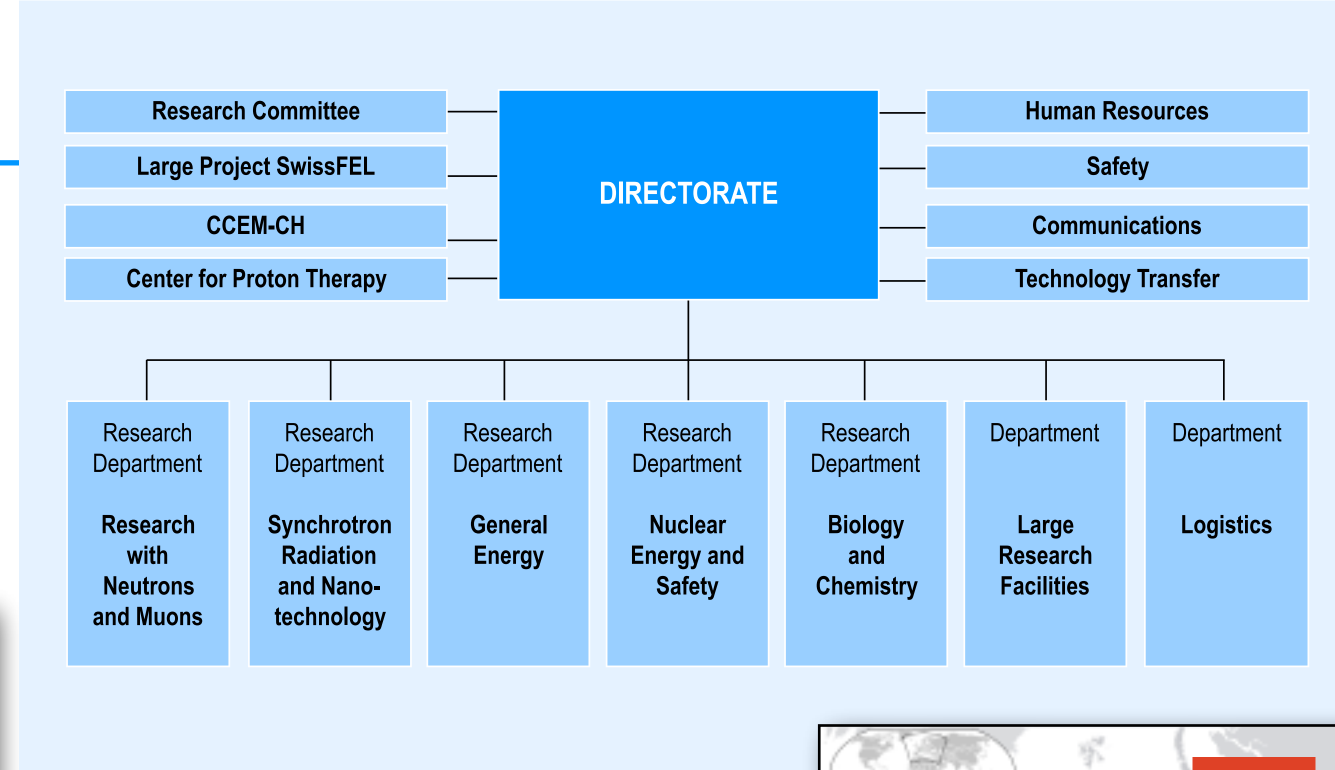
Wir schaffen Wissen – heute für morgen

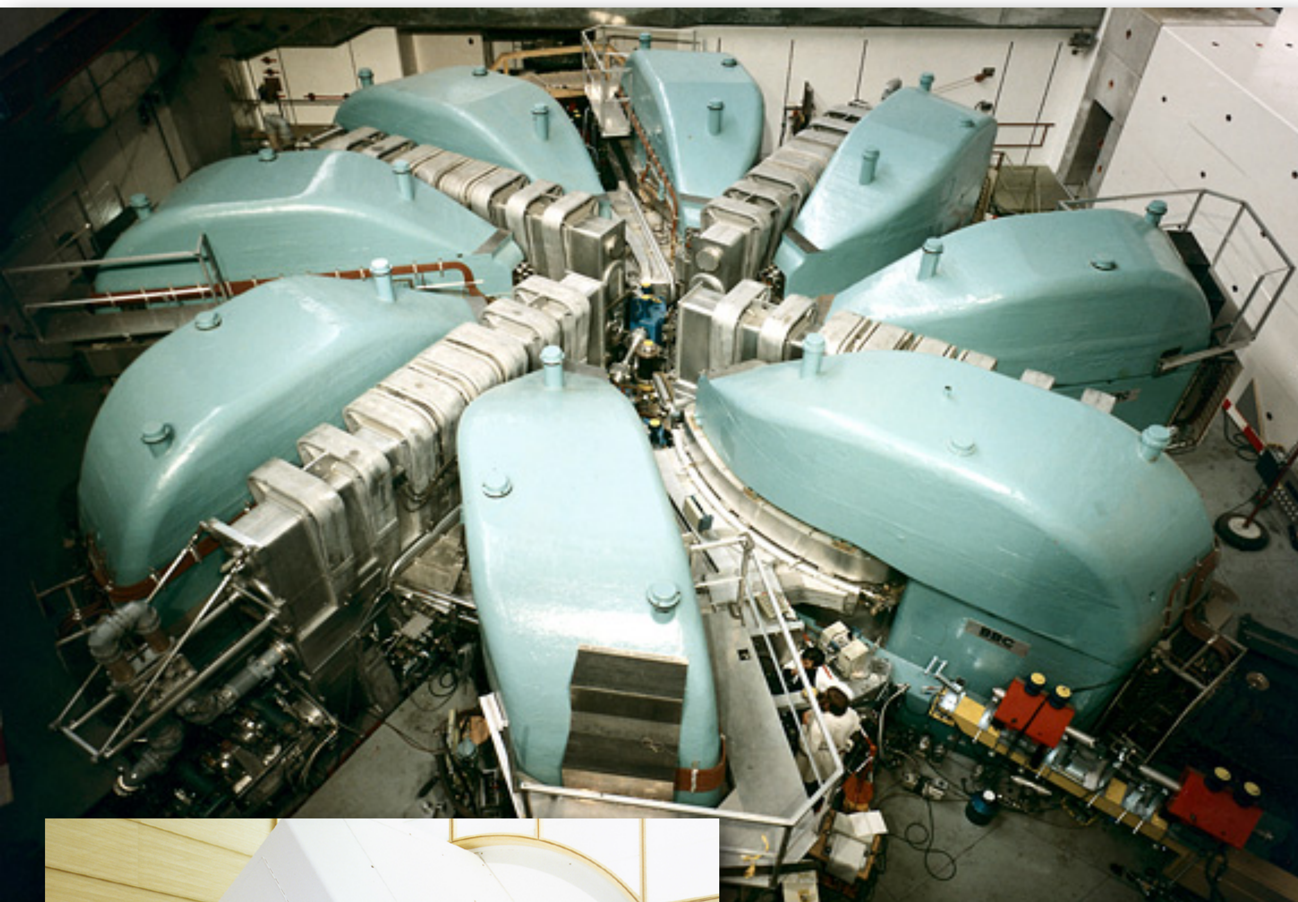
Layout and Opportunities SwissFEL

Chris Milne on behalf of R. Abela, B. Patterson, J. Szlachetko, G. Ingold, P. Beaud, L. Patthey, U. Flechsig, R. Follath, C. Erny, J. Schneider, C. Hess, A. Oggenfuss, B. Pedrini, P. Juranic, J. Rehanek, P. Heimgartner, P. Wiegand, P. Fischer, J. Czapla-Masztafiak, T.J. Penfold, G. Knopp, M. van Daalen, H. Braun, R. Ganter, M. Calvi, T. Schmitt, C. Pradervand, C. Seiler, J. Réhault, Y. Deng, J. Stettler, S. Reiche, A. Mathys, A. Alarcon, F. Lohl, C. Vicario, A. Trisorio, M. Divall, L. Sala, M. Radovic, Ch. Hauri, M. Pedrozzi…

Paul Scherrer Institute

- Home of the Swiss Light Source synchrotron, a proton accelerator, and a spallation neutron source
- 1500 staff, 300 PhD students
- PSI Forum has 15,000 visitors per year
- Proton therapy facility





Fall 2012: Swiss Parliament approved SwissFEL

Brief project history at PSI

2003-2005 Low-Emittance Gun (LEG) Project at PSI

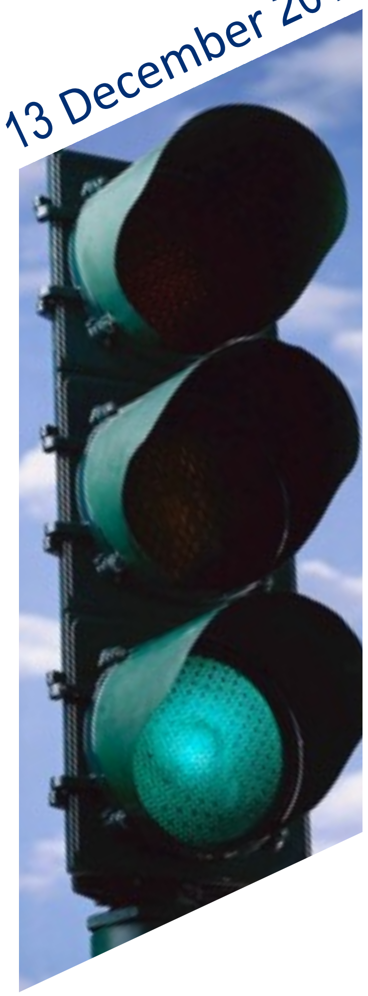
2005-2008 PSI-XFEL Project

2009 Beginning of SwissFEL Project

25 September 2012

Swiss Parliament decides research funding law 2013-16 including mandate for PSI to build SwissFEL

13 December 2012



Parliament approves 2013 government budget including funding for SwissFEL building

December 2012: We received the green light to start building SwissFEL

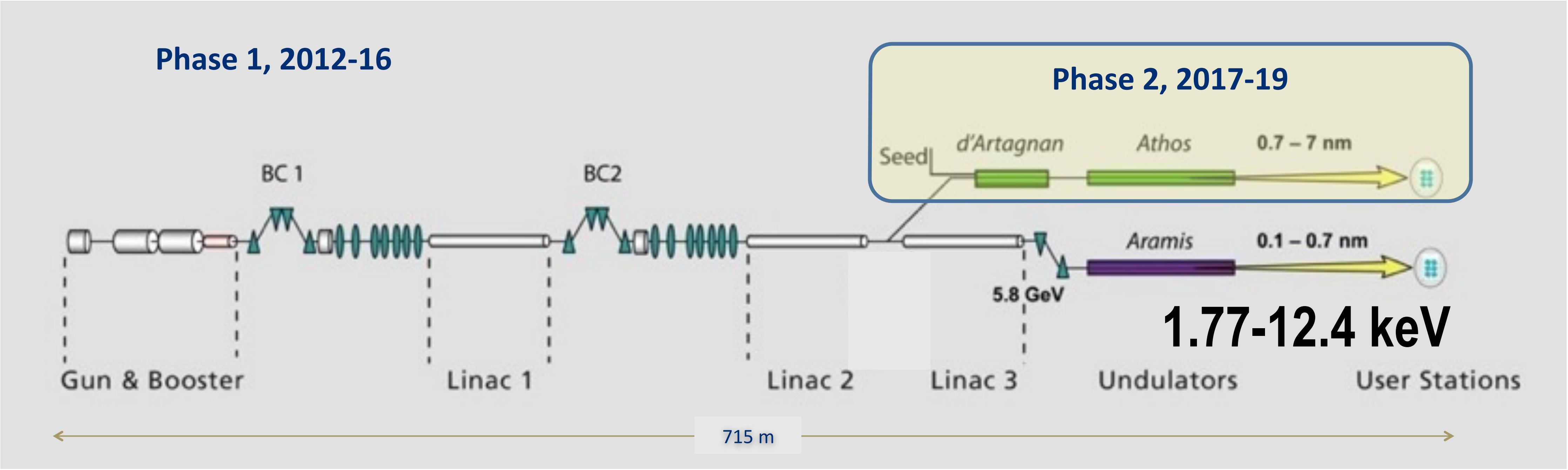
SwissFEL location at the Paul Scherrer Institute

SwissFEL: June 27, 2013

SwissFEL under construction

What are we going to put into this building ?

Hans Braun
and co-workers



2012-2017

Aramis: 1-7 Å (**2-12.4 keV**) hard X-ray SASE FEL,
In-vacuum , planar undulators with variable gap
User operation from mid 2017

after 2017

Athos : (2nd phase) 7-70 Å (**200-1700 eV**) soft X-ray FEL for SASE/seeded operation
APPLE II undulators with variable gap and full polarization control
To be implemented after 2017

Aramis: Hard X-ray self-seeding

SwissFEL parameters	
Wavelength from	1 Å - 70 Å
Photon energy	0.2-12 keV
Photon / pulse (1Å)	7.3E+10
Pulse duration	1 fs - 20 fs
Energy bandwidth	0.05-0.16%
e^- Energy	5.8 GeV
e^- Bunch charge	10-200 pC
Repetition rate	100 Hz

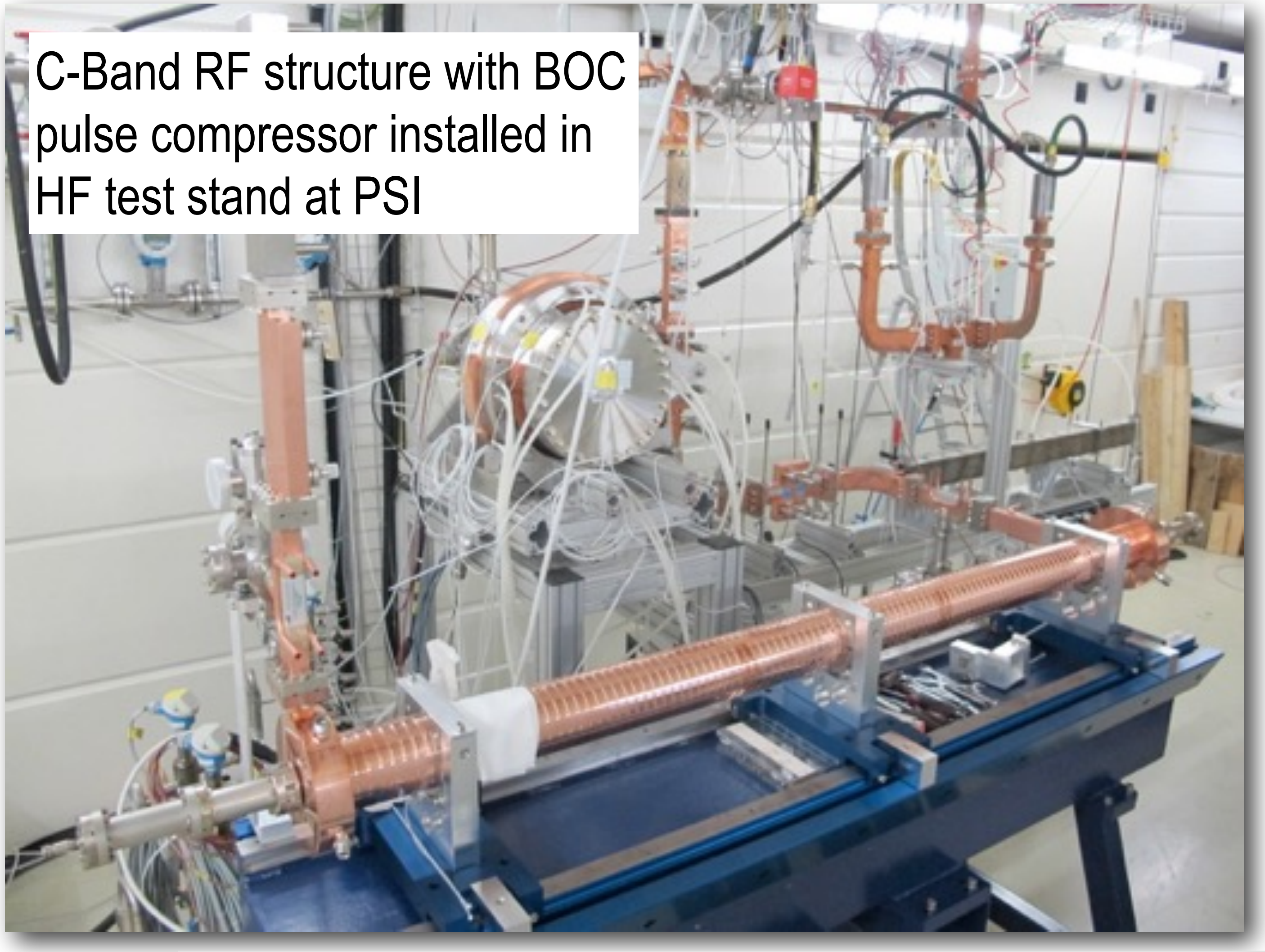
SwissFEL design parameters at 1 Å (12.4 keV)

Sven Reiche and co-workers

FEL Beam Design Parameters	Nominal Operation Mode		Special Operation Mode	
	Long Pulses	Short Pulses	Large Bandwidth	Ultra-Short Pulses
Undulator period (mm)	15	15	15	15
Undulator parameter	1.2	1.2	1.2	1.2
Energy spread (keV)	350	250	17000 (FW)	1000
Saturation length (m)	47	50	50	50
Saturation pulse energy (µJ)	150 (*)	3	100	15
Effective saturation power (GW)	2.8	0.6	2	50
Photon pulse length (fs, rms)	21	2.1	15	0.06
Beam radius (µm)	26.1	17	26	17
Divergence (µrad)	1.9	2	2	2.5
Number of photons	$7,3.10^{10}$	$1,7.\ 10^{9}$	5.10^{10}	$7.5.\ 10^{9}$
Spectral Bandwidth, rms (%)	0.05	0.04	3.5 (FW)	0.05
Peak brightness (# photon/mm^2.mrad^2.s^1.0.1% bandwidth)	7.10^{32}	1.10^{32}	8.10^{30}	$1,3.10^{33}$
Average brightness (# photon/mm^2.mrad^2.s^1.0.1% bandwidth)	$2,3.10^{21}$	$5,7.10^{18}$	3.10^{19}	$7,5.10^{18}$

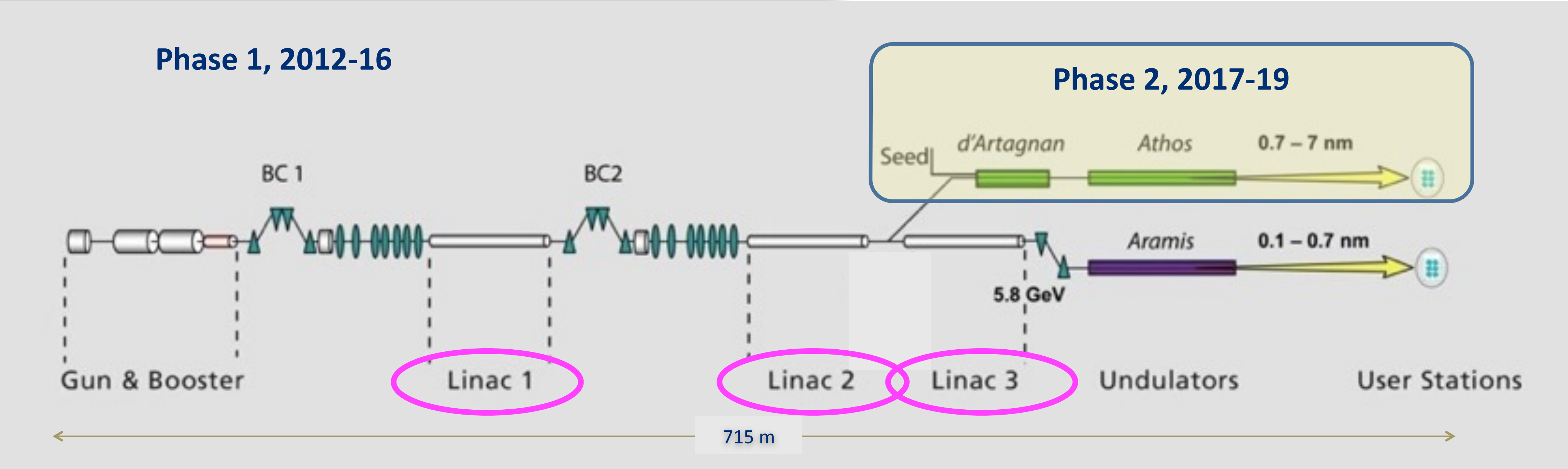
SwissFEL Linac Modules

Florian Löhl
and co-workers



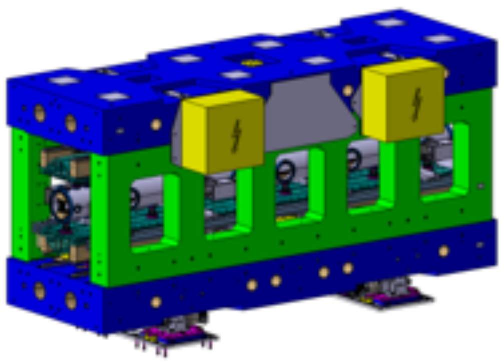
C-Band RF structure with BOC pulse compressor installed in HF test stand at PSI

	# RF stations	*E* (GeV)
Injector	1+1+4 S-band, 1 X band	0.355
Linac 1	9 C-band	2.1
Linac 2	4 C-band	3.0
Linac 3	13 C-band	5.8

