
# Layout and Opportunities with 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…

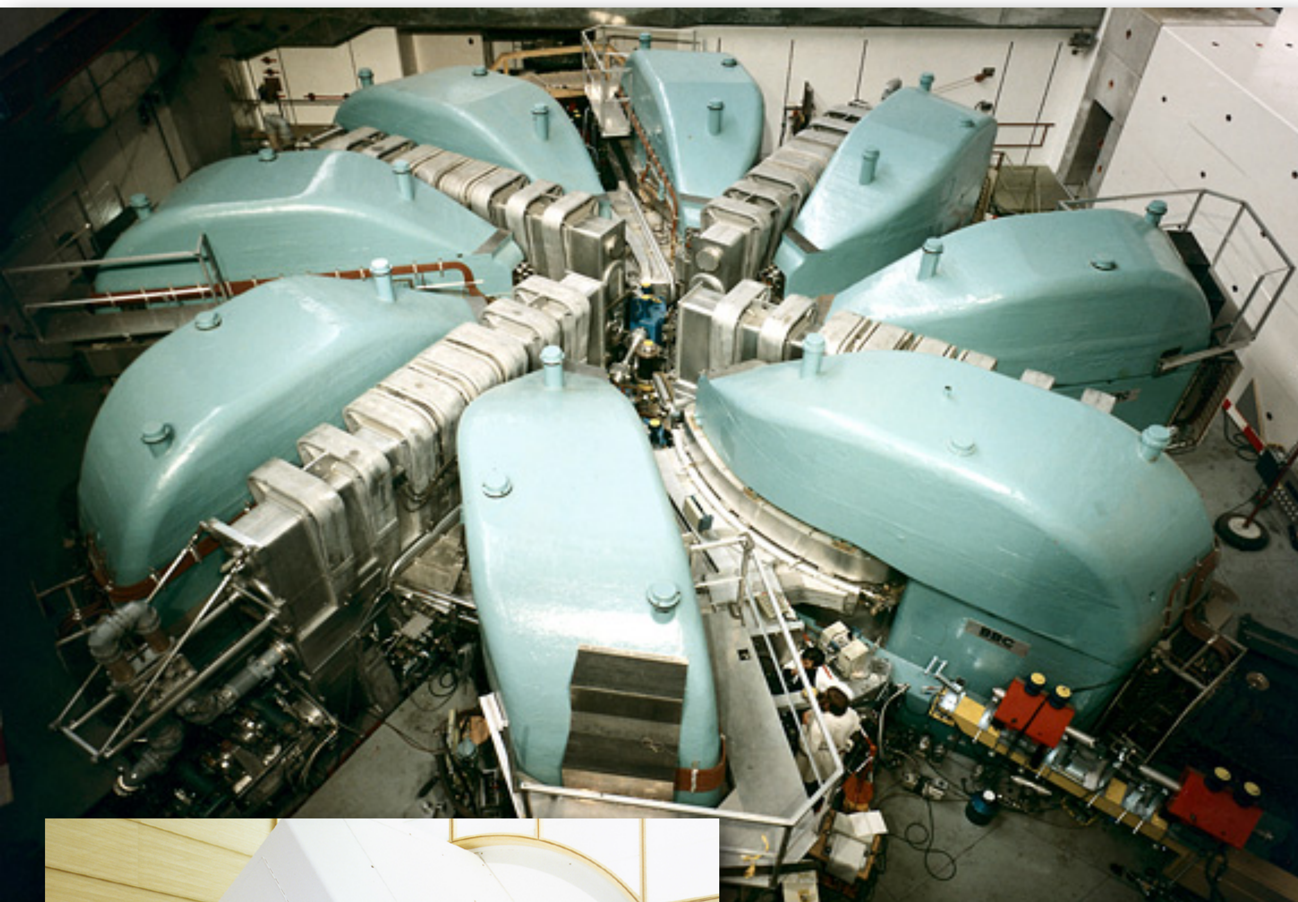
# Paul Scherrer Institute

- 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

**DIRECTORATE**

| | |
|---|---|
| Research Committee | Human Resources |
| Large Project SwissFEL | Safety |
| CCEM-CH | Communications |
| Center for Proton Therapy | Technology Transfer |

| Research Department | Research Department | Research Department | Research Department | Research Department | Department | Department |
|---|---|---|---|---|---|---|
| Research with Neutrons and Muons | Synchrotron Radiation and Nano-technology | General Energy | Nuclear Energy and Safety | Biology and Chemistry | Large Research Facilities | Logistics |



