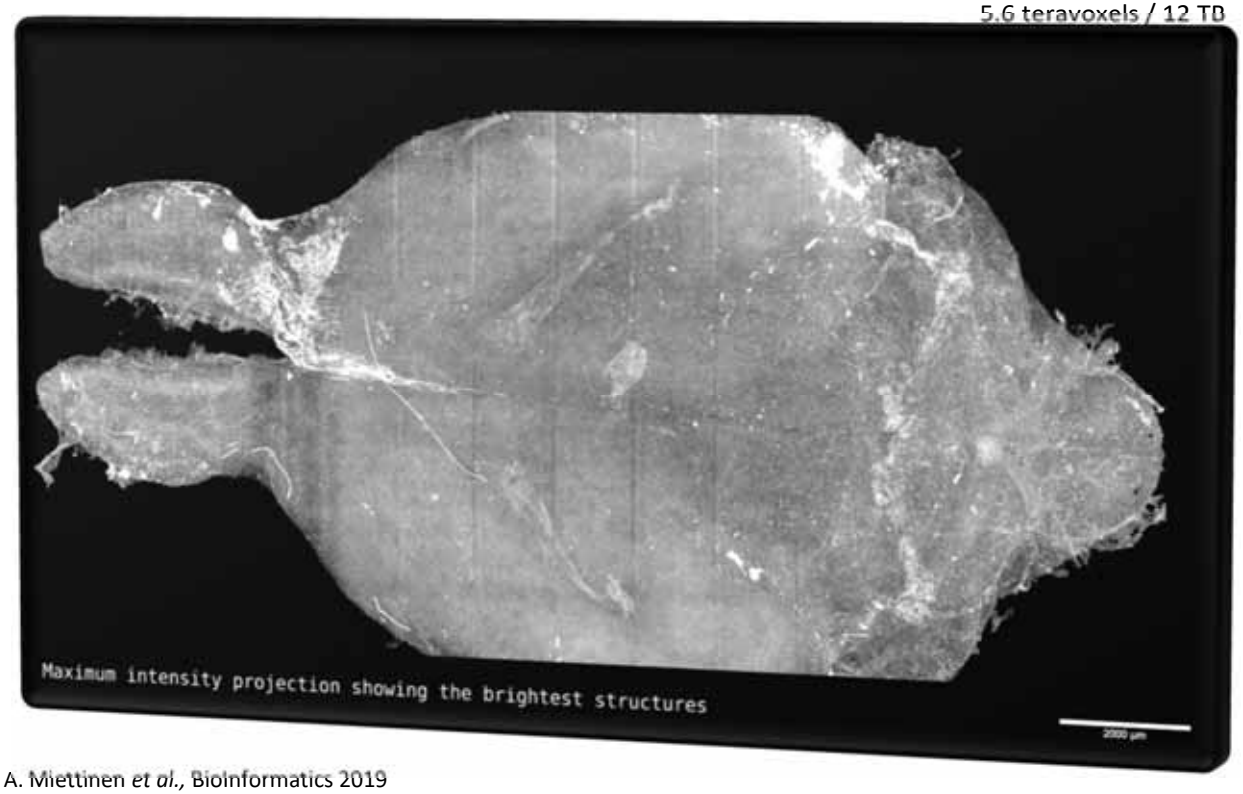
Hunting the complete mouse brain microvascular architecture



Human Brain Project

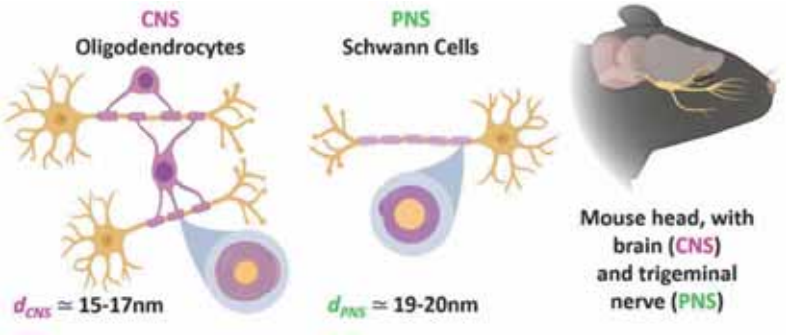
This is a stitched tomogram of more than 1000 single volumes, assembled non-rigidly.