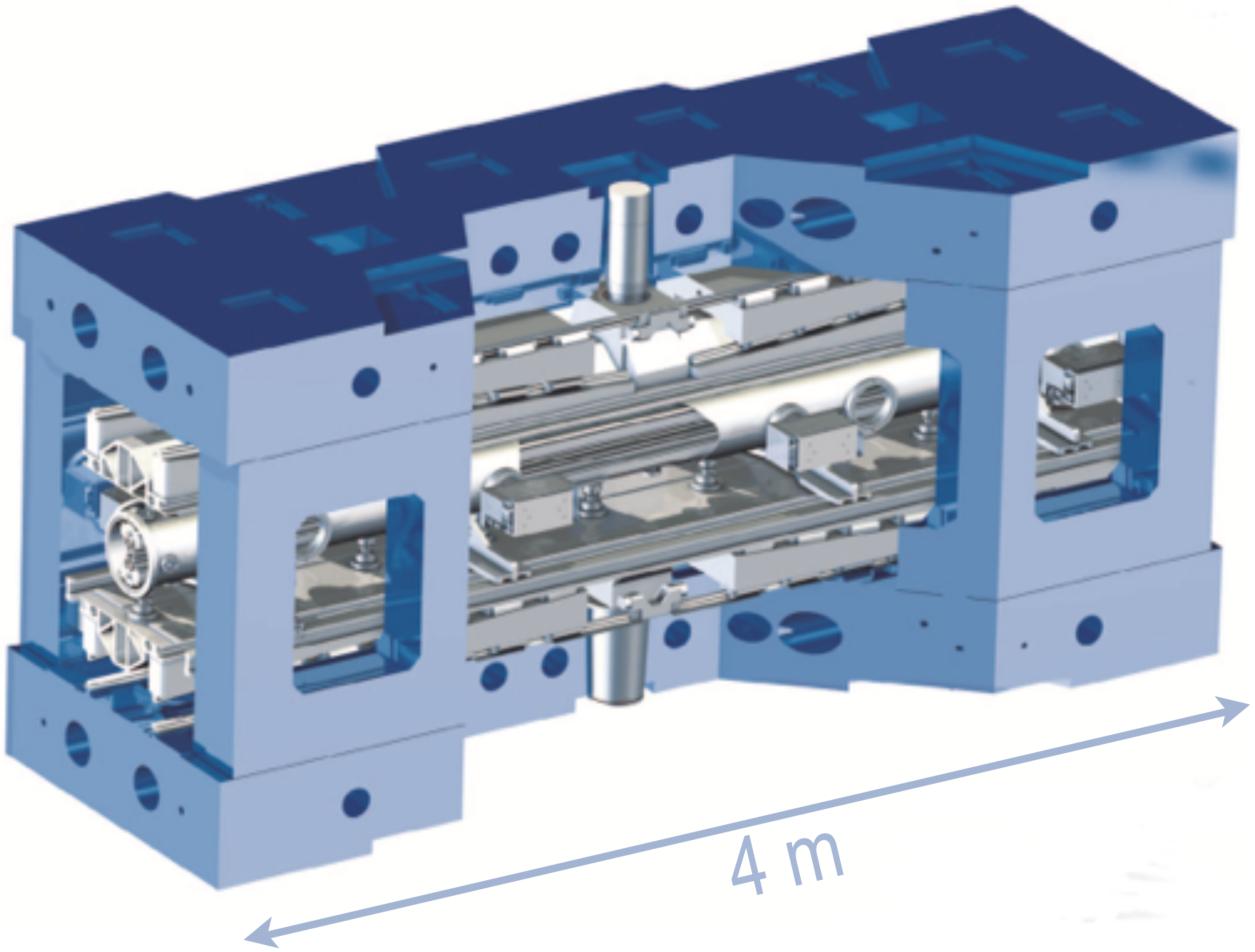


SwissFEL Hard X-ray Undulators

Romain Ganter
and co-workers



Symmetric Support Structure: Stability & Cost effective
Mineral Cast: Mechanical Rigidity
Gap Adjustment with Wedge system: Precision (0.3 μm)



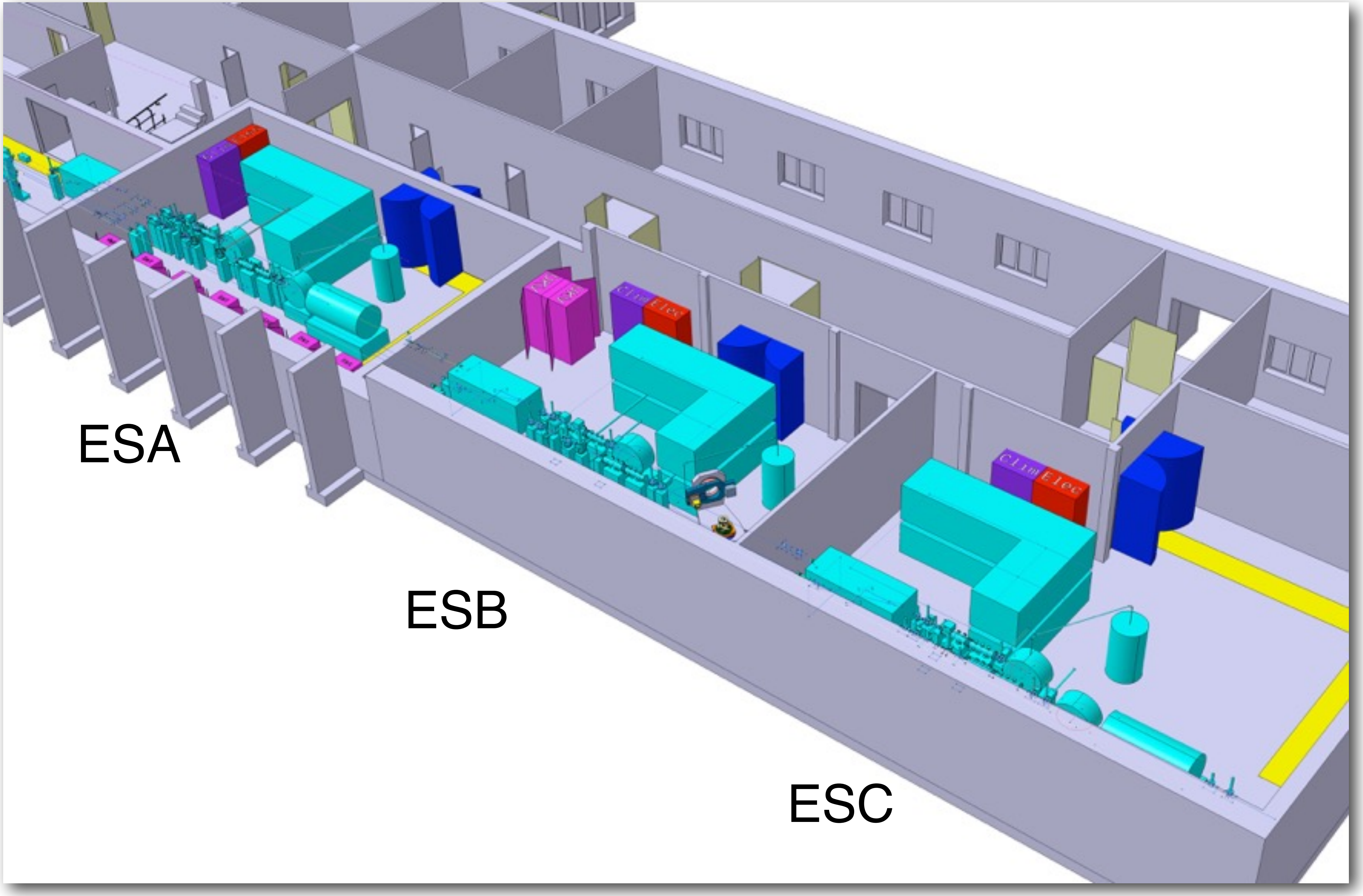
Undulator Type	Hybrid – In Vacuum
Undulator Magnetic Length	3990 mm
Number of Undulators	12
Undulator Period	15 mm
Nominal K value	1.2
Nominal gap	4.7 mm
Magnetic material	NdFeB-Dy
Pole Material	CoFeVa

Key building block for SwissFEL beamlines
12 x 17t of precision mechanic

First **U15** is getting ready for installation in WLHA injector test facility Q4-2013

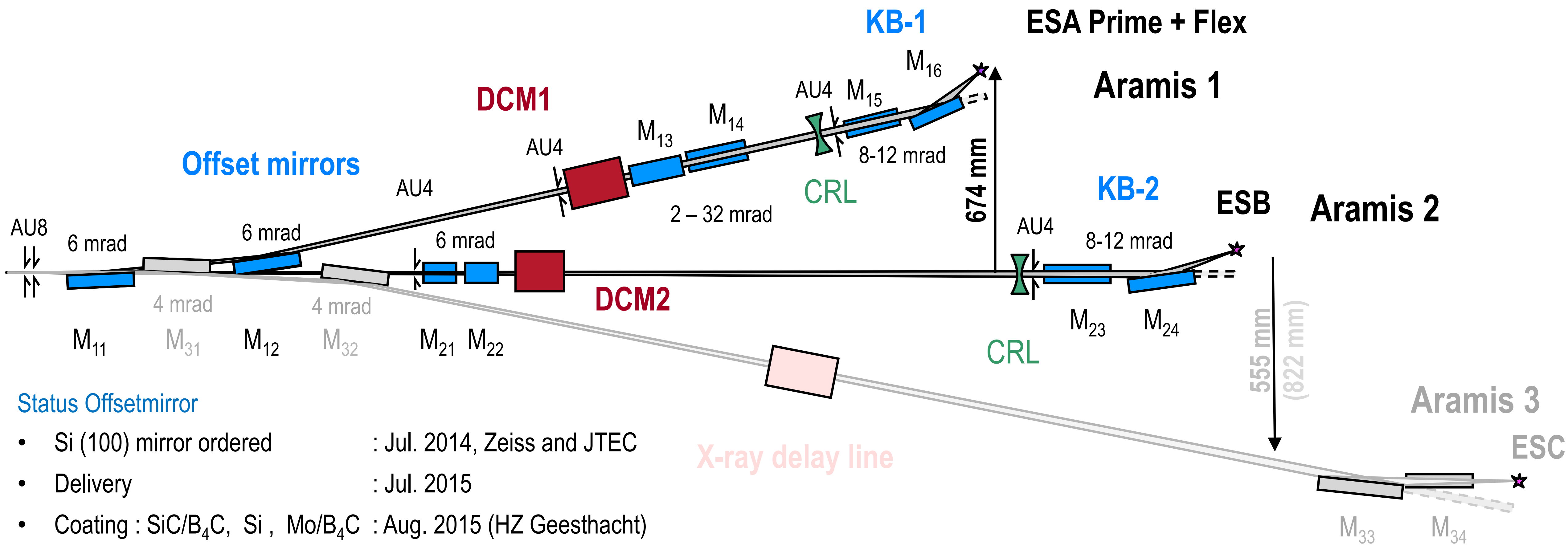
Key industry partners:
- **MDC Daetwyler Industries (CH)**
- Bruker (D)
- Hitachi (Jp)
- Micro-Waterjet (CH)
- Vakuumschmelze (D)

Aramis Experimental Hutches



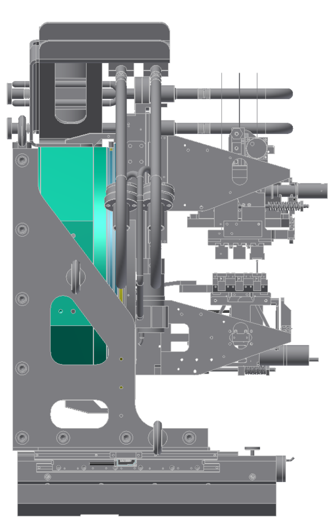
ARAMIS optical layout

L. Patthey, U. Flechsig and R. Follath



Status Offsetmirror

- Si (100) mirror ordered : Jul. 2014, Zeiss and JTEC
- Delivery : Jul. 2015
- Coating : SiC/B_4C, Si , Mo/B_4C : Aug. 2015 (HZ Geesthacht)
- Installation : Spring 2016

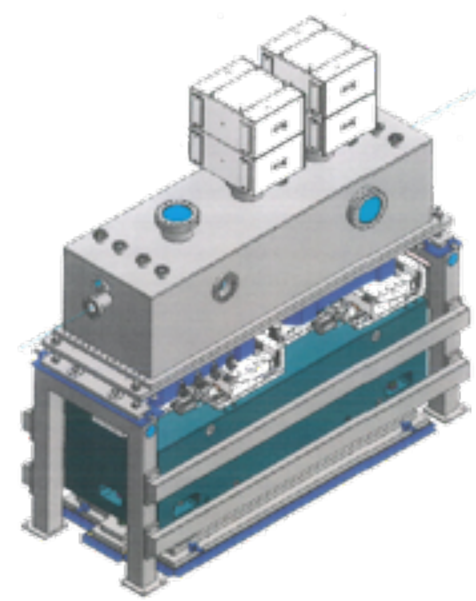


Double Crystal Monochromator

research instruments

- Fixed offset (20 mm) and variable offset (4 – 42 mm)
- 3 crystal pairs, Si (111), Si (311), tbd
- Common Bragg axis 5 – 80 deg
- 4500 eV – 12400 eV
- Pink / Monochromatic mode
- Delivery & Installation Oct. / Nov. 2015

R. Follath et. al., *SRI Proceedings* (2015)



KB-System

Pioneering New Horizons in Science TOYAMA

Specification

- full energy range 1.7 – 12.4 keV
- Variable spot size
- Mo / B_4C coating

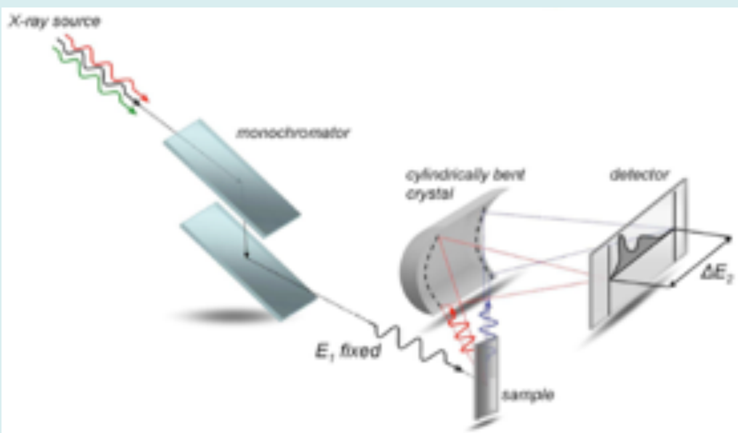
Status

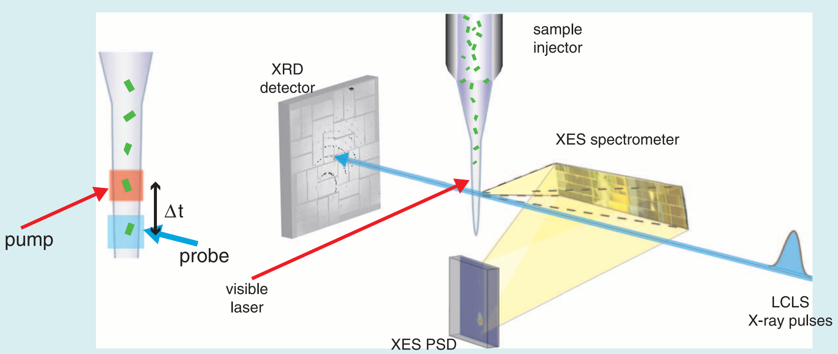
- WTO tender published 12. Dec. 2014
- KO-Meeting 30. Jun 2015
- Delivery & Installation Nov. / Dec. 2016

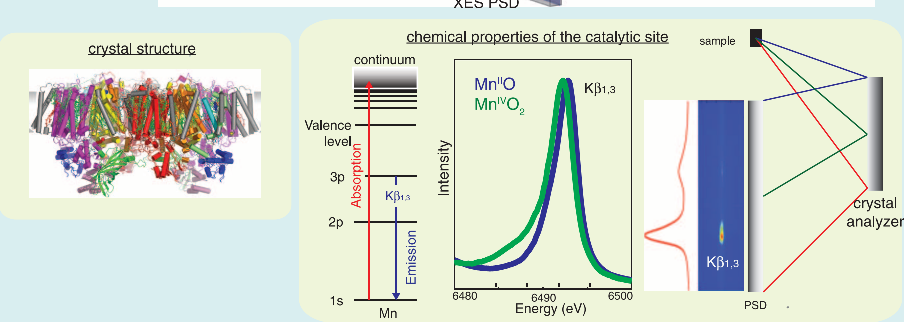
SwissFEL Experimental Stations

Bruce Patterson
and co-workers

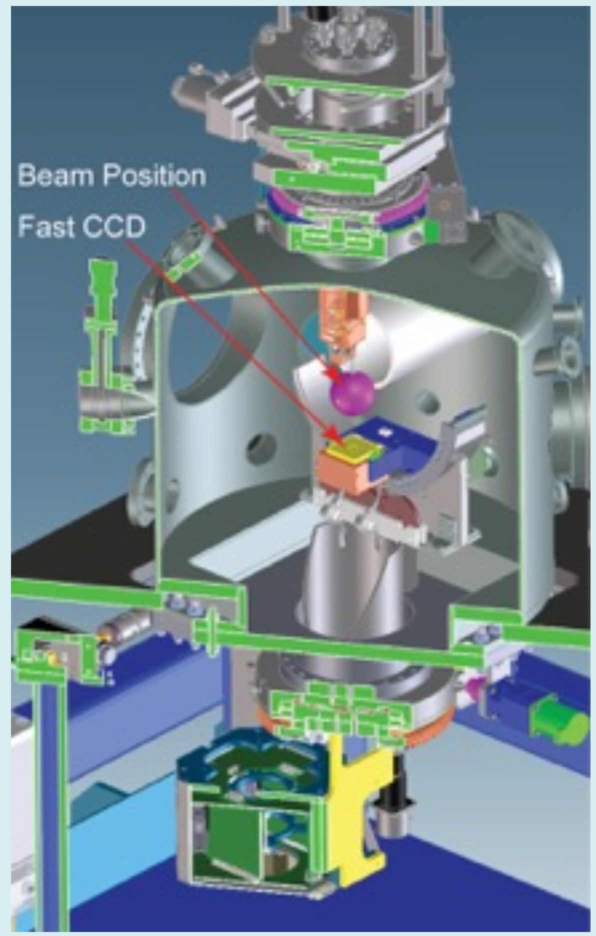
ESA:
Ultrafast photochemistry and photobiology







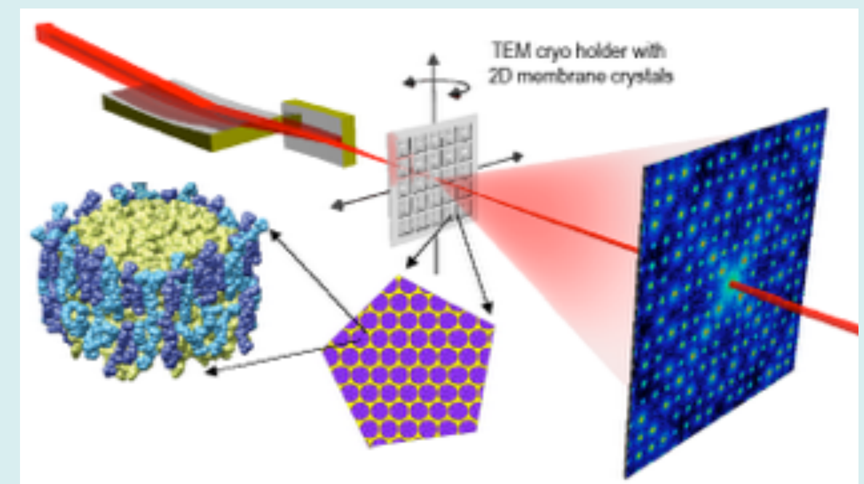
ESB:
Pump-probe crystallography



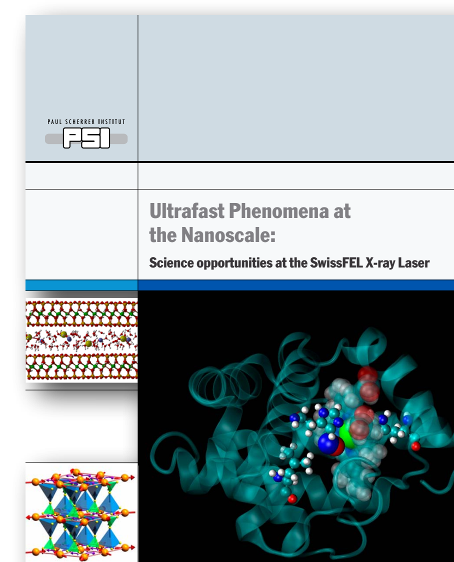
Phase I:
Ready by 2017

B. Patterson et. al., *CHIMIA* **68**, 73 (2014)

ESC: **Phase II: >2017**
Materials science and nanocrystallography



Scientific Case
B. Patterson
editor



http://www.psi.ch/swissfel/

ESA: Ultrafast photochemistry and photobiology

C. Milne,
J. Szlachetko
and G. Knopp

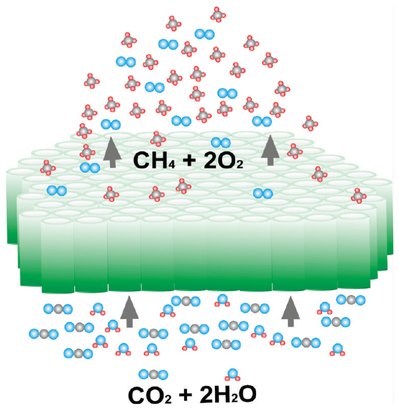
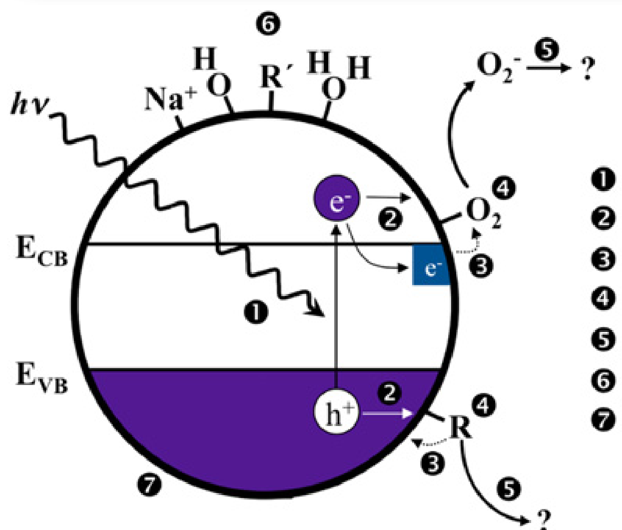


Figure 16. Depiction of flow-through photocatalytic membrane for CO_2 conversion.