# Fall 2012: Swiss Parliament approved SwissFEL

**Brief project history at PSI**

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

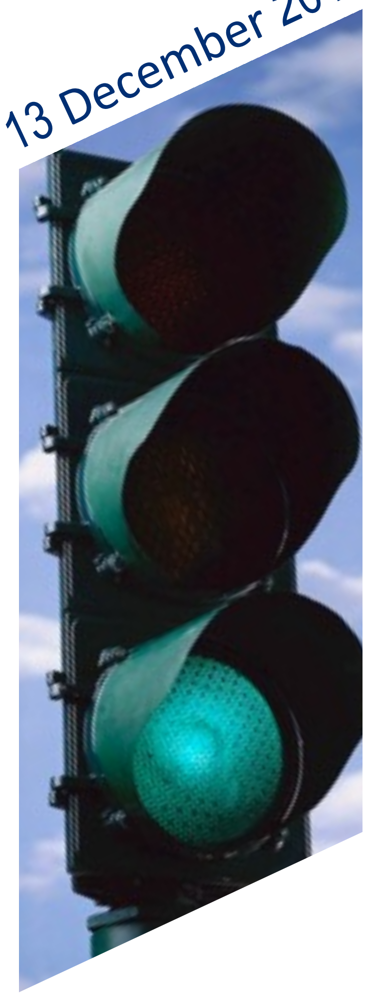
2005-2008 PSI-XFEL Project

2009 Beginning of SwissFEL Project

25 September 2012