5.6 teravoxels / 12 TB

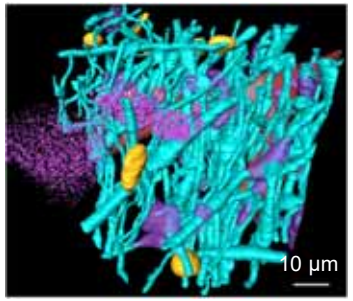


A. Miettinen *et al.*, Bioinformatics 2019

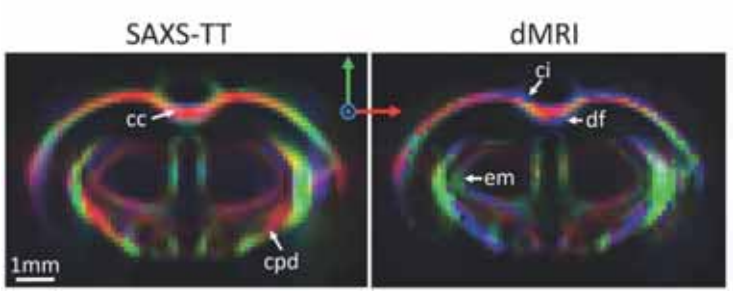
X-ray neuroimaging: 3+ complementary methods



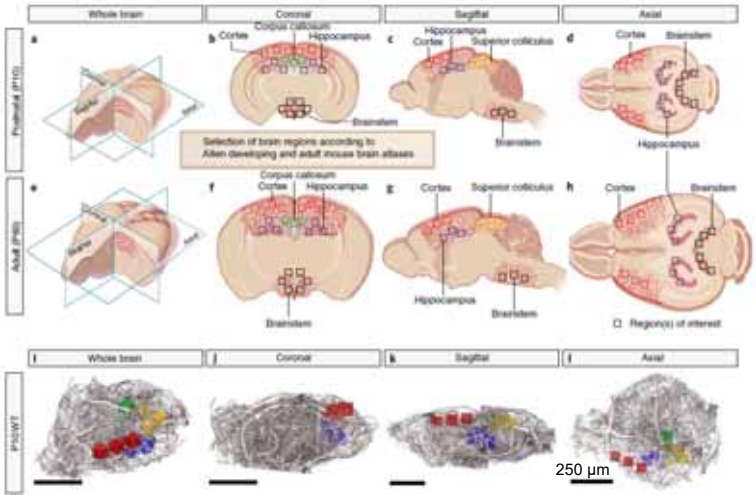
Cryo ptychographic tomography using OMNY at cSAXS



Full-field tomography (with 'stitching') at S- and I-TOMCAT



Scanning SAXS tomography at cSAXS or PX I



M. Georgiadis *et al.*, Nature Comm. **12**, 2941 (2021)
H.T. Tran *et al.*, Front. Neurosci. **14**, 570019 (2020)
T. Wälchli *et al.*, Nature Protocols **16**, 4564 (2021).

The TOMCAT crew is working on it!

2019…

2021

2020-2021…

TOMCAT2.0 - Brainstorming

Summary

The future for your science at SLS hard X-ray crystallography and imaging beamlines is bright.

We are looking forward to collaborate with you on your challenging and fascinating scientific projects.

https://www.luzern.com/en/highlights/listicals/top-five-sunrise-locations-in-central-switzerland/

LSB Mission

Excellence from source to detector / excellence in life and materials science
We are at the forefront of method and instrumentation developments to render otherwise inaccessible information accessible via X-ray based techniques. In collaborations with Swiss and international scientists we employ these strengths for state-of-the-art research with focus on life and materials science. We are competent partners for academic and industrial users.