Electronic relaxation in nanoparticles

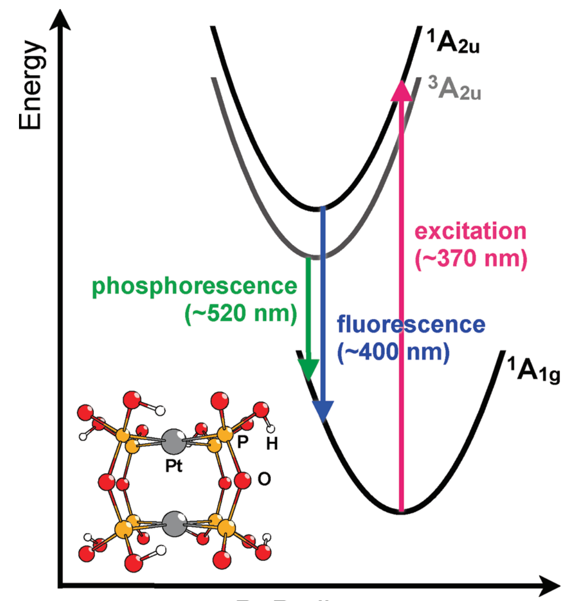


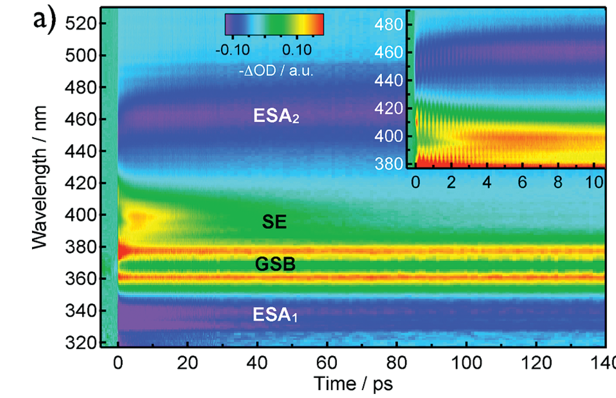
Important issues

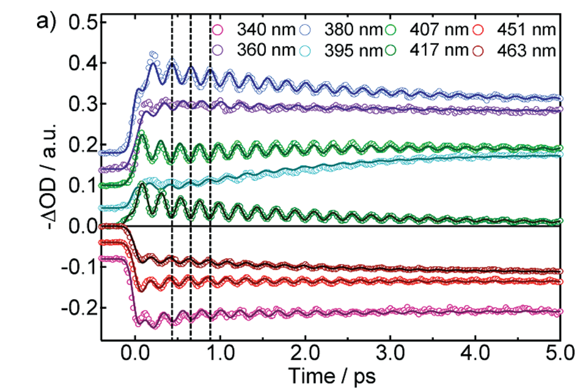
1. excitation
2. charge transport and trapping
3. charge transfer
4. molecular adsorption
5. reaction mechanisms
6. poisons and promoters
7. surface and material structure

A. Listorti et al. *Rev. Chem. Mater.* **23**, 3381 (2011);
A. Hagfeldt et al. *Chem. Rev.* **110**, 6595 (2010);
M. Henderson *Surf. Sci. Rep.* **66**, 185 (2011);
S.C. Roy et al. *ACS Nano* **4**, 1259 (2010)

Photochemistry



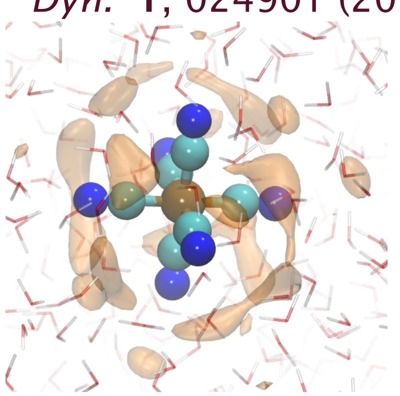




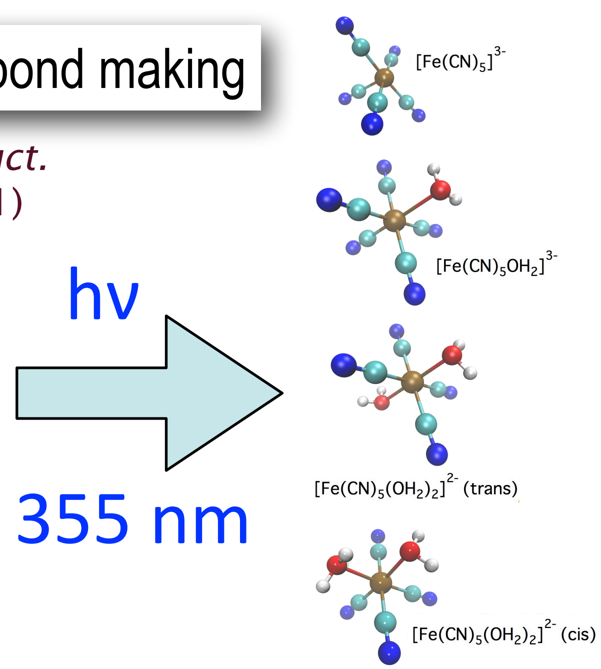
R. van der Veen et al. *JACS* **133**, 305 (2011)

Bond breaking and bond making

M. Reinhard et al. *Struct. Dyn.* **1**, 024901 (2011)

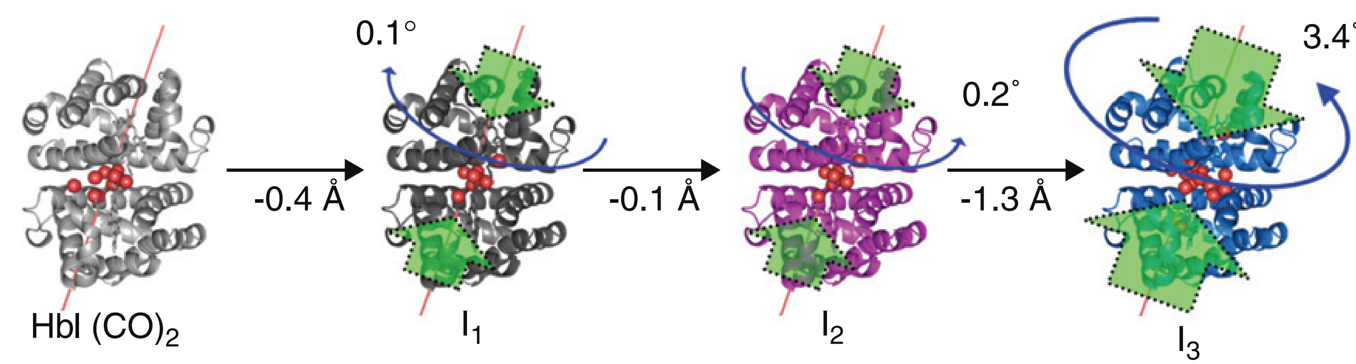


$[Fe(CN)_6]^{4-}$



Protein function

Intermediate states of homodimeric hemoglobin (HbI) ligated with CO

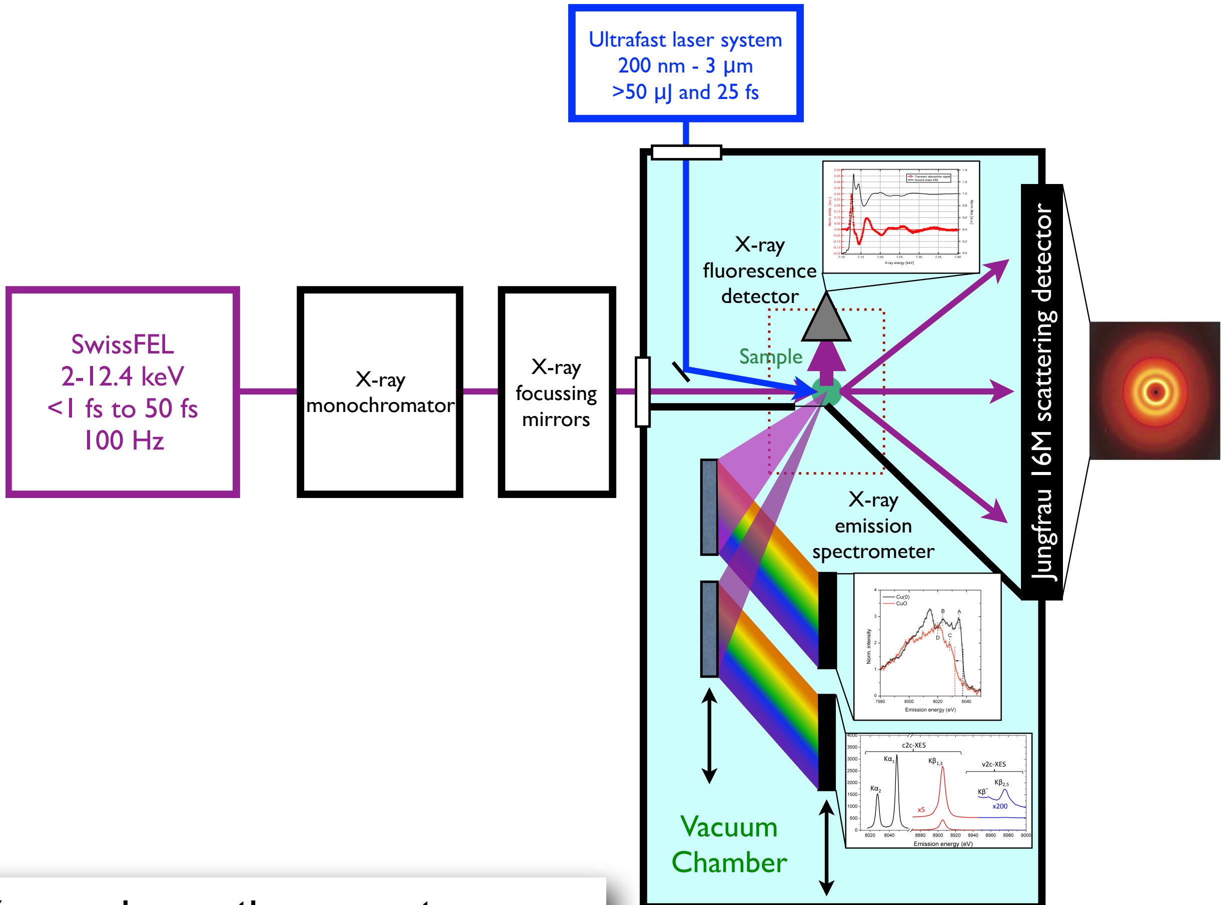


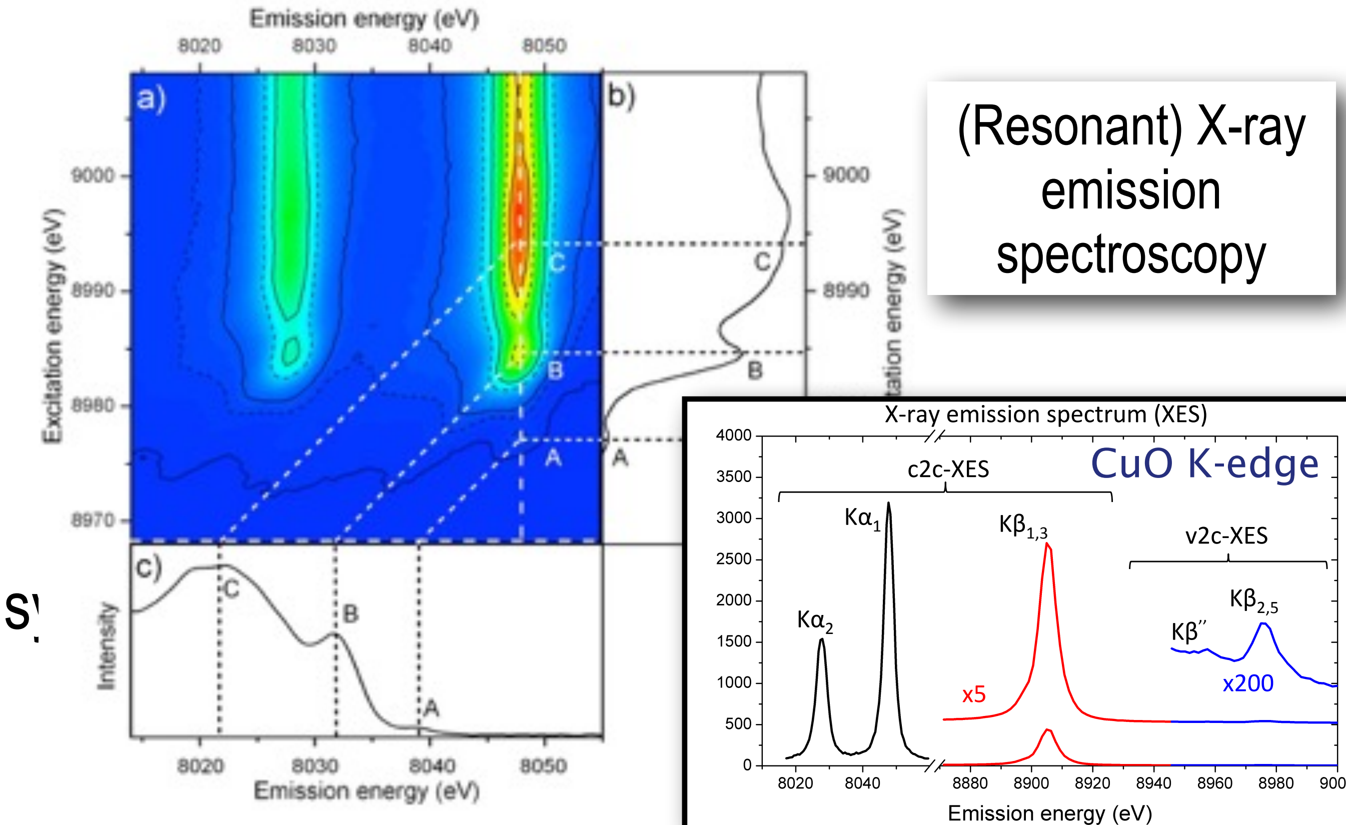
R. Neutze and K. Moffat *Curr. Op. Struc. Bio.* **22**, 651 (2012)

We want time-resolved electronic and structural information on these systems as they evolve

ESA: The X-ray probe techniques

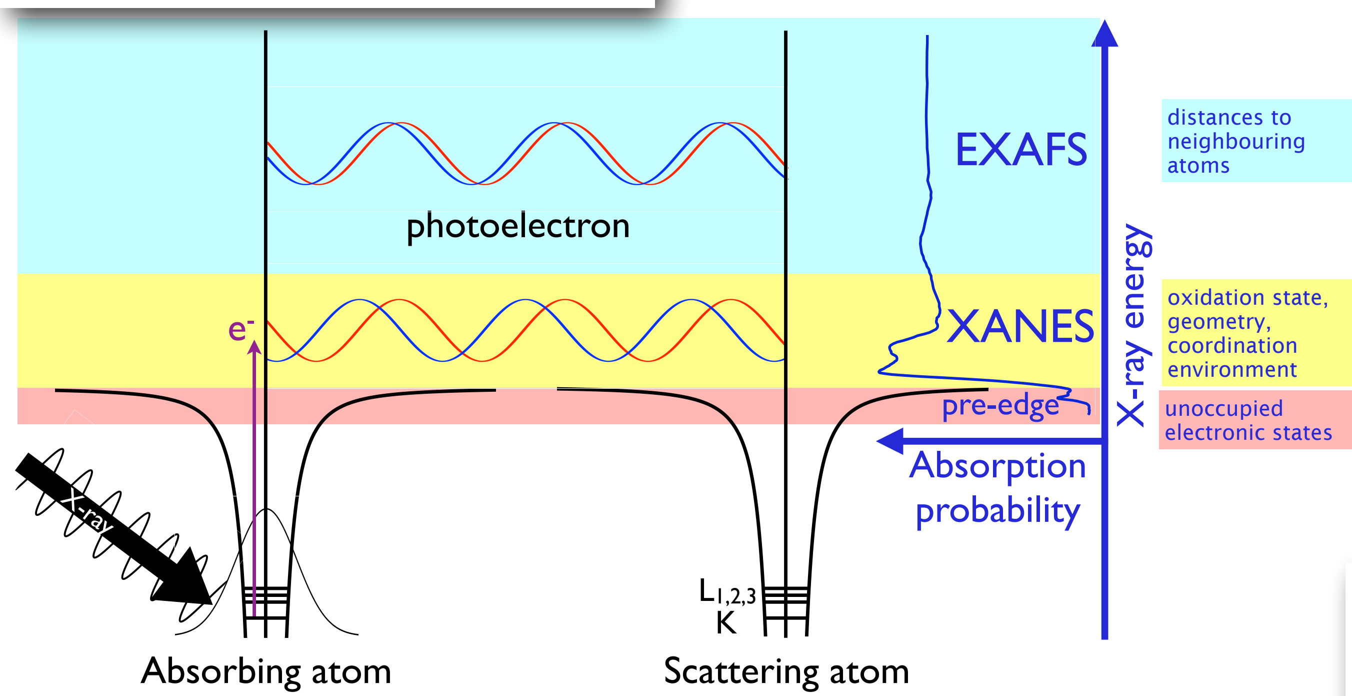
C. Milne,
J. Szlachetko
and G. Knopp





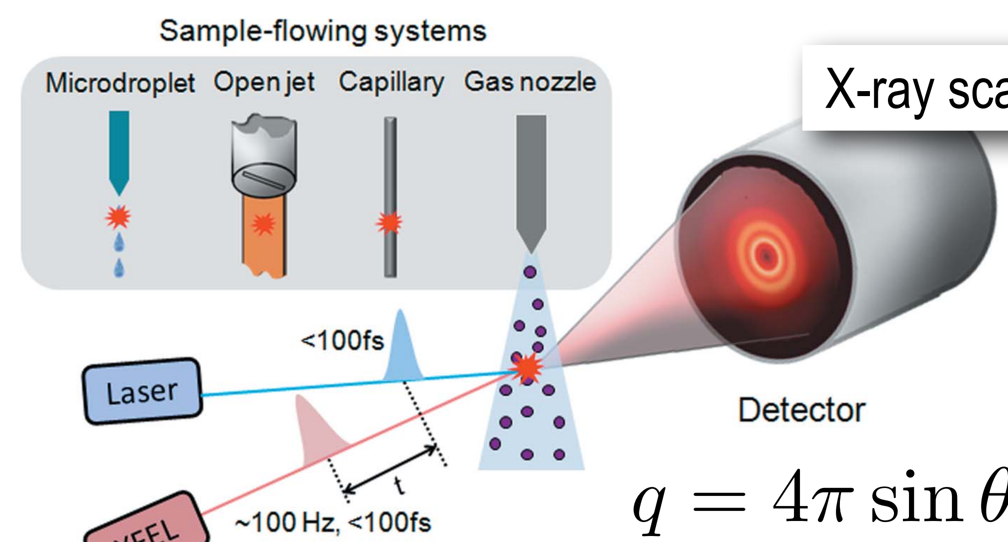
(Resonant) X-ray emission spectroscopy

X-ray absorption spectroscopy



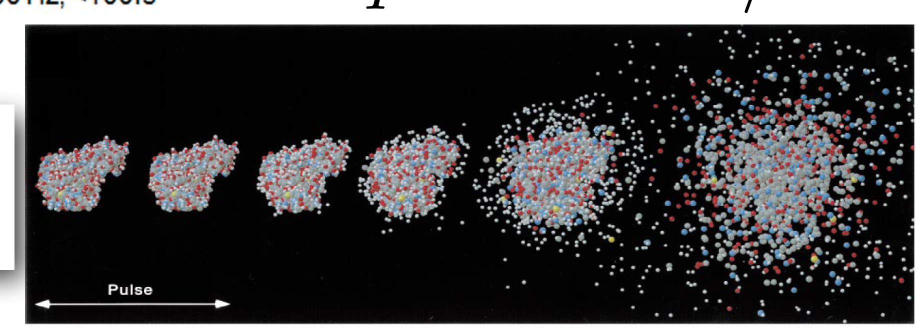
C.J. Milne et al. *Coord. Chem. Rev.* **277** 44 (2014)