Swiss Parliament passes 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

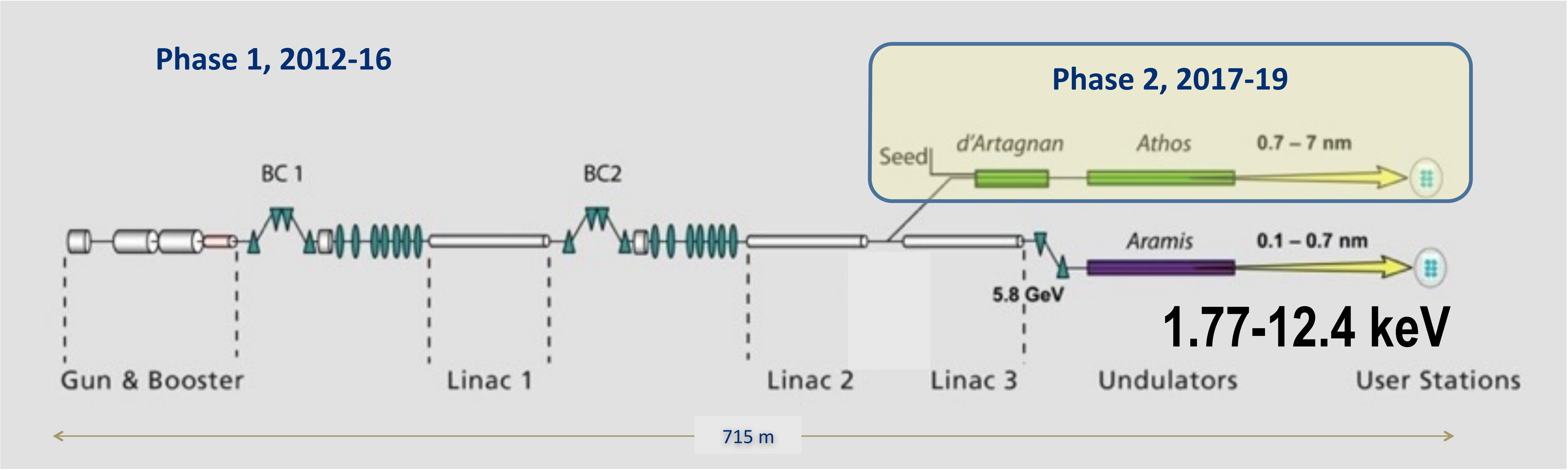
# SwissFEL: June 27, 2013

# 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 |

PAUL SCHERRER INSTITUT PSI

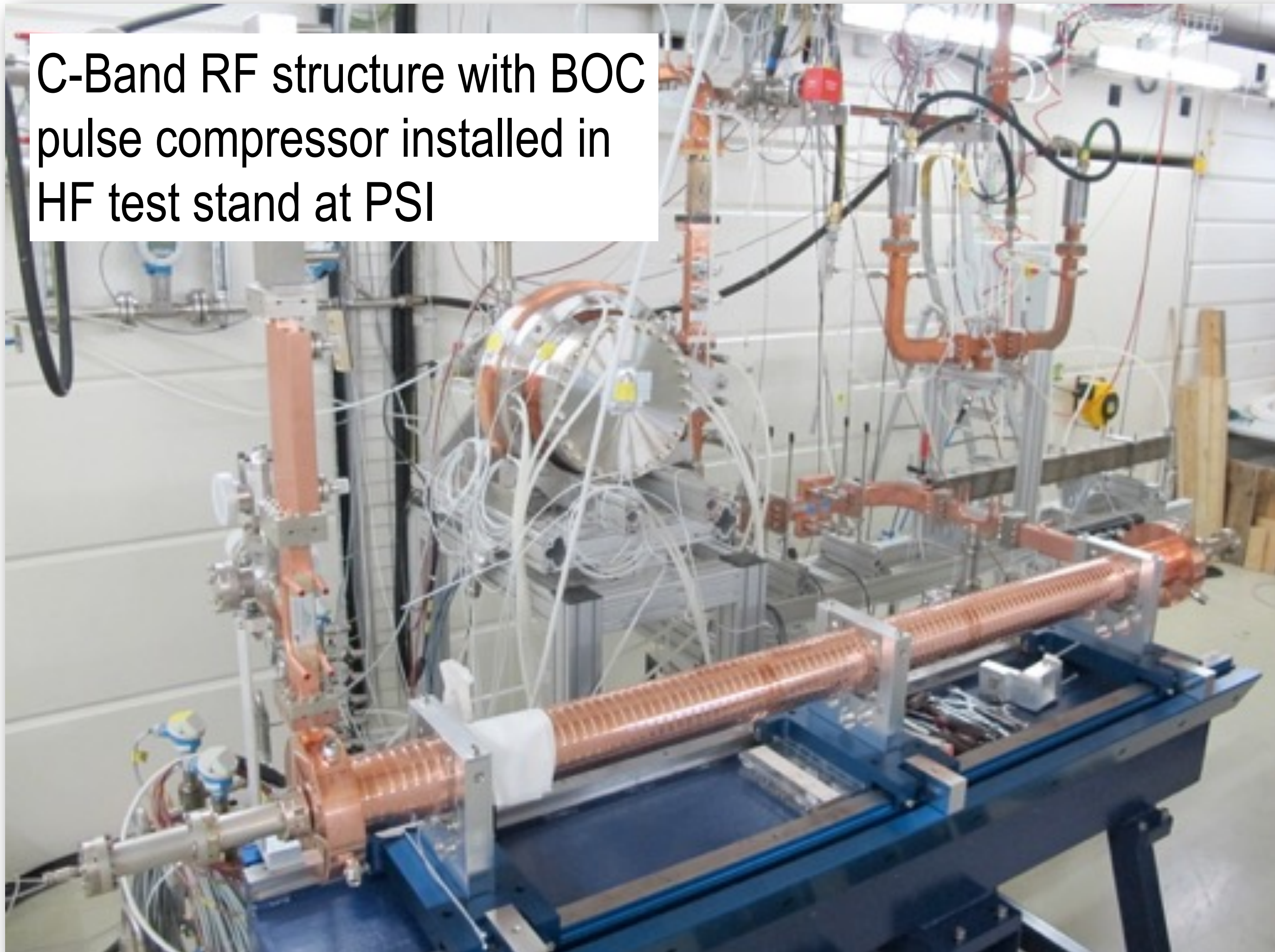
# SwissFEL design parameters at 1 Å (12.4 keV)