X-ray scattering



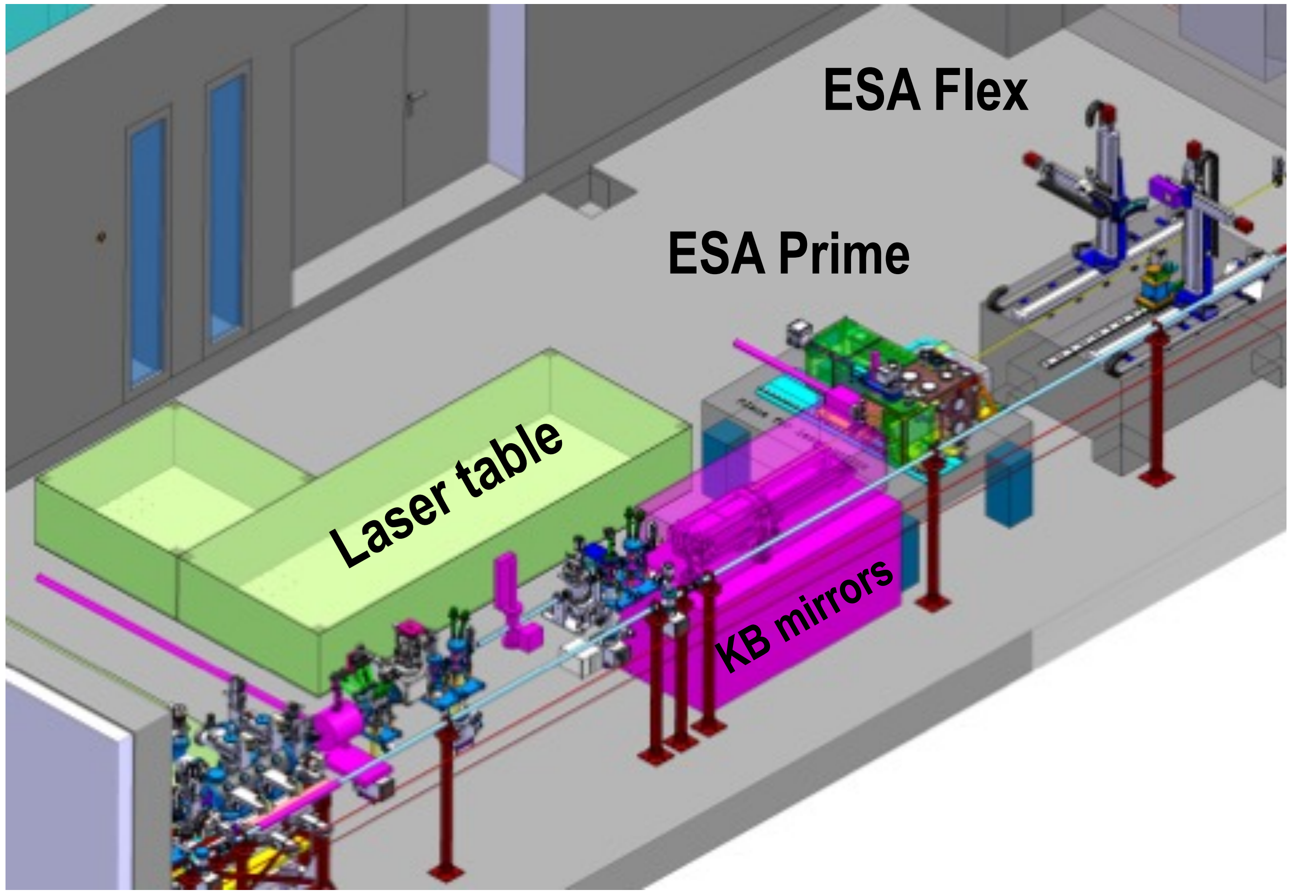
$$q = 4\pi \sin\theta/\lambda$$

R. Neutze et al. *Nature.* **406** 752 (2000)



The ESA Instruments: Prime and Flex

C. Milne,
J. Szlachetko
and G. Knopp

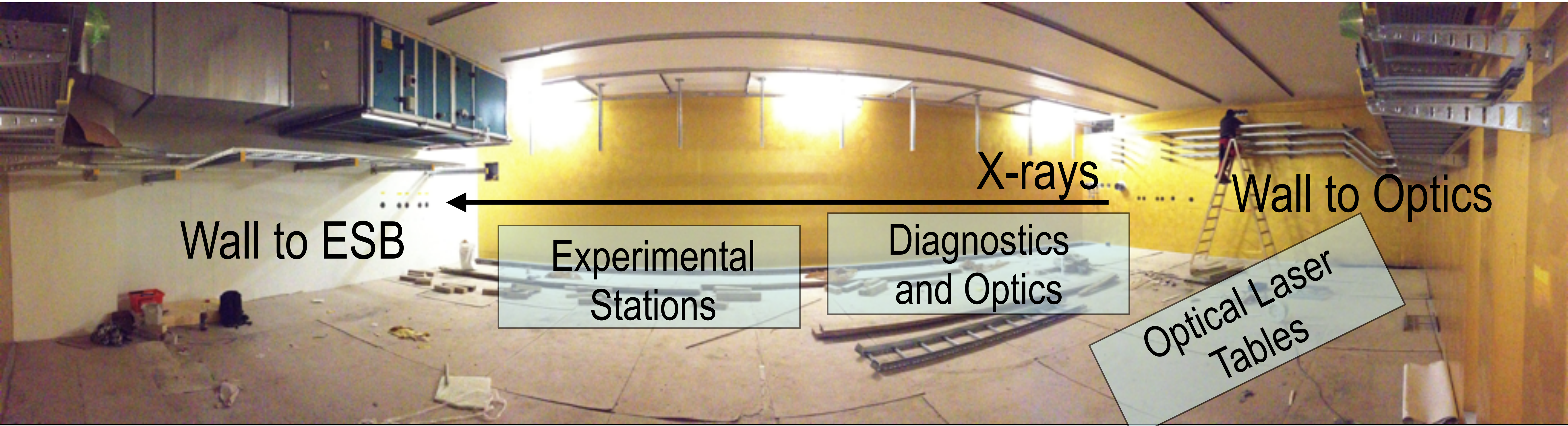


ESA Prime

- works under He or vacuum to use the 2-5 keV range
- located at the 1 µm achromatic X-ray focus (KB mirrors)
- emphasis is on **combined scattering and spectroscopy measurements**

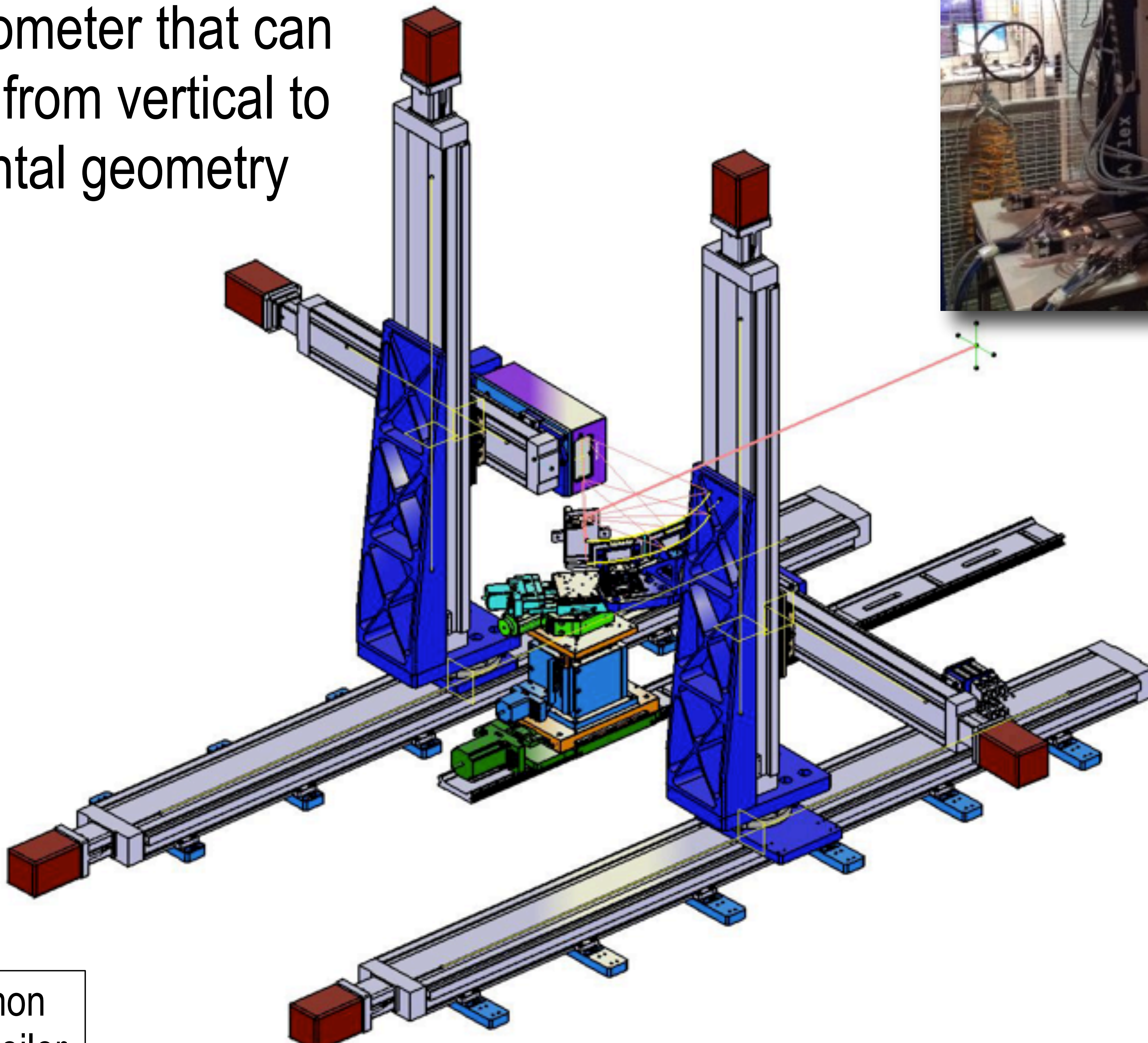
ESA Flex

- **flexible station** to accommodate user chambers and constrained geometries
- ability to easily change the spectrometer position will provide the highest energy resolution and the ability to change the scattering geometry



ESA Flex: In Action !

In-air flexible X-ray spectrometer that can switch from vertical to horizontal geometry