Sven Reiche and co-workers

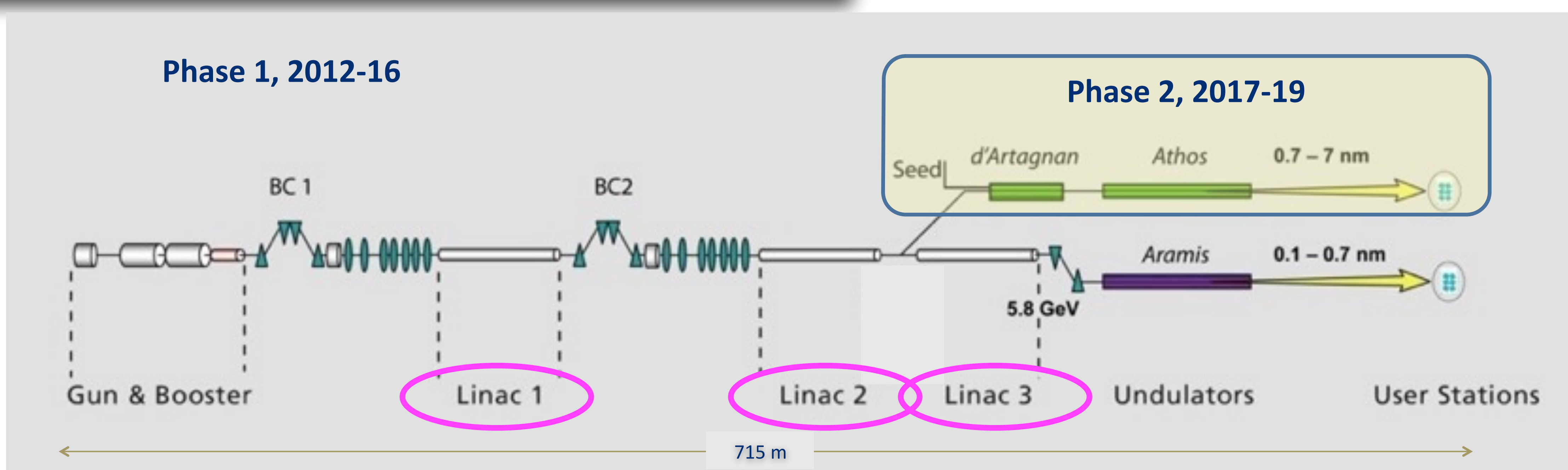
| FEL Beam Design Parameters | Nominal Operation Mode | | Special Operation Mode | |
|---|---|---|---|---|
| | Long Pulses | Short Pulses | Large Bandwidth | Ultra-Short Pulses |
| Undulator period (mm) | 15 | 15 | 15 | 15 |
| Undulator parameter | 1.2 | 1.2 | 1.2 | 1.2 |
| Energy spread (keV) | 350 | 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

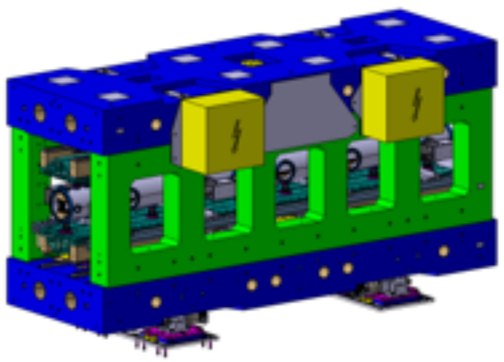



| | # RF stations | *E* (GeV) |
|---|---|---|
| Injector | 1+1+4 S-band, 1 X band | 0.355 |
| Linac 1 | 9 C-band | 2.1 |
| Linac 2 | 4 C-band | 3.0 |
| Linac 3 | 13 C-band | 5.8 |