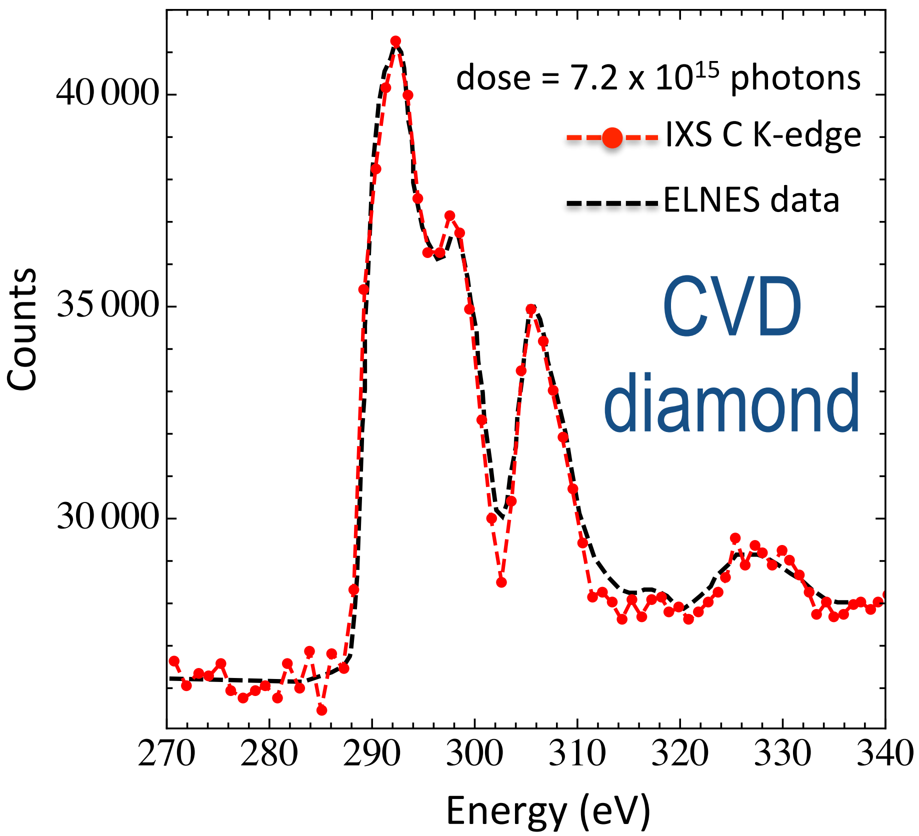


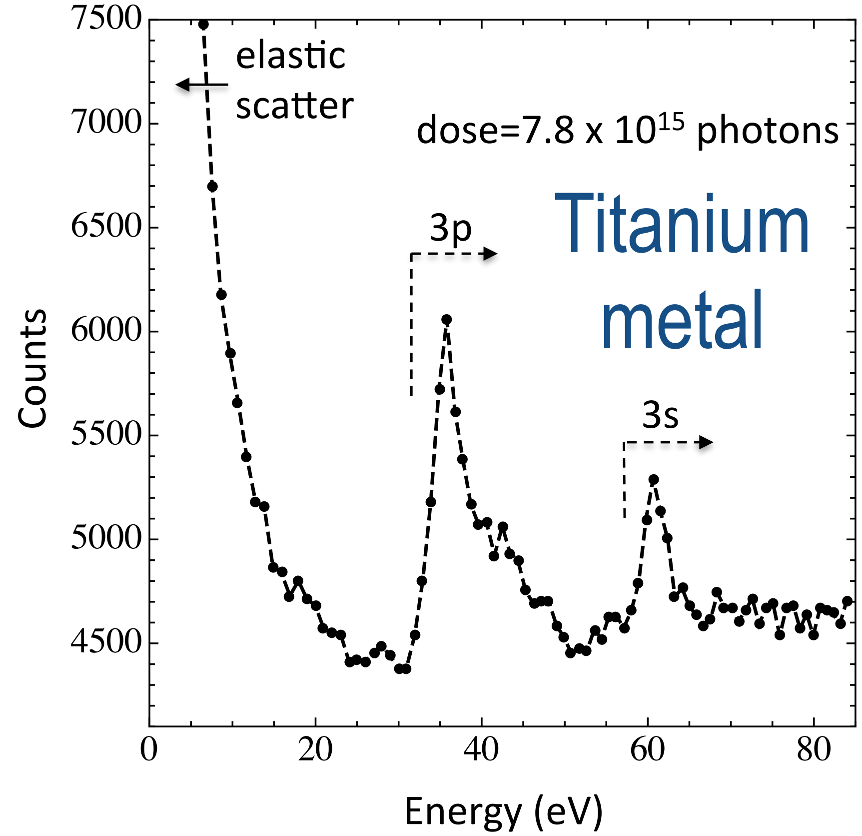
A. Ammon and C. Seiler

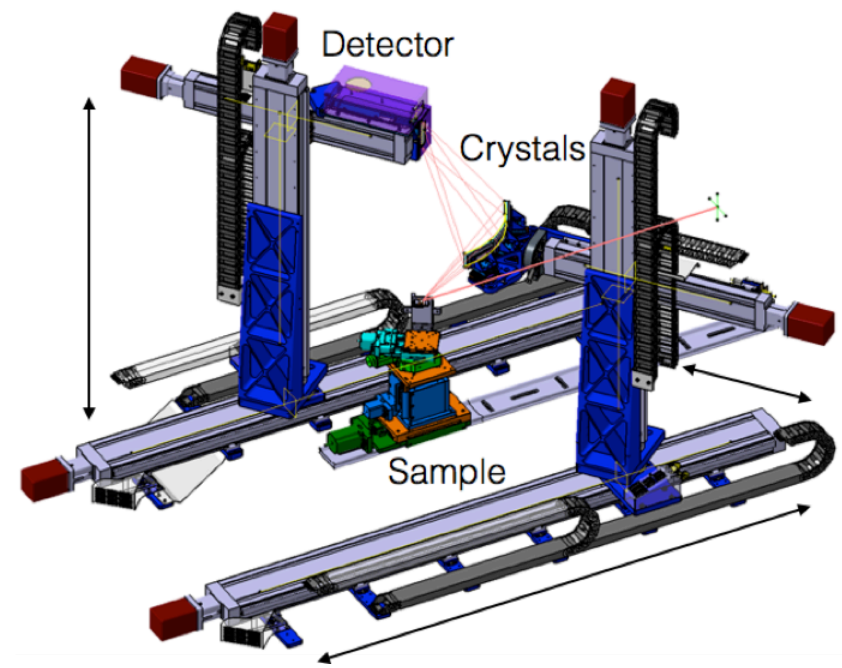
Commissioned at the SLS May 5-12

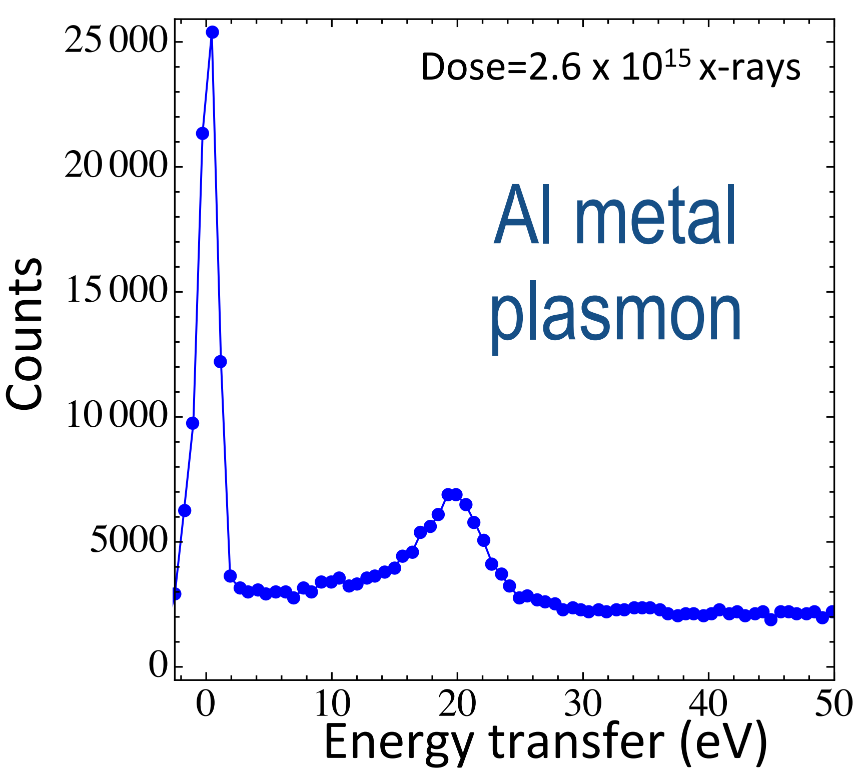
Inelastic X-ray Scattering at ESA Flex

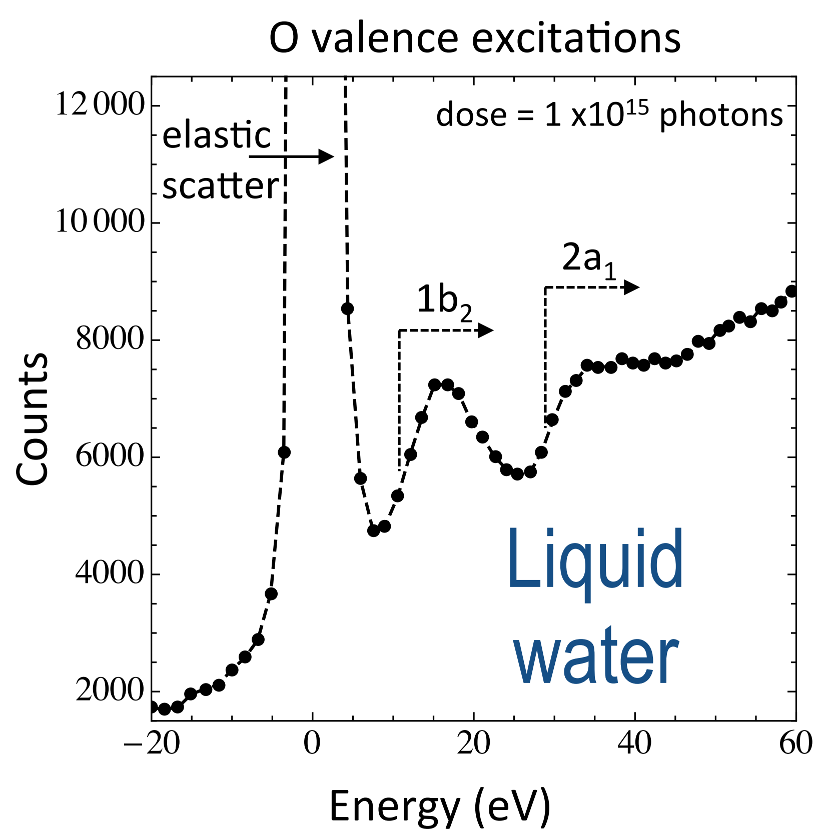
Collaboration with SuperXAS beamline

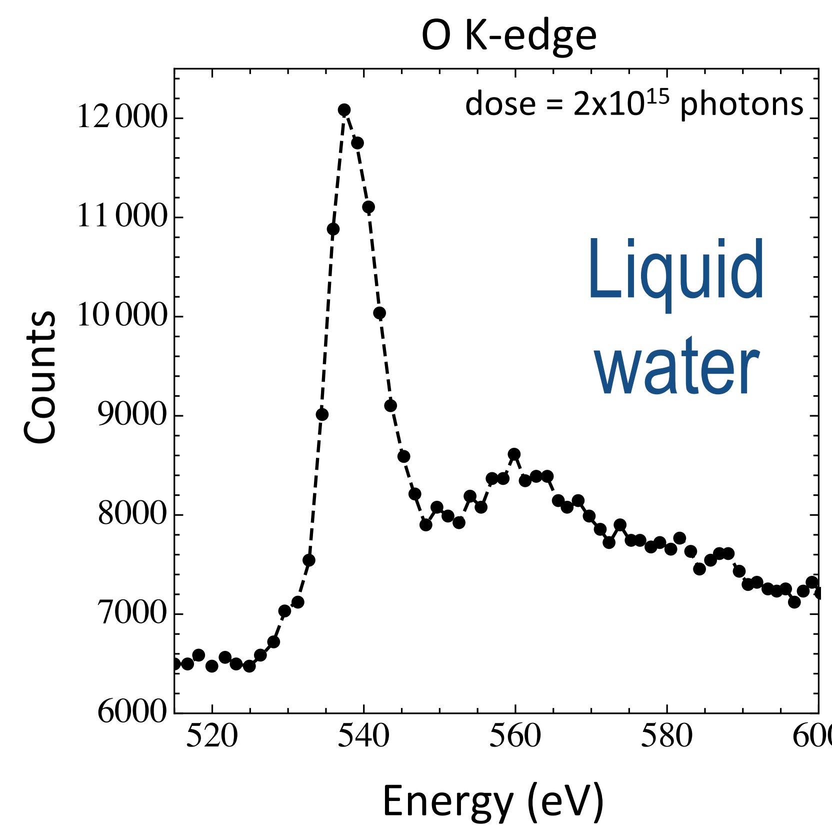








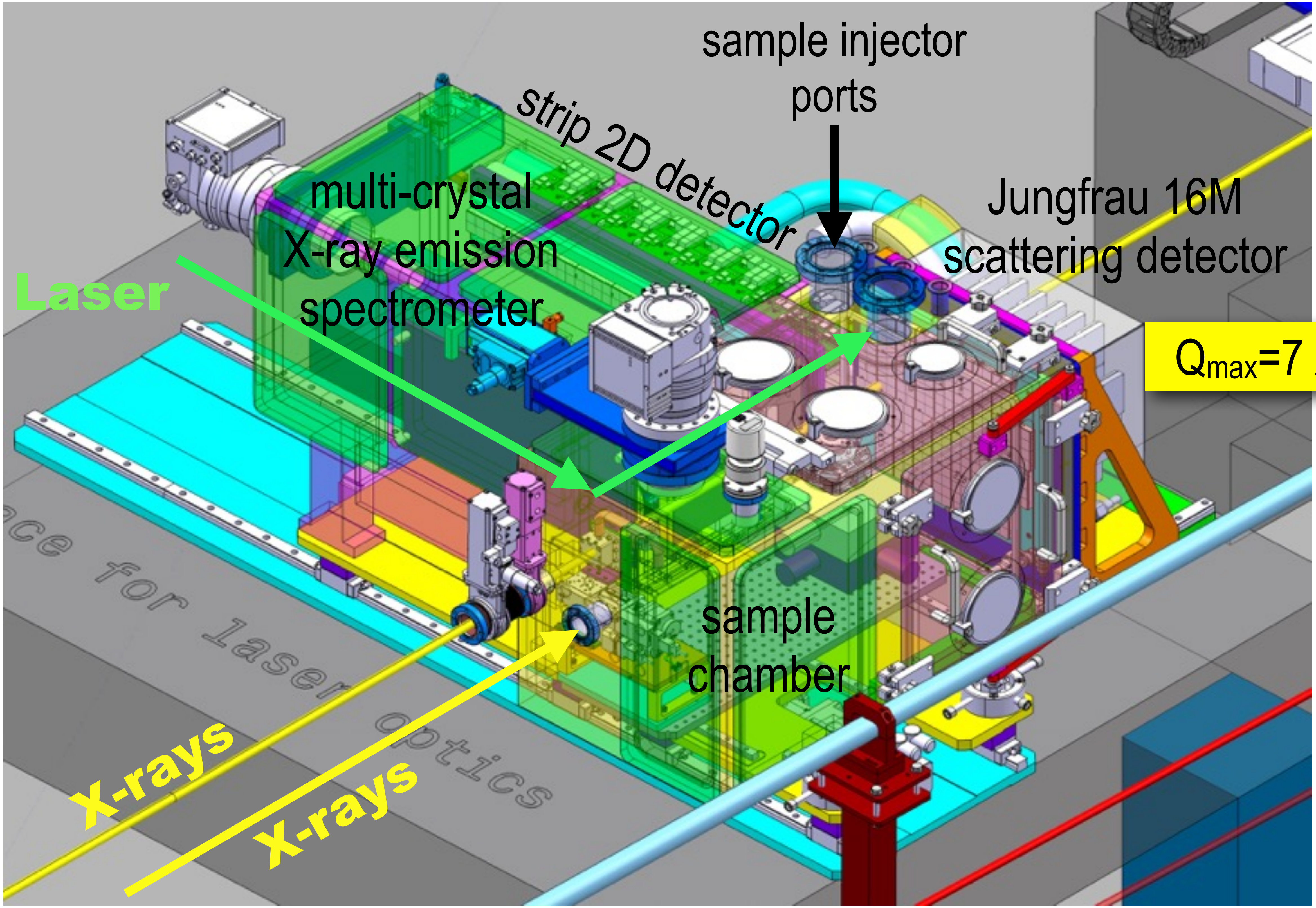




chris.milne@psi.ch

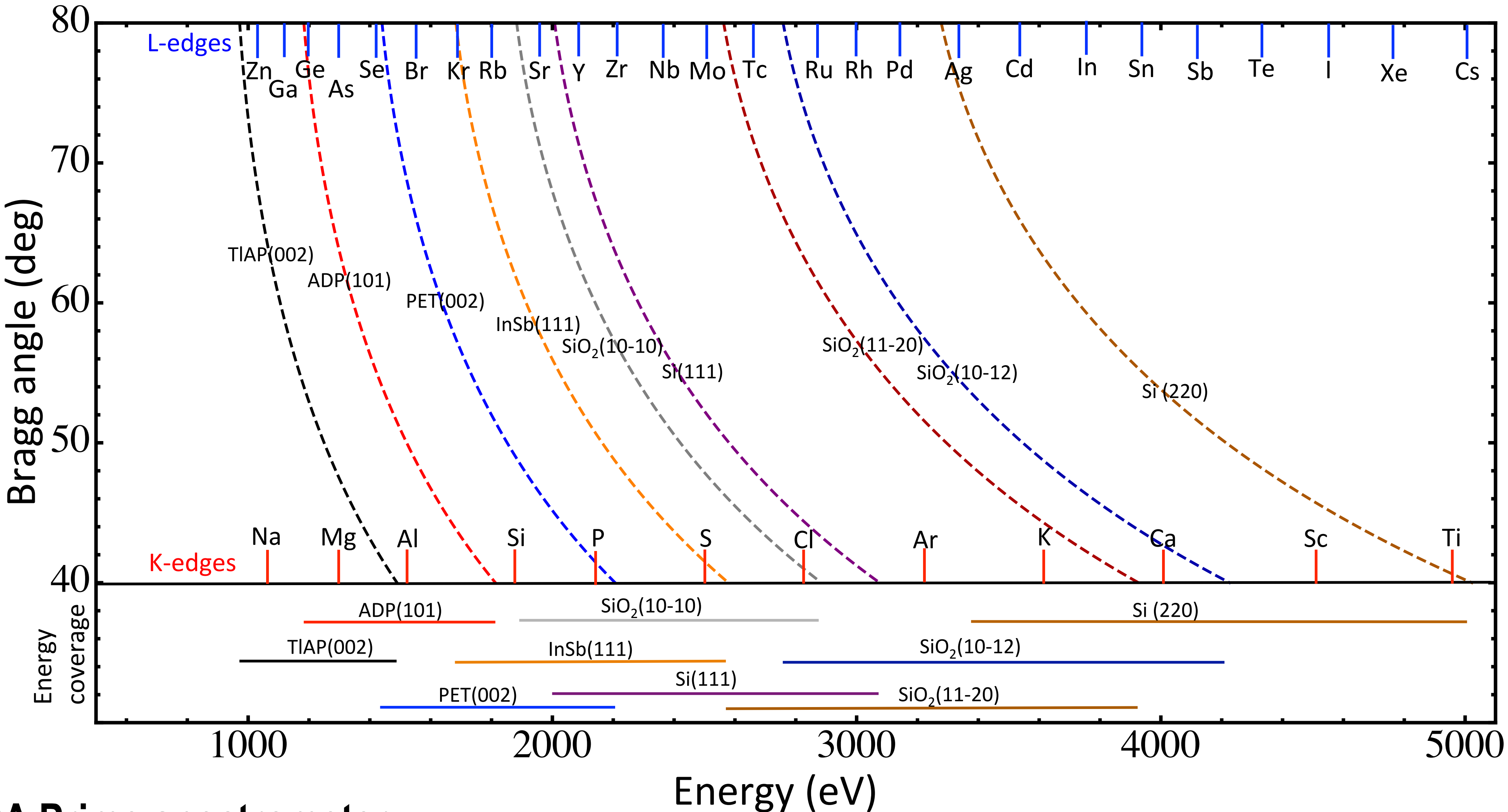
ESA Prime: Pre-final design

Markus Vitins and Jérome Stettler



ESA Prime status: design completion goal July 2015

ESA Prime: ‘Tender’ X-ray von Hamos spectrometer

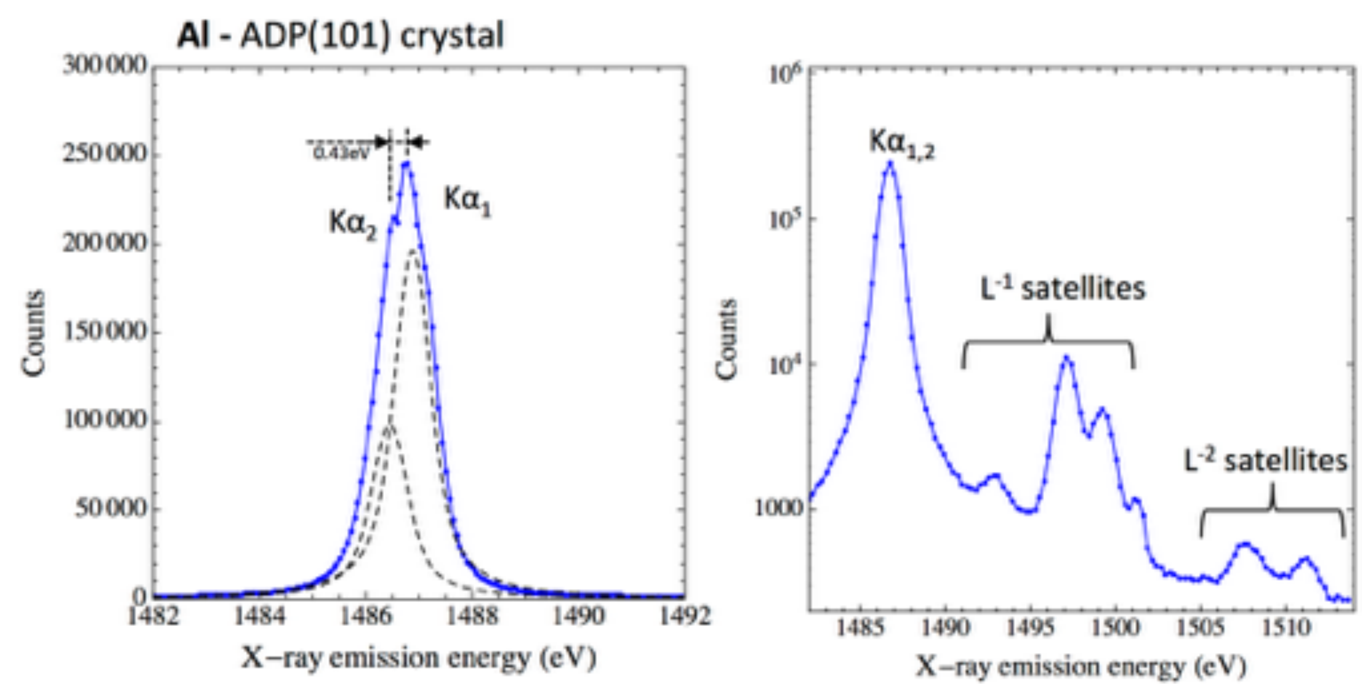


Tender X-ray crystals tested:

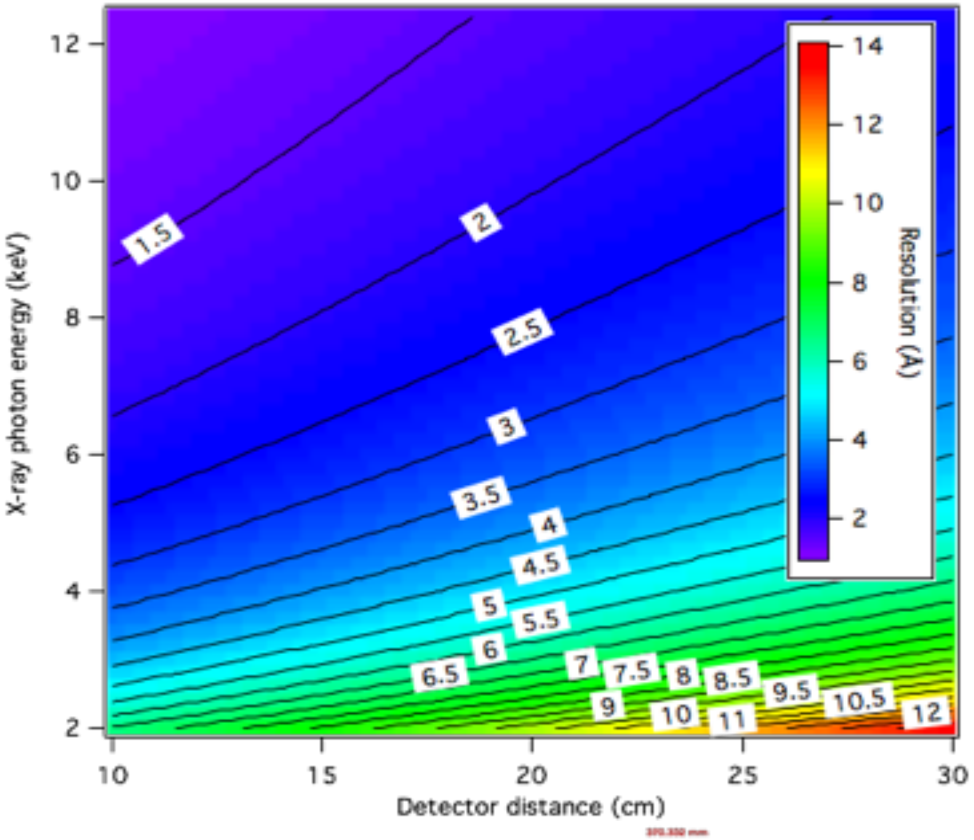
- ADP
- PET
- InSb

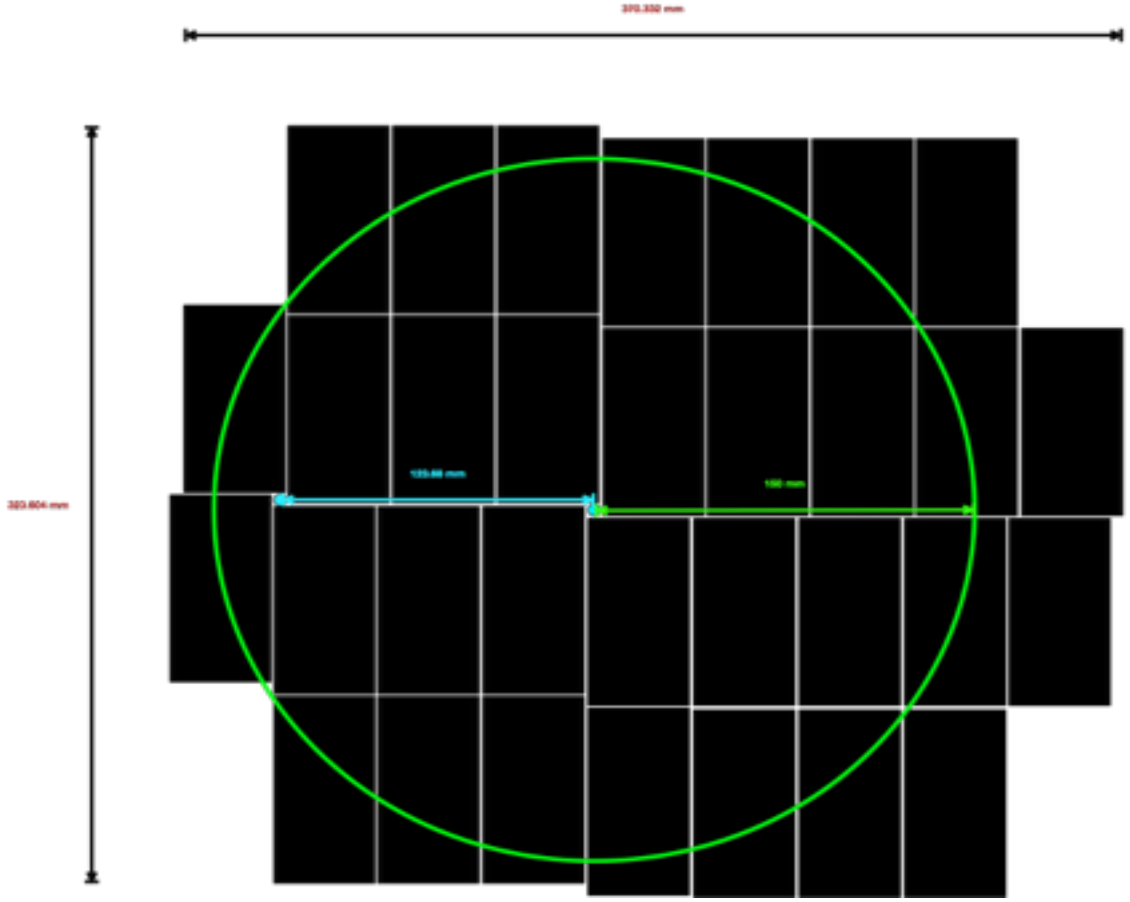
ESA Prime spectrometer

- To cover 1-5 keV X-ray emission energies we need exotic crystals
- Needs to operate in vacuum to avoid X-ray loss
- Spectrometer compartment should be isolated from sample compartment
- Crystals and detectors need some travel range to cover the desired X-ray energies
- This X-ray energy range is a priority for SwissFEL



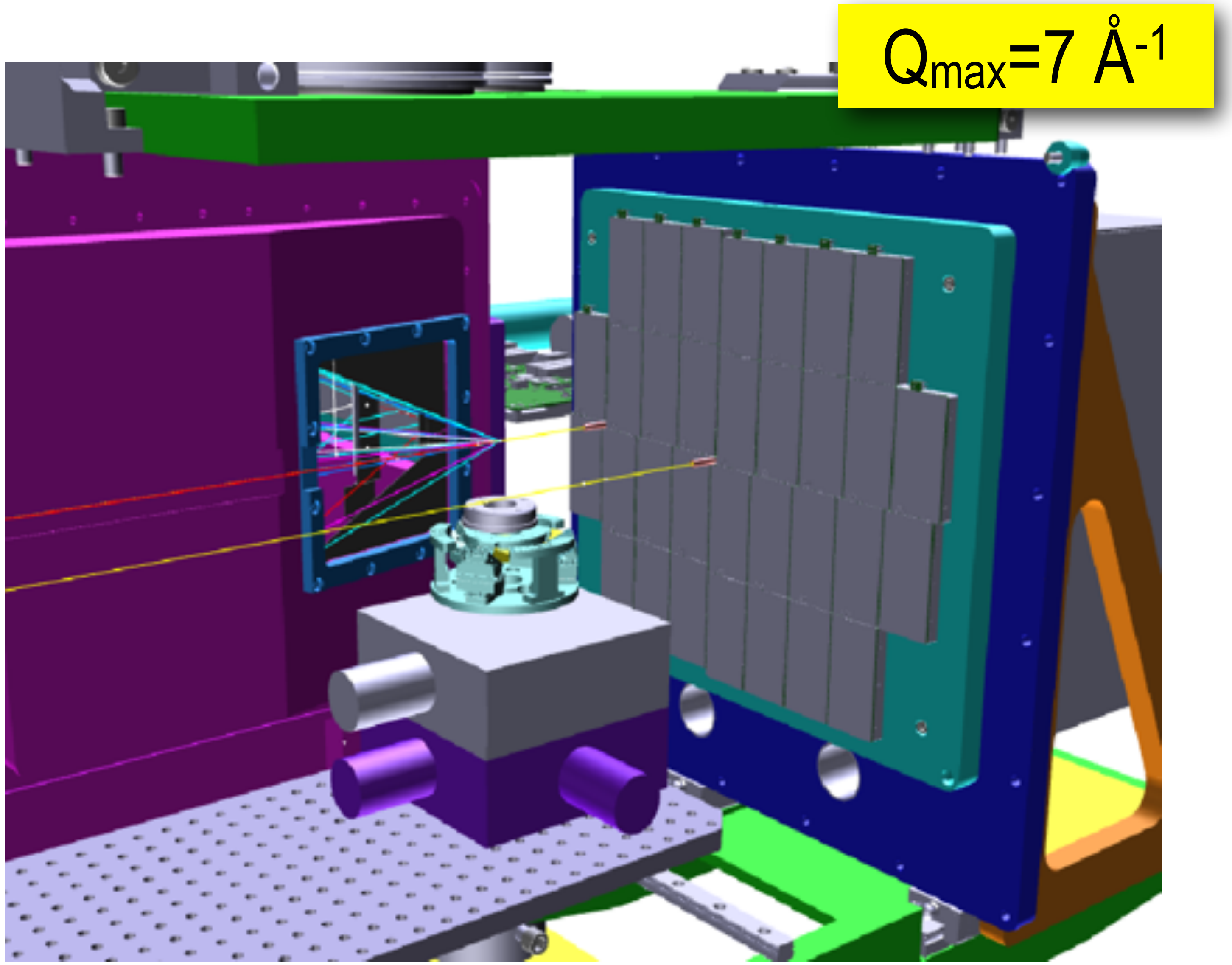
ESA Prime: Scattering experiments





Goals

- Detector as close as possible (100 mm)
- Protect detector from sample/He/mechanical damage/optical laser with window (Kapton/Mylar)
- Simultaneous use of spectrometer and Jungfrau 16M
- Two horizontal chamber positions for different experimental priorities (scattering/diffraction Vs spectroscopy)



Lipidic-cubic phase jets for SFX

J. Standfuss, P. Nogly,
G. Schertler (BIO)

Tested LCP jet at ESRF microfocus beamline and under pump-probe conditions at LCLS (CXI)

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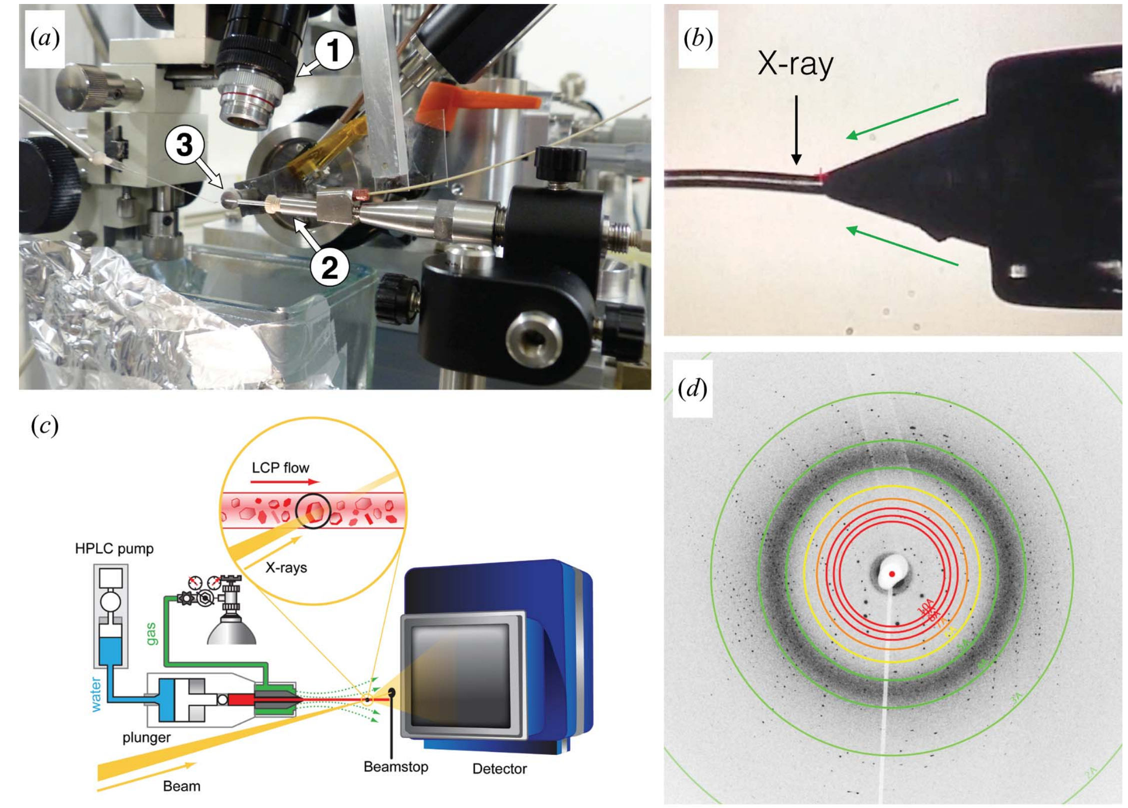
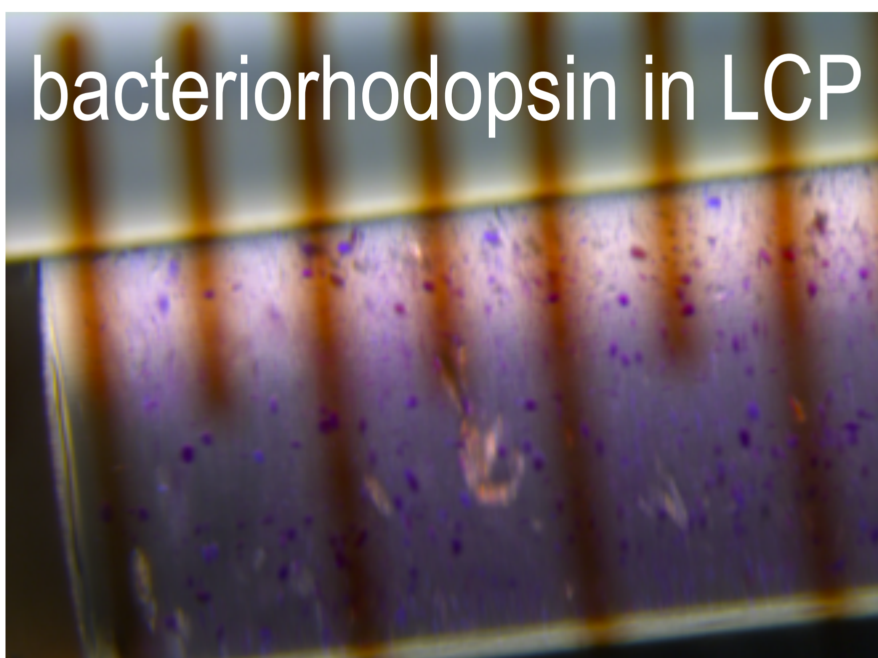
Received 16 October 2014
Accepted 1 December 2014

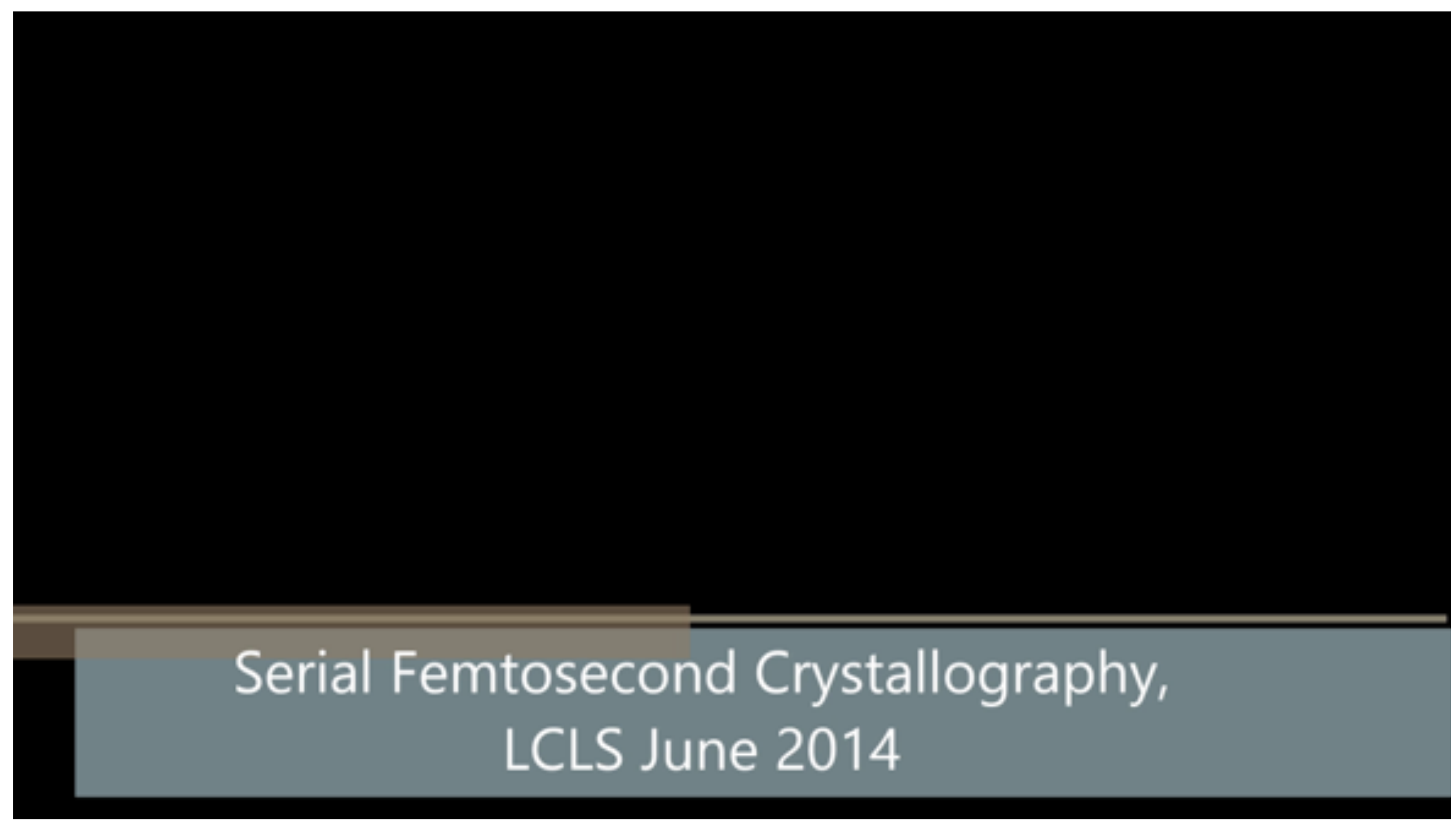
Lipidic cubic phase serial millisecond crystallography using synchrotron radiation

Przemyslaw Nogly,[a] Daniel James,[b] Dingjie Wang,[b] Thomas A. White,[c] Nadia Zatsepin,[b] Anastasya Shilova,[d] Garrett Nelson,[b] Haiguang Liu,[b] Linda Johansson,[e] Michael Heymann,[c] Kathrin Jaeger,[a] Markus Metz,[c,f] Cecilia Wickstrand,[g] Wenting Wu,[a] Petra Båth,[g] Peter Berntsen,[g] Dominik Oberthuer,[c,f] Valerie Panneels,[a] Vadim Cherezov,[e] Henry Chapman,[c,h] Gebhard Schertler,[a,i] Richard Neutze,[g] John Spence,[b] Isabel Moraes,[j,k,l] Manfred Burghammer,[d,m]* Joerg Standfuss[a]* and Uwe Weierstall[b]*



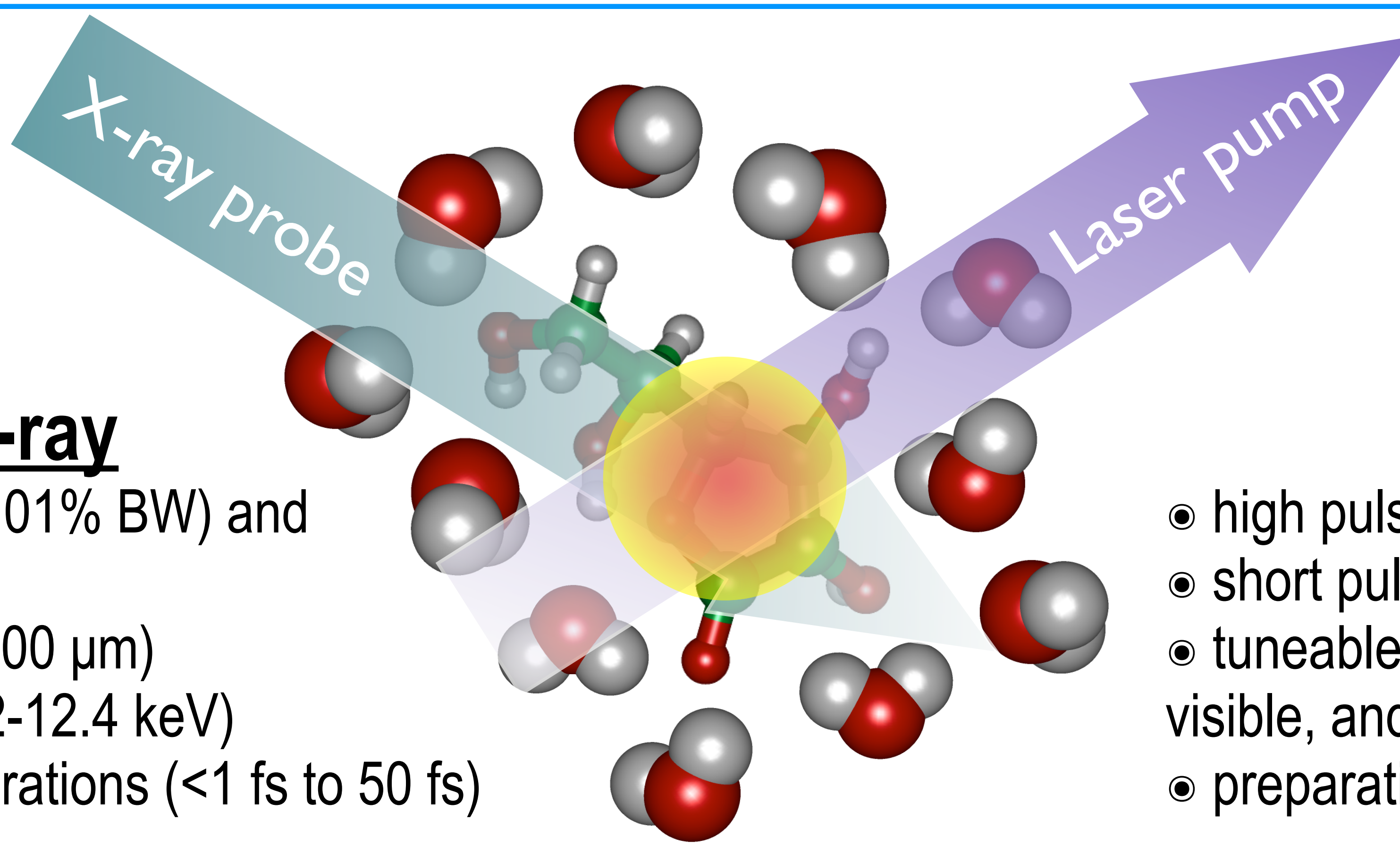


media courtesy of Przemek Nogly



SwissFEL Experimental Station A

Goal: To have this ready by 2017



X-ray

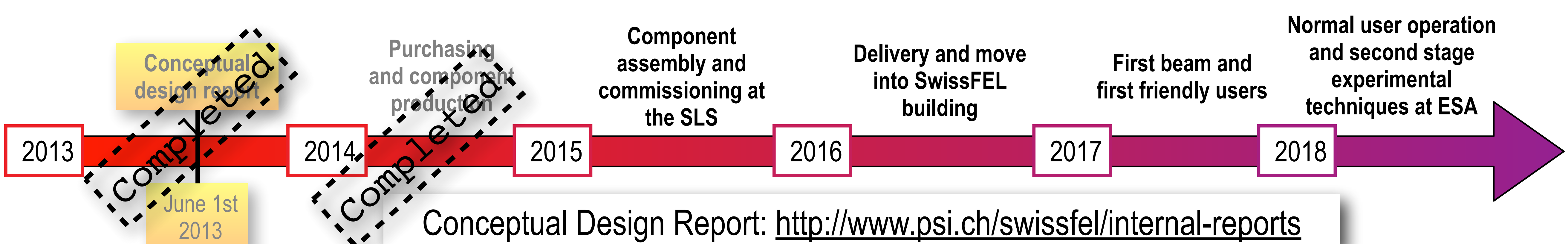
- monochromatic (0.01% BW) and broadband (1-4%)
- variable focus (1-100 μm)
- tuneable energy (2-12.4 keV)
- ultrashort pulse durations (<1 fs to 50 fs)

Laser

- high pulse energies (5-10 mJ)
- short pulses (20-50 fs)
- tuneable wavelengths including IR, visible, and UV
- preparation for THz and <10 fs

Available experimental configurations

- pump-probe sample chamber for use at low pressure and controlled environments with all probe techniques
- 2D scattering detector (PSI 16M Jungfrau, 75 μm pixels, 10^4 dynamic gain)
- **ESA Prime instrument covering the 1-12 keV range (XES, HEROS, IXS, RXES)**
- jets for solution samples (100 μm) and serial fs crystallography (4 μm)

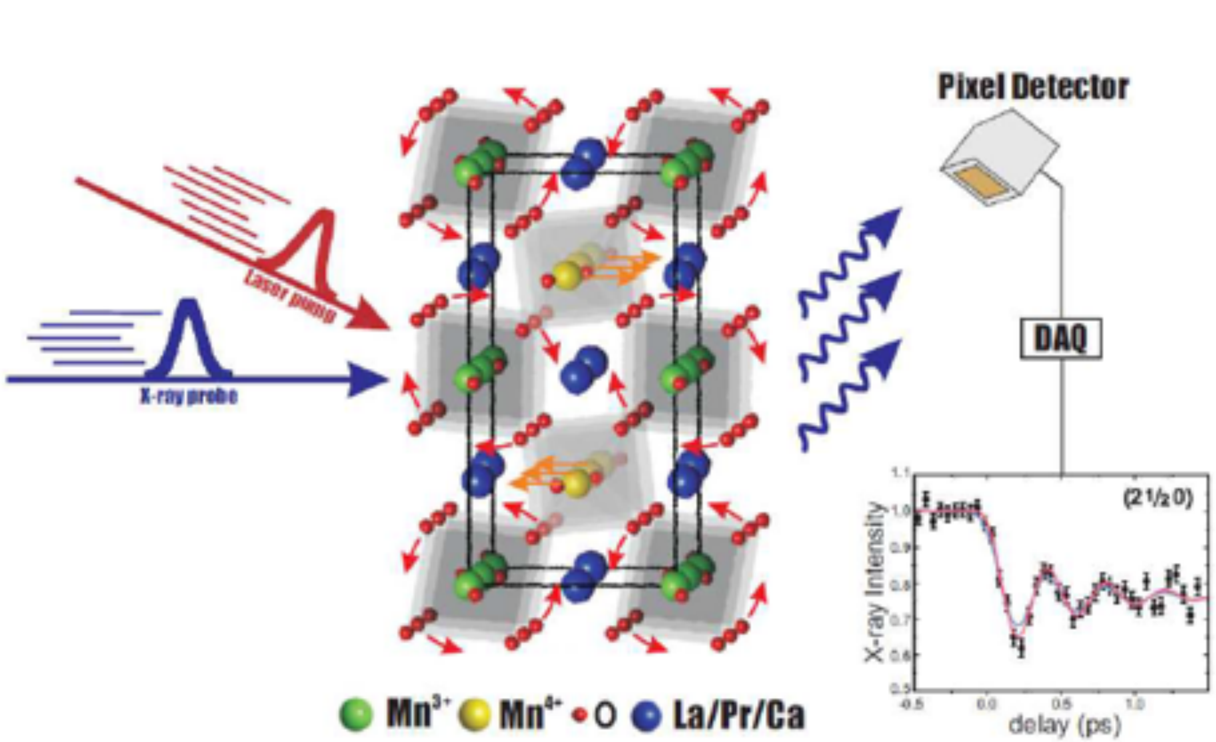


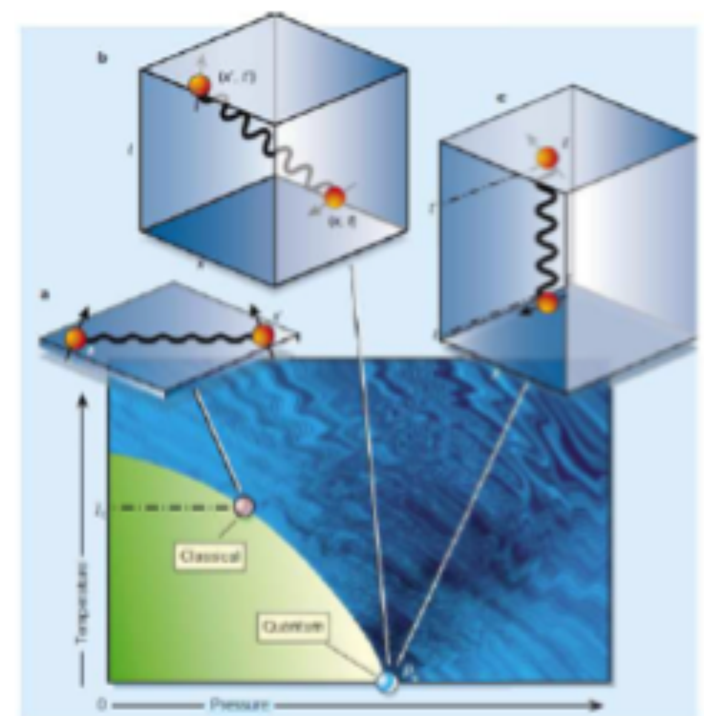
Conceptual Design Report: http://www.psi.ch/swissfel/internal-reports

ESB: Probing Correlated Coupled Dynamics & Fluctuations

→ **pump: launch coherent excitation**
(phonon, spin wave, charge wave, orbital wave, ...)

→ **tune system close to critical point**
(apply static pressure or B-field at low T)





[P. Coleman, Nature 413 (2001)]

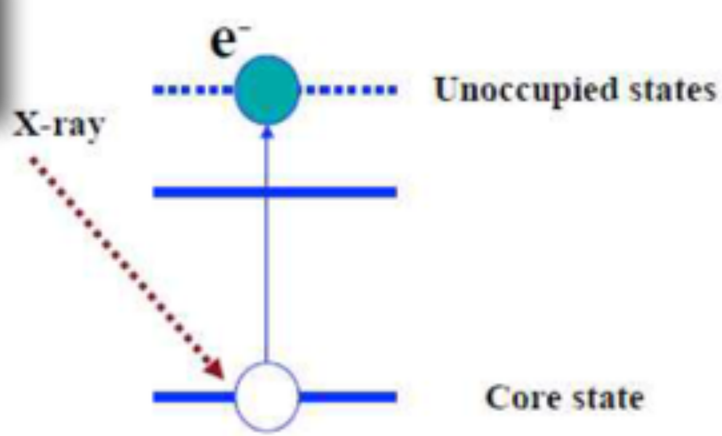
→ X-ray probe: how does the (coherent) excitation evolve in time ?