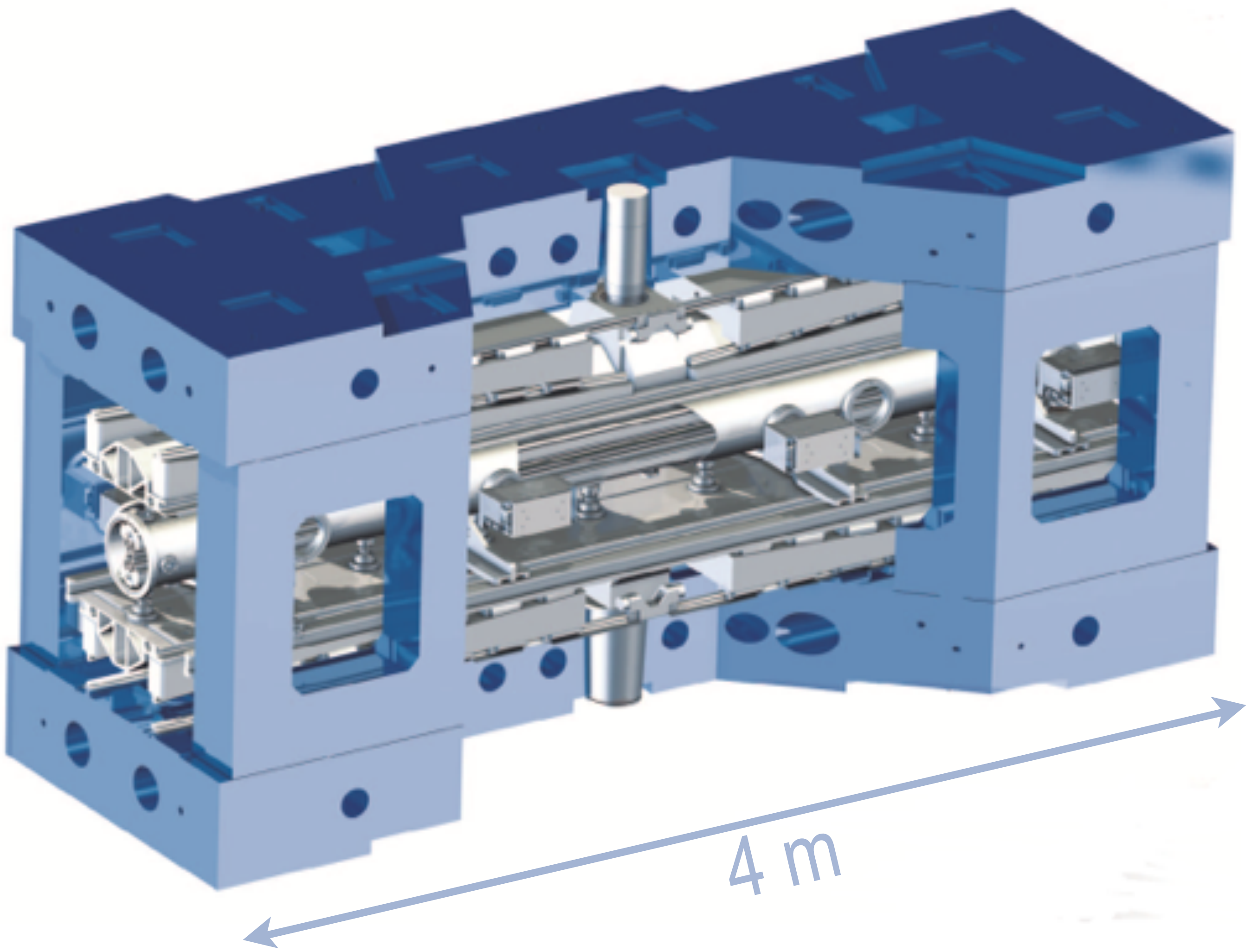
# SwissFEL Hard X-ray Undulators

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 |

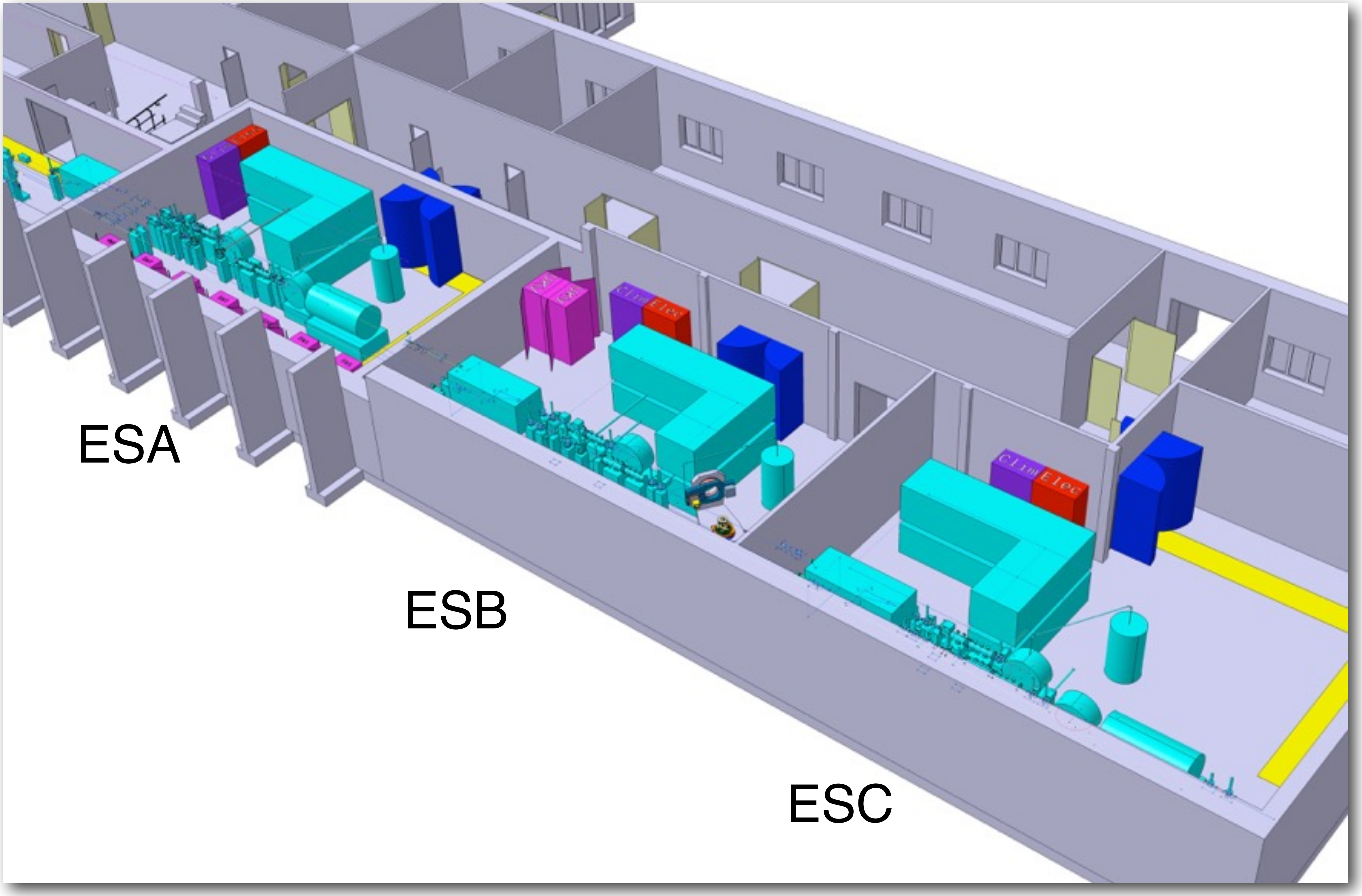



Key building block for SwissFEL beamlines
12 x 17t of precision mechanic