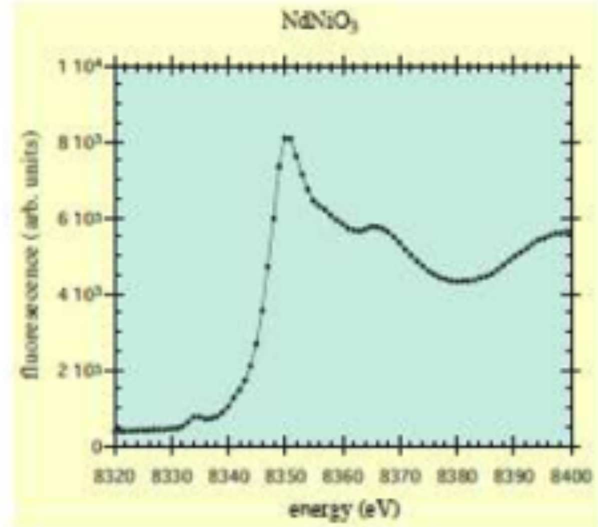
↔ tr-XRD: measures changes in lattice constants & symmetry
↔ tr-RXRD: sensitive to coupling of charge-, orbital- and spin-order (↔ polarization)
↔ tr-(N)TDS: measures S(**q**,ω = 0) & fluctuating coherence length ξ_F
↔ tr-(R)IXS: measures S(**q**,ω) & change of momentum dispersion

ESB: The X-ray probe techniques

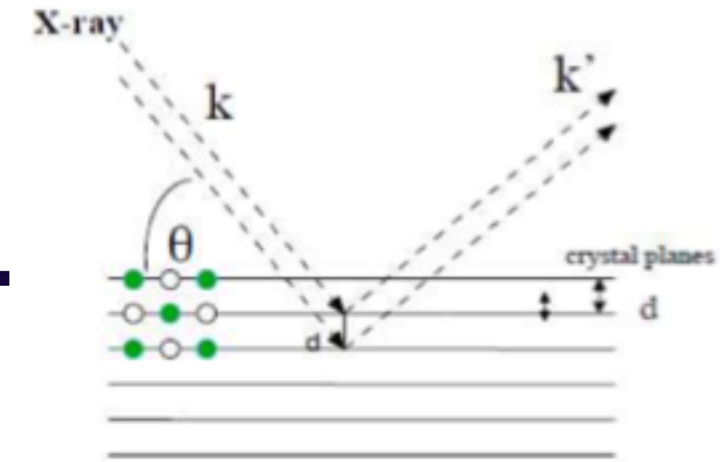
Gerhard Ingold and Paul Beaud

Resonant X-ray Diffraction



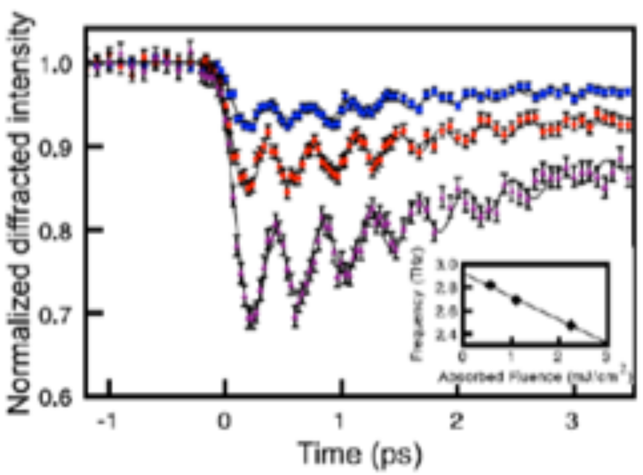


+



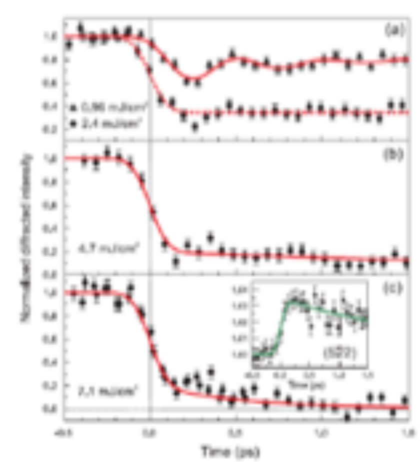
X-ray Diffraction

Peierls system: coherent phonons (Bi)



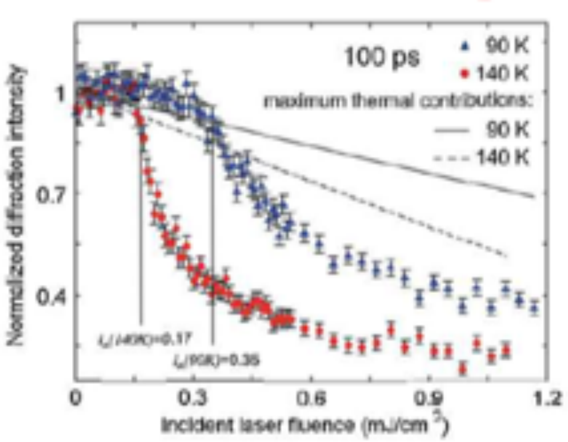
[Johnson PRL 2008]

Jahn-Teller dynamics (LCMO)



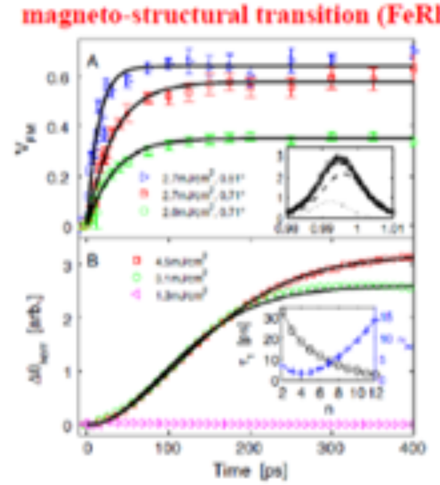
[Beaud PRL 2009]

excitonic CDW system ($TiSe_2$)



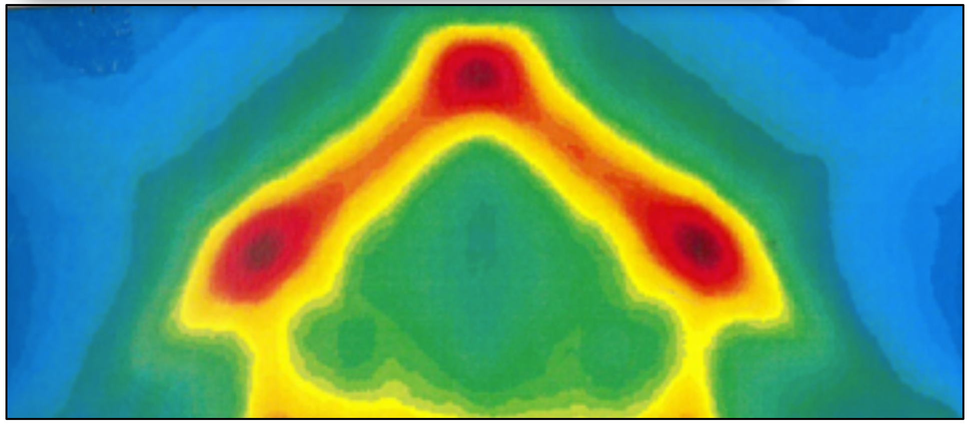
[Vorobeva PRL 2011]

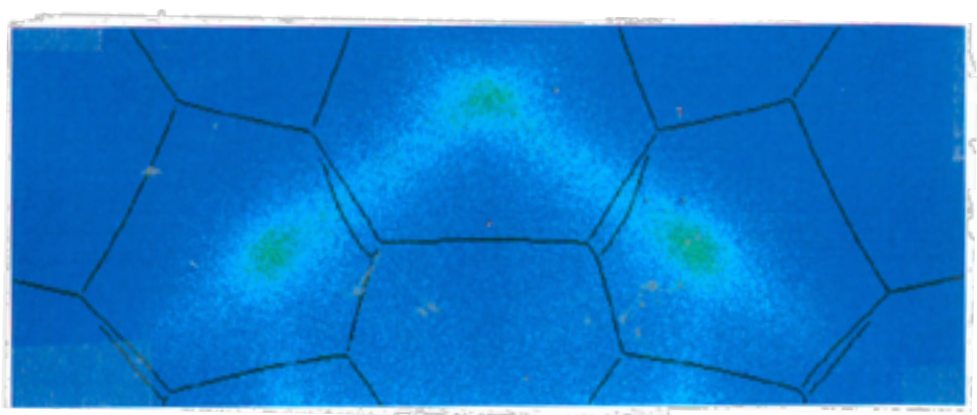
magneto-structural transition (FeRh)



[Mariager PRL 2012]

Elastic X-ray Diffuse Scattering

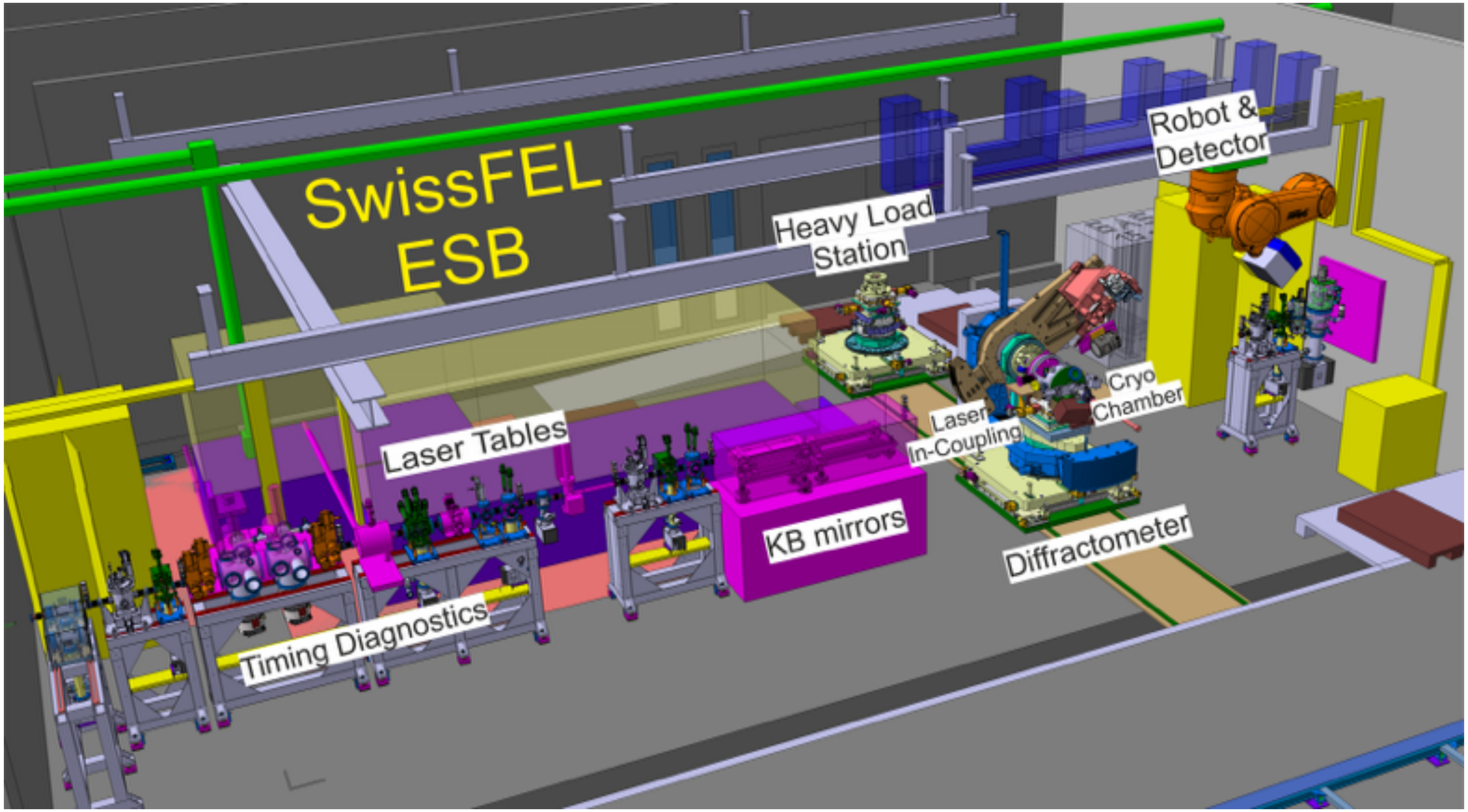




TDS from Si(100) measured at the SLS (courtesy J. Johnson)

SwissFEL ESB: General Layout

Femtosecond Pump-Probe X-ray Diffraction and Scattering (Crystalline Samples)
Energy Range 4.5 - 12.4 keV, X-ray Spot Size 2 - 200 μm

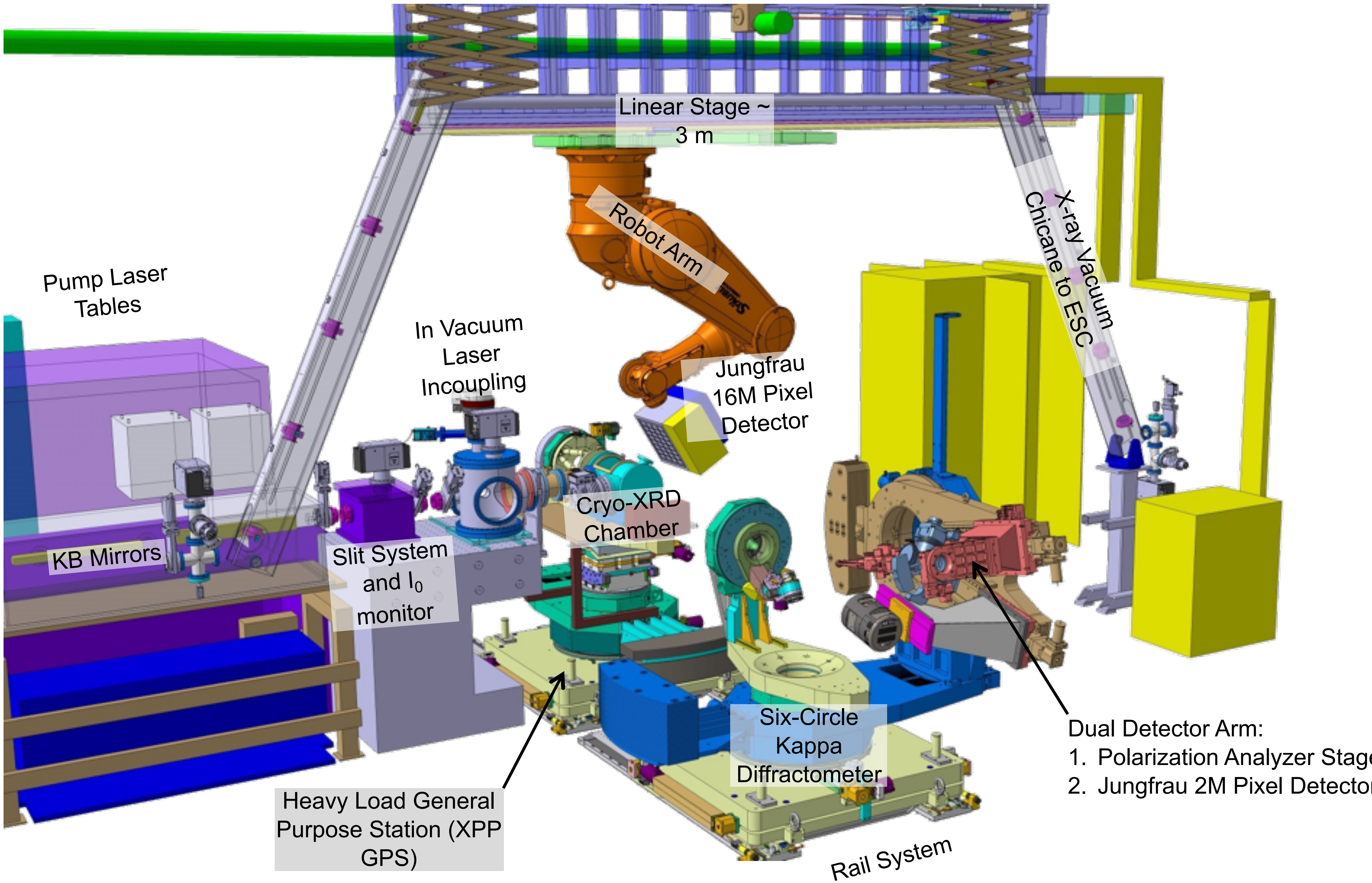


Single X-ray focus position – two Endstations:

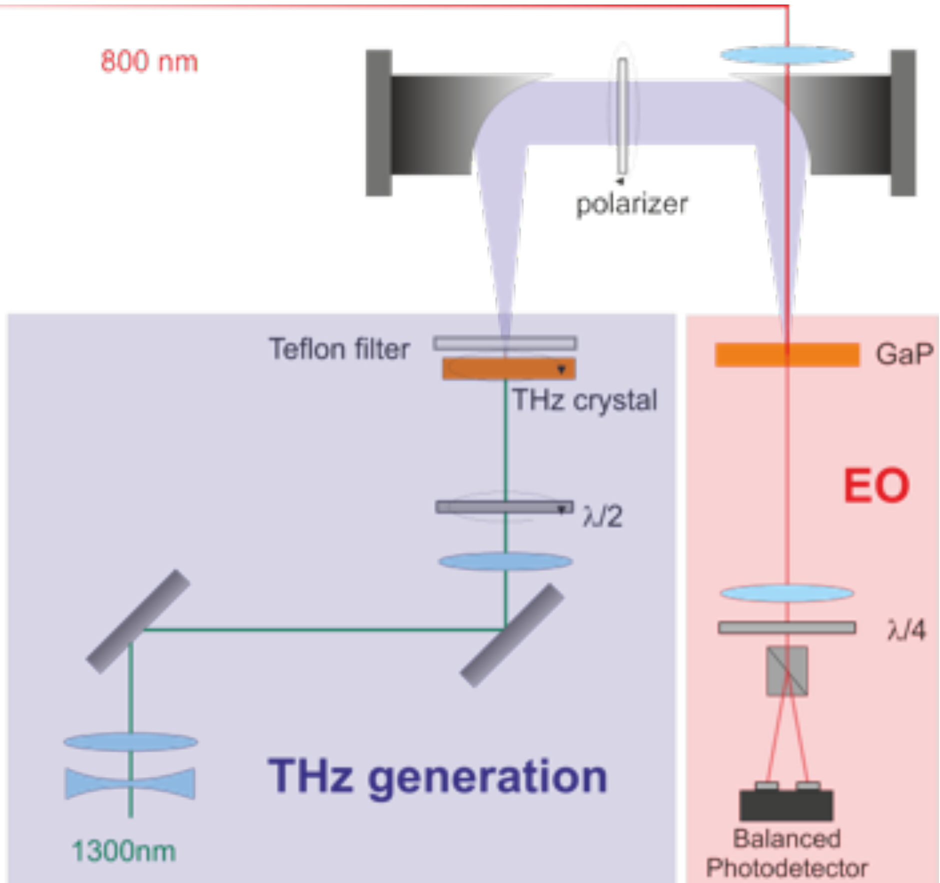
- **Pump-Probe General Purpose Station: XPP GPS (Heavy Load Station + Robot Detector Arm)**
- **Pump-Probe (Resonant) Diffraction: XPP XRD (Six-Circle Kappa Diffractometer)**

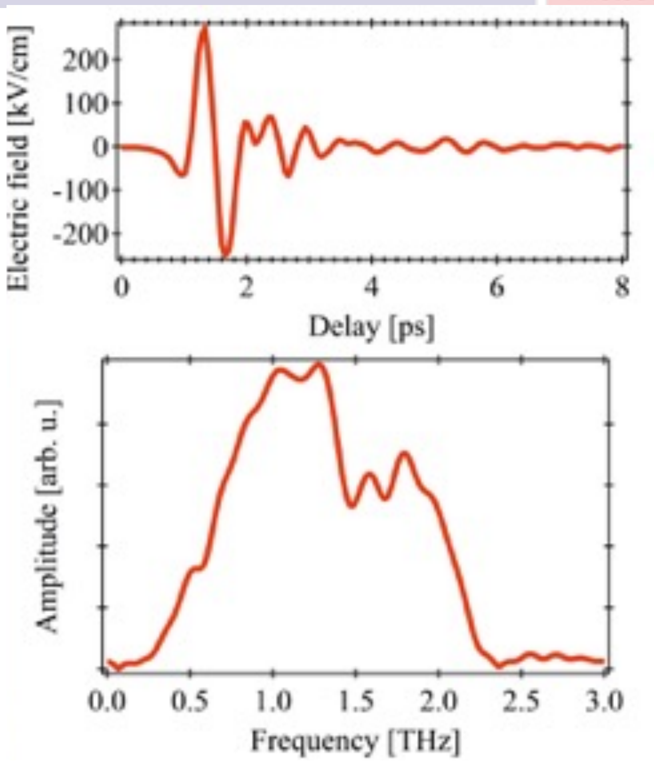
(Cryo Diffraction Chambers mounted on both stations)

SwissFEL ESB: Two Endstations



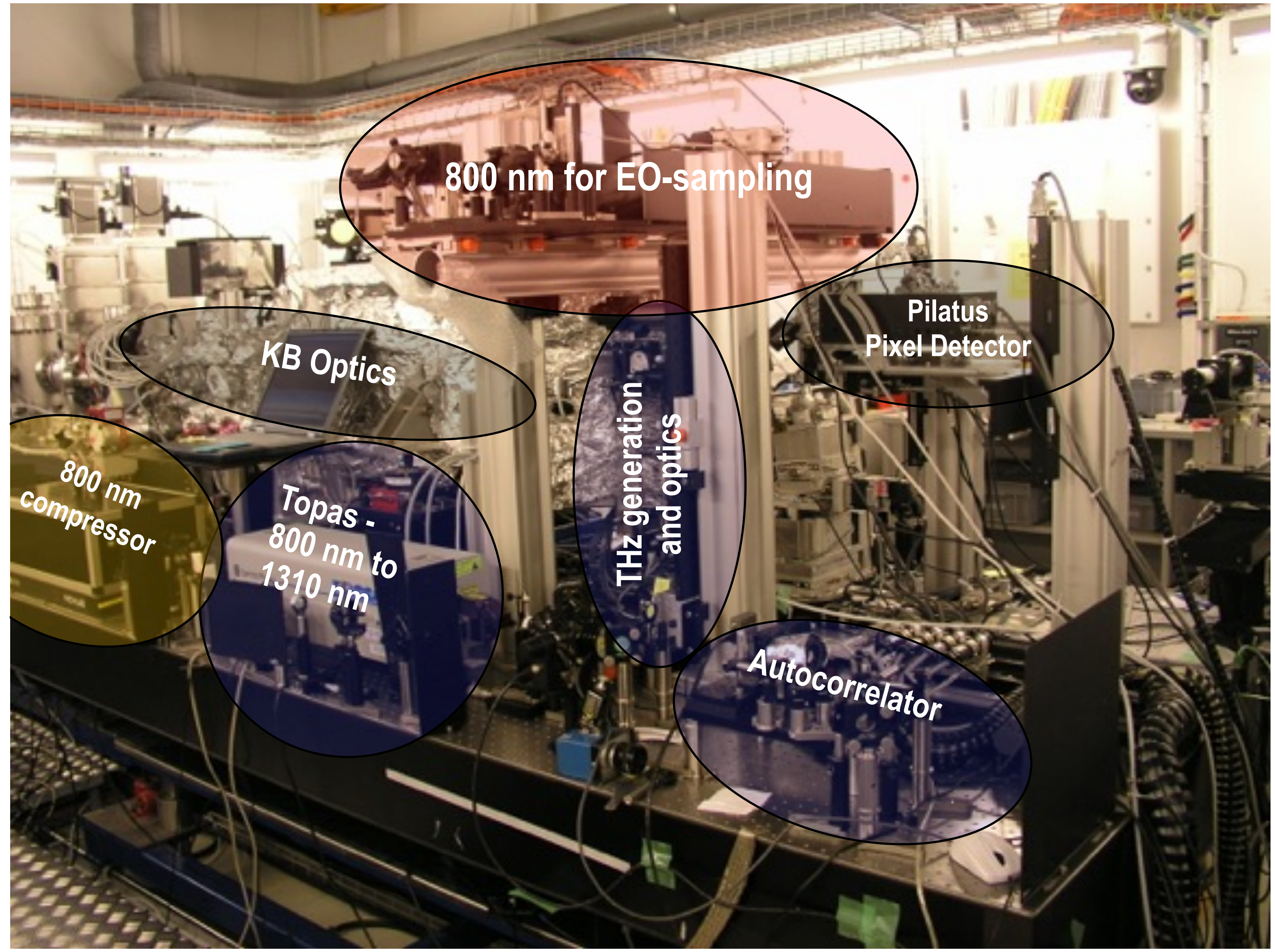
THz Pump – XRD Probe Setup (R&D FEMTO@MicroXAS)

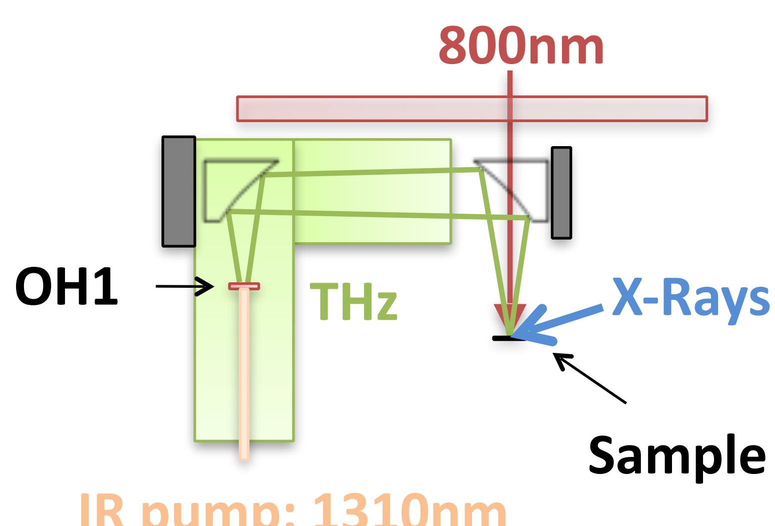


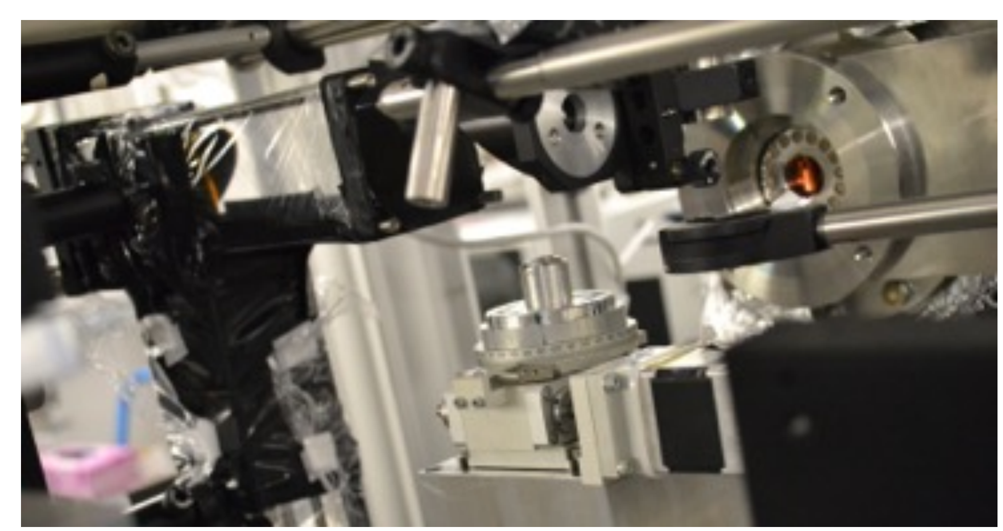


Structural Order in $Sn_2P_2S_6$: Ferroelectric Polarization

Grübel et. al. (in preparation)

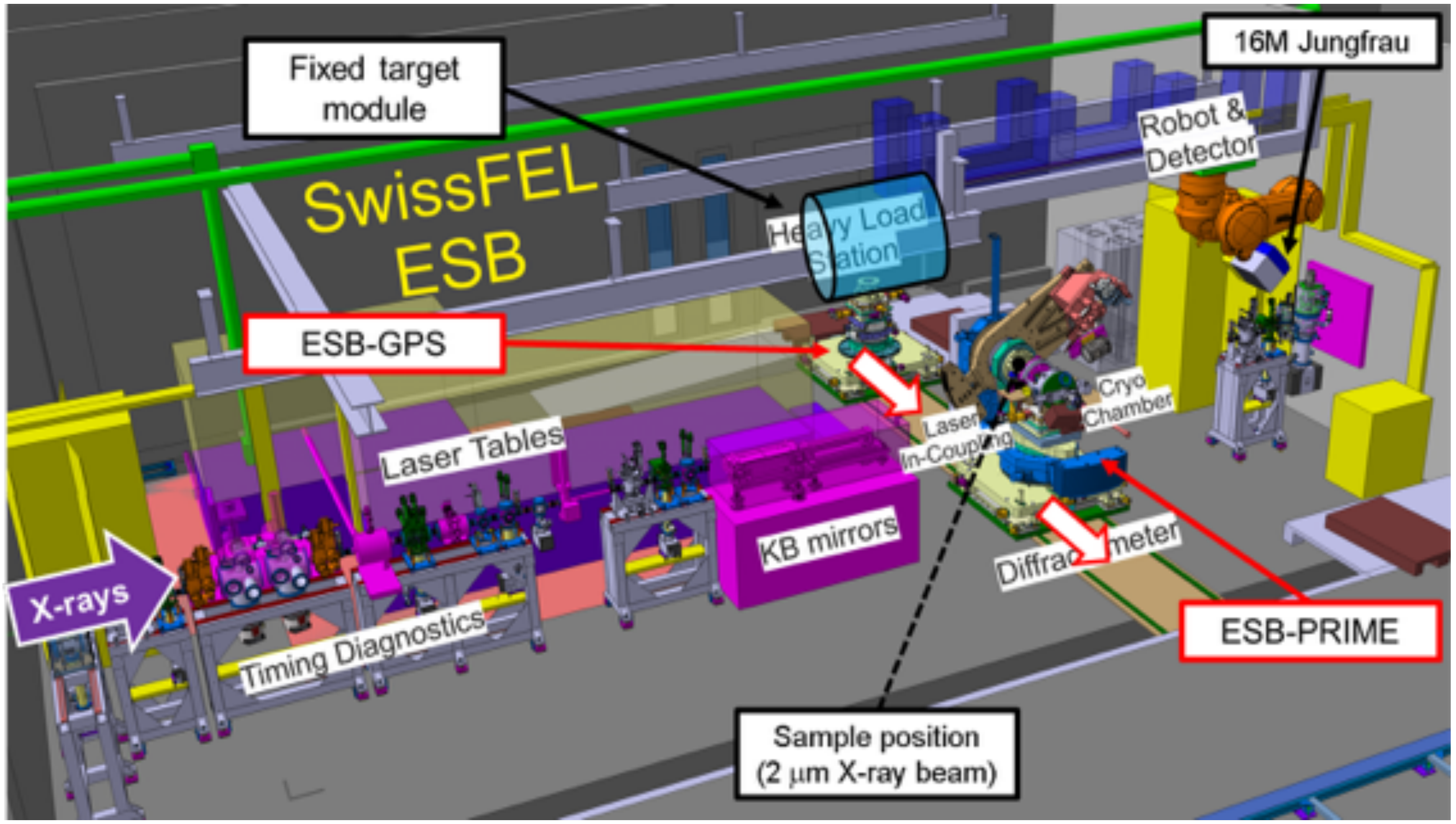




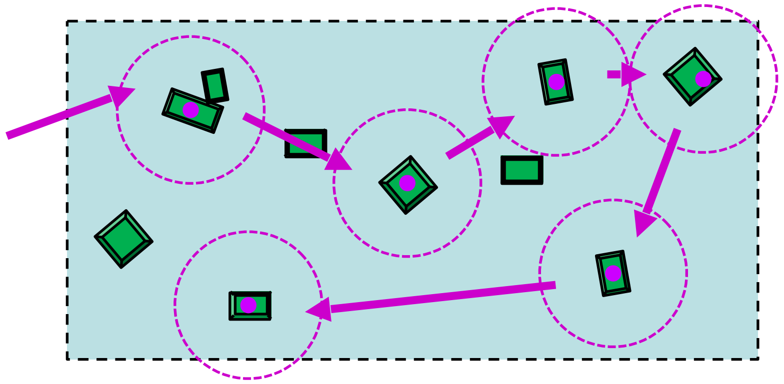


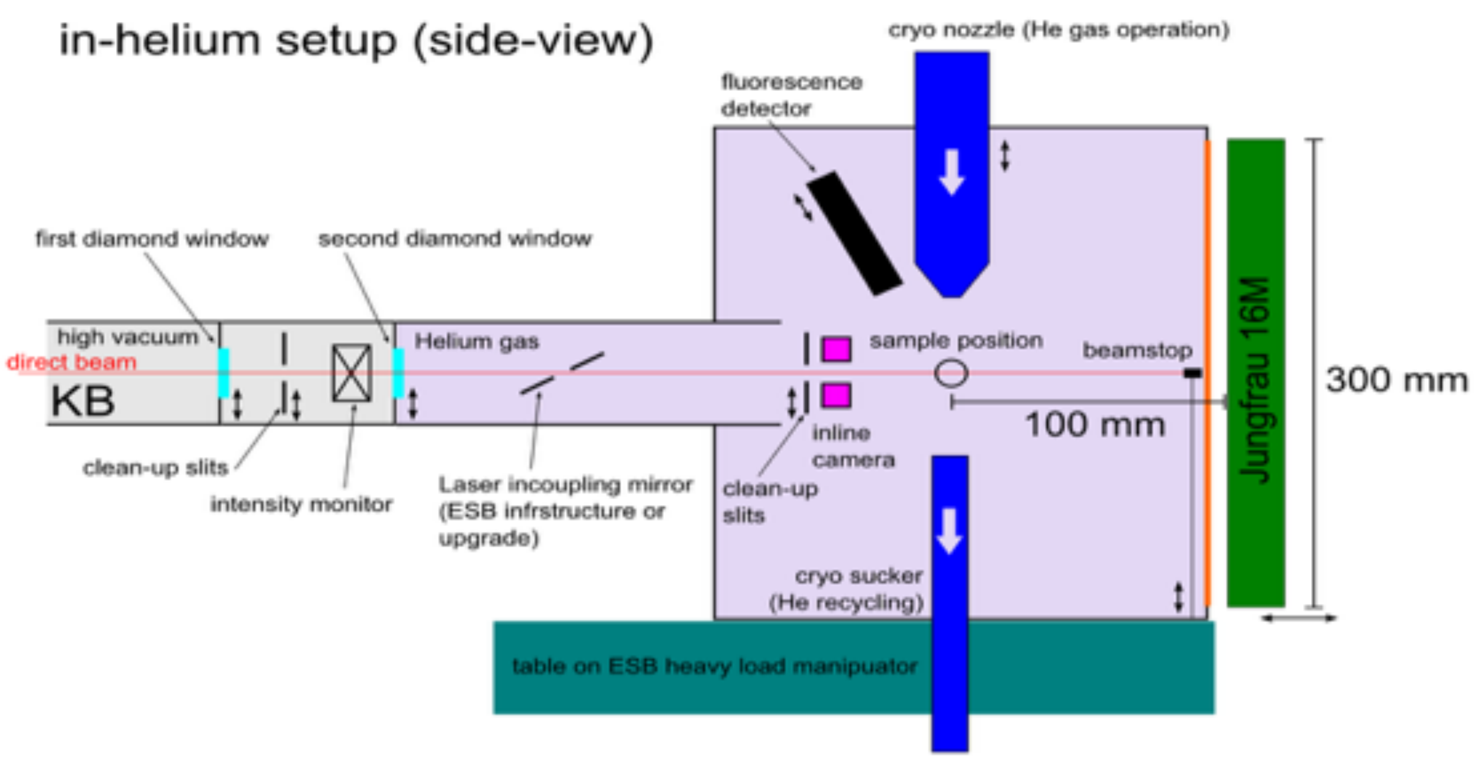
Fixed target protein crystallography module at ESB-GPS

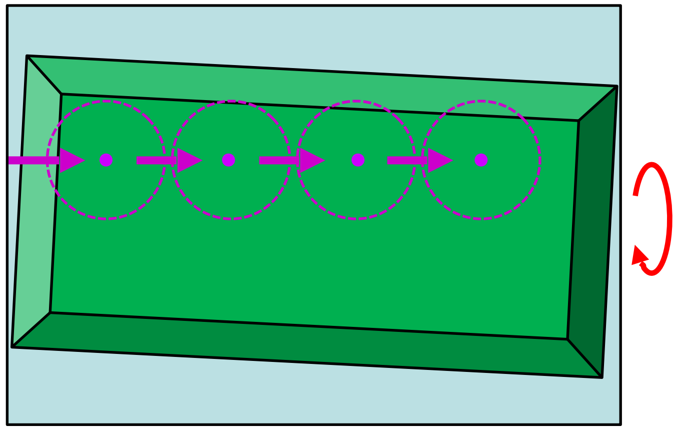
- Movable, suitable for ESB-GPS
- Room temperature AND Cryo
- In-air AND In-helium
- 100 Hz serial (scanning) femtosecond crystallography (< 5 μm xtals)
- Synchrotron-like femtosecond crystallography (> 5 μm xtals)



Serial (scanning) femtosecond crystallography



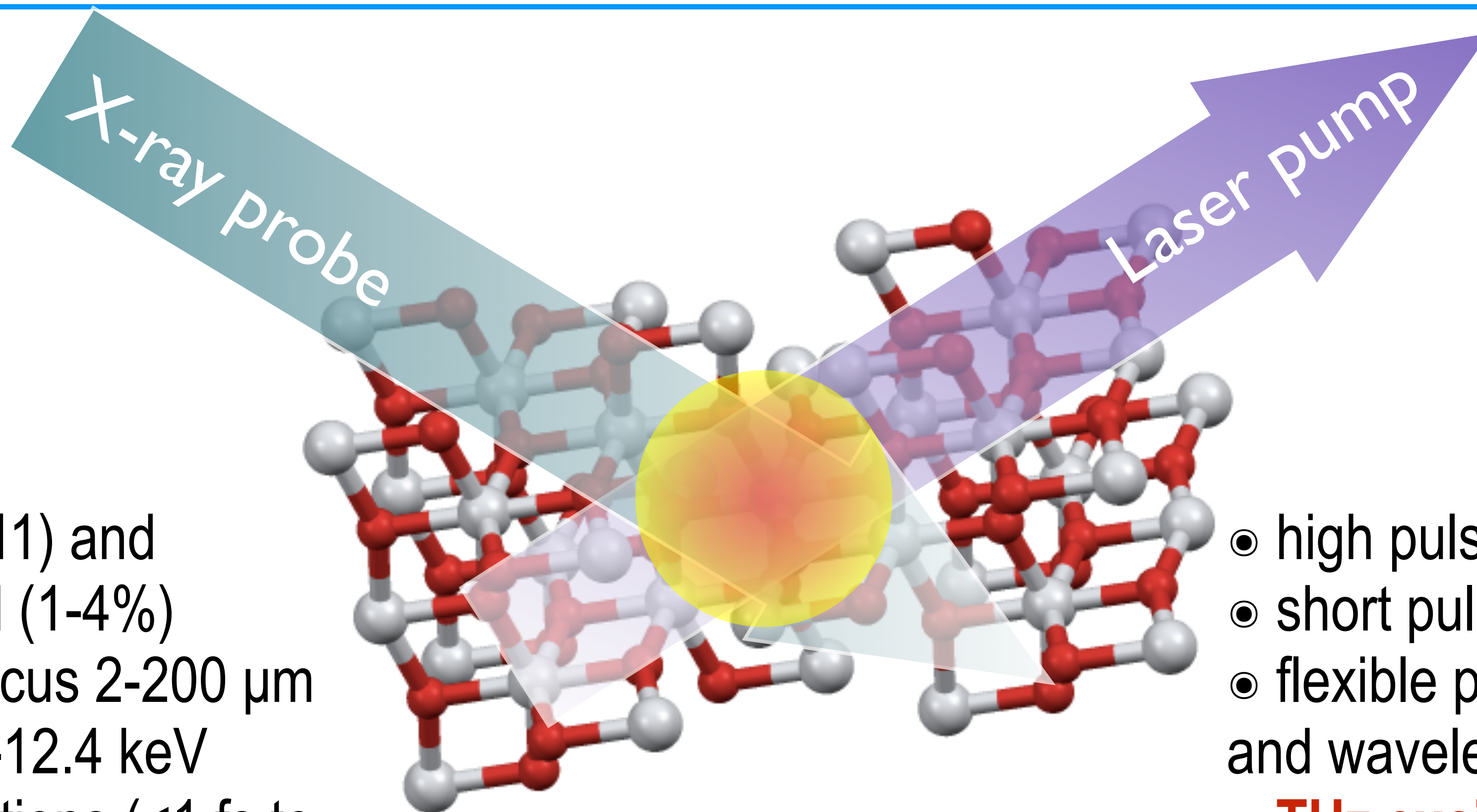




Synchrotron-like femtosecond crystallography

SwissFEL Experimental Station B

Goal: To have this ready by 2017



X-ray

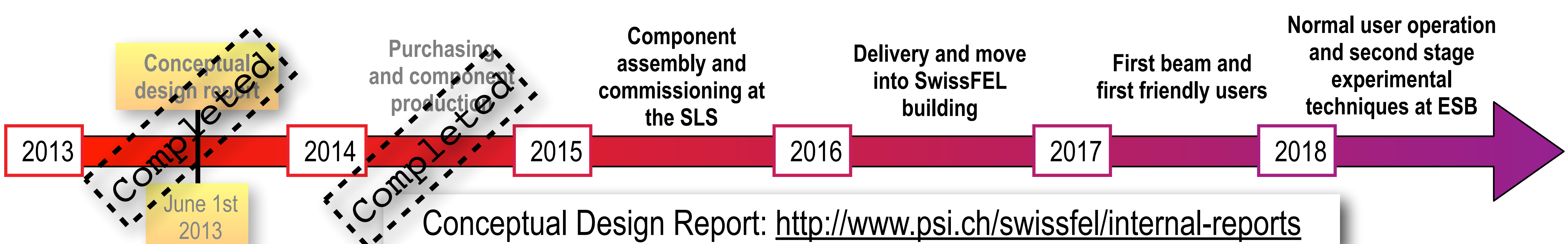
- monochromatic Si(111) and Si(311) and broadband (1-4%)
- variable KB mirror focus 2-200 μm
- tuneable energy 4.5-12.4 keV
- ultrashort pulse durations (<1 fs to 50 fs)

Laser

- high pulse energies (5-10 mJ)
- short pulses (10-20 fs)
- flexible pump setup (polarization and wavelength UV to NIR)
- **THz excitation** and <10 fs

Available experimental configurations

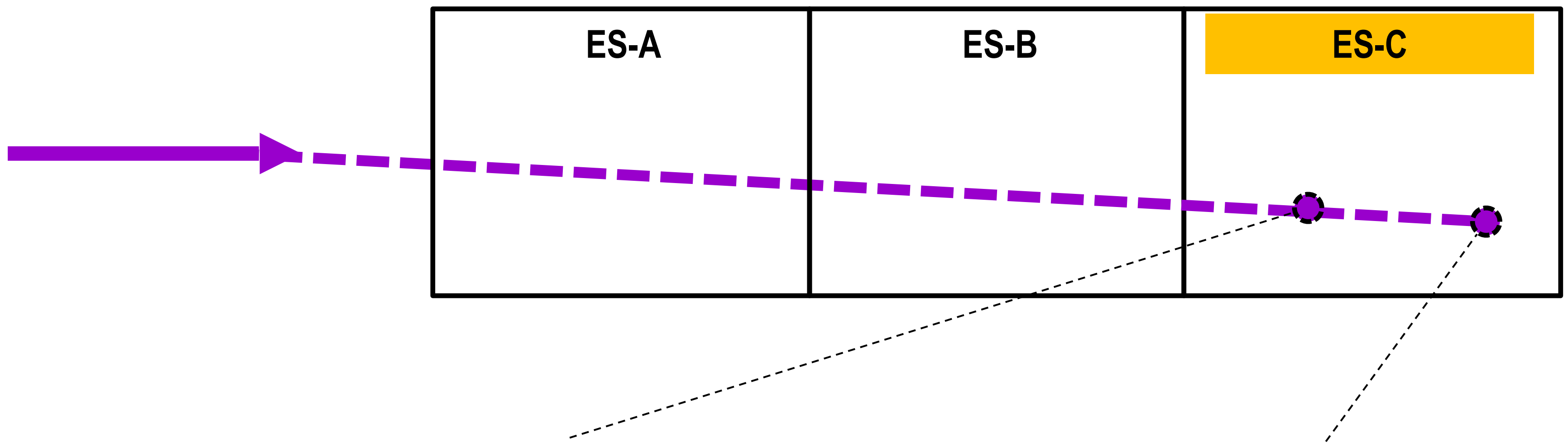
- 6-circle diffractometer
- 2D scattering detector (PSI 16M Jungfrau, 75 μm pixels, 10^4 dynamic range)
- **HV/UHV diffraction chamber with cryo cooling (10-700 K)**
- Time arrival monitor <10 fs (P. Juranić et. al., Opt. Expt. **22**, 30004 (2014).)
- General-purpose station for hosting user setups (e.g. fixed-target protein crystallography)



Conceptual Design Report: http://www.psi.ch/swissfel/internal-reports

Experimental Station C

Material science and nanocrystallography



Phase alpha 201X

Parameter	Value
Focusing scheme	*KB*
Photon energy	*4.0 – 12.6 keV*
Focus size	***150 nm***
Transmission	*0.7 – 0.8*
Distance from last mirror	*350 mm*

Phase beta 20XX

Parameter	Value
Focusing scheme	*Multilayer KB*
Photon energy	*12.2 – 12.8 keV (e.g.)*
Focus size	***20 nm***
Transmission	*0.2 – 0.5*
Distance from last mirror	*30 mm*

- **Material science at the nanoscale**
- **Non/linear X-ray optics**
- **Protein 2D crystallography**
- **(Single particle imaging)**

Send your great ideas to
Bill Pedrini
bill.pedrini@psi.ch

Calculations by **Rolf Follath**

In progress, stay tuned…

PAUL SCHERRER INSTITUT

Acknowledgements

SwissFEL project: R. Abela, P. Juranic, B. Pedrini, L. Patthey, Ch. Erny, B. Patterson, L. Sala, T. Penfold, P. Heimgartner, P. Wiegand, J. Szlachetko, G. Knopp, J. Réhault, Y. Deng

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DTU: K. Haldrup;

Wigner: G. Vankó;

Rennes: M. Lorenc;

Fribourg: J-C. Dousse, J. Hoszowska;

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