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

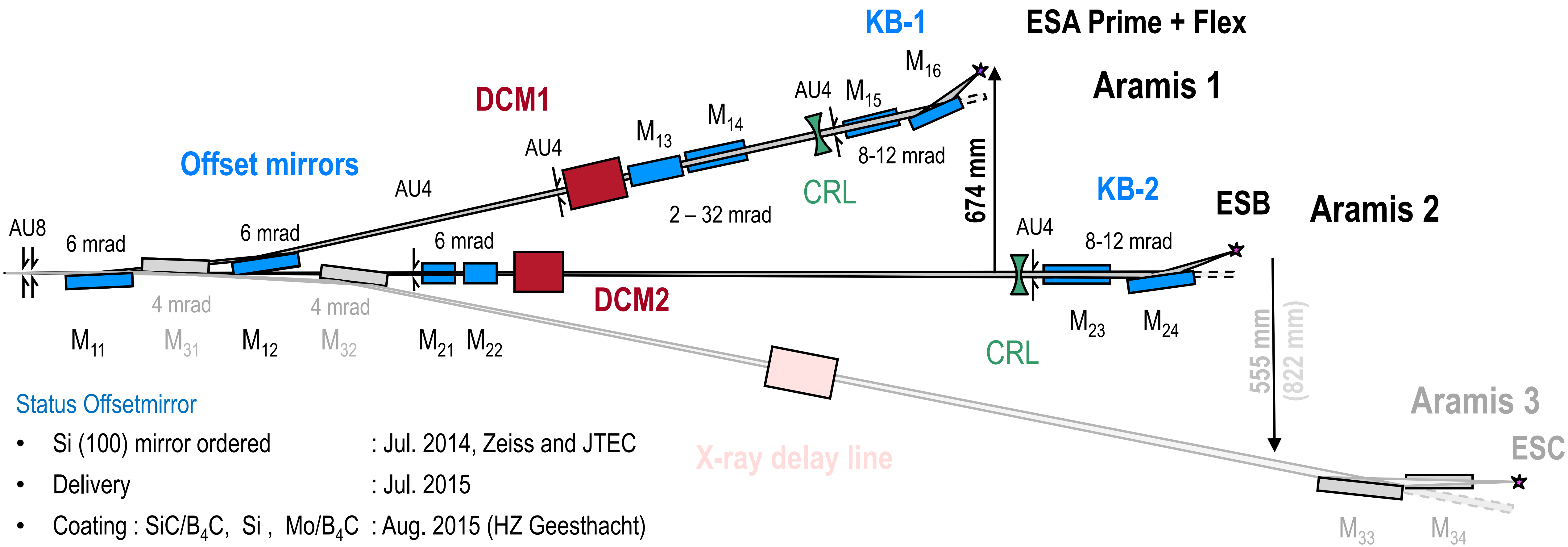
Key industry partners:
- **MDC Daetwyler Industries (CH)**
- Bruker (D)
- Hitachi (Jp)
- Micro-Waterjet (CH)
- Vakuumschmelze (D)

# Aramis Experimental Hutches



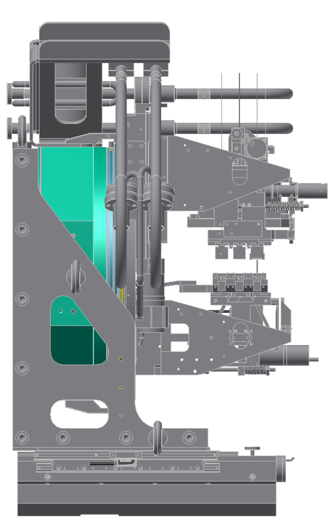
# ARAMIS optical layout

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

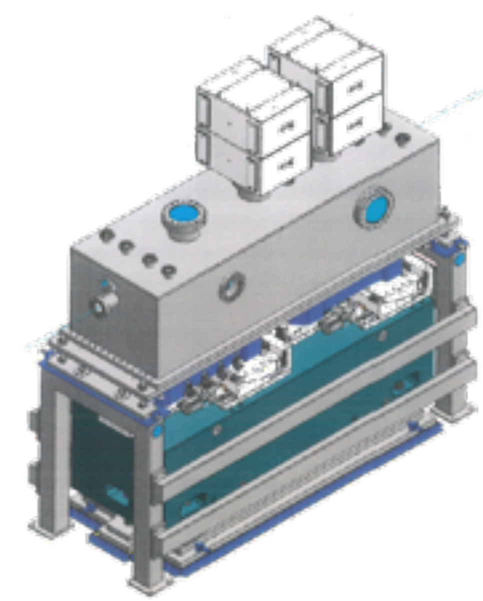


### Double Crystal Monochromator

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

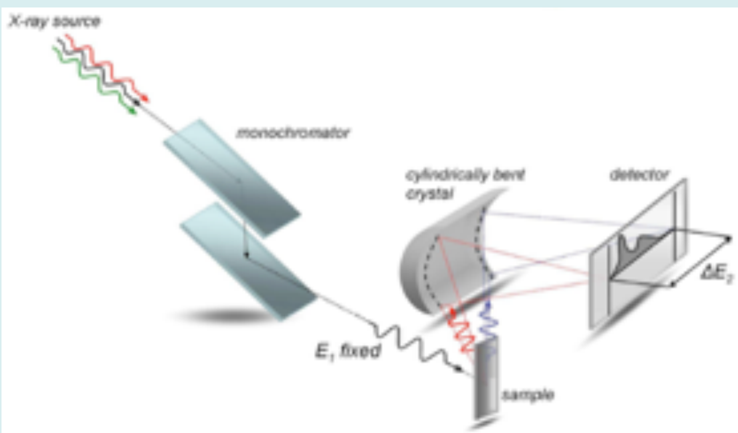
**Status**

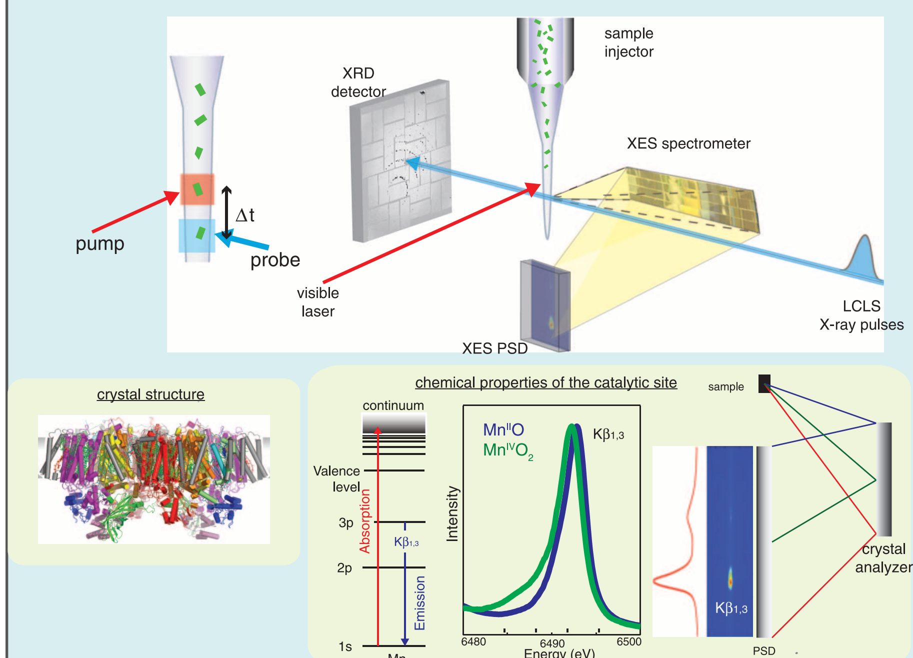
- WTO tender published 12. Dec. 2014
- KO-Meeting 30. Jun 2015
- Delivery & Installation Nov. / Dec. 2016

# SwissFEL Experimental Stations

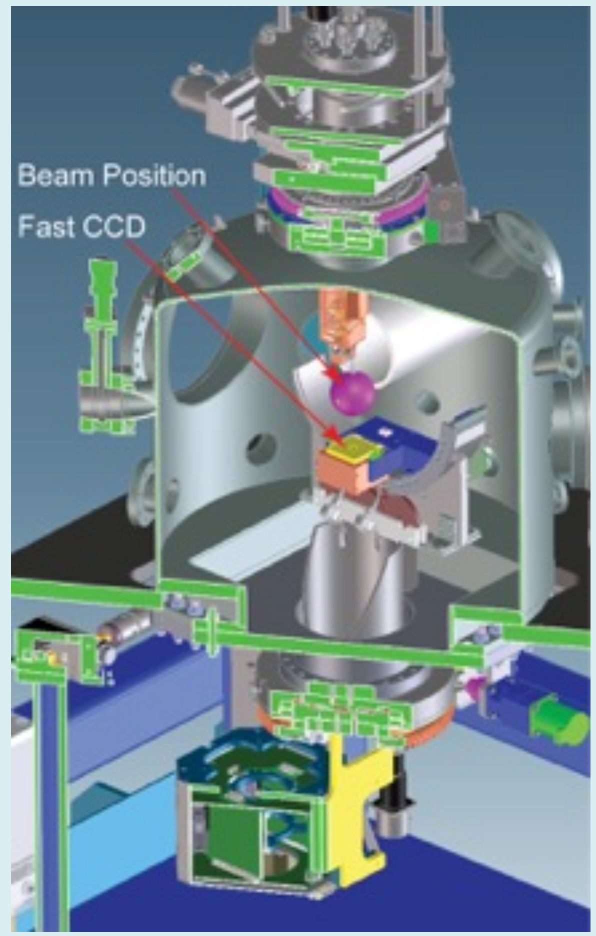
Bruce Patterson
and co-workers

## ESA:
Ultrafast photochemistry and photobiology




## ESB:
Pump-probe crystallography

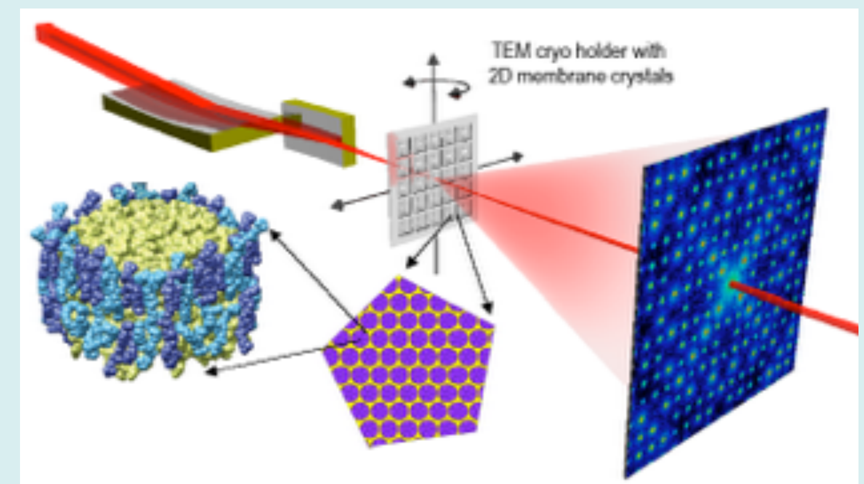



**Phase I:**
**Ready by 2017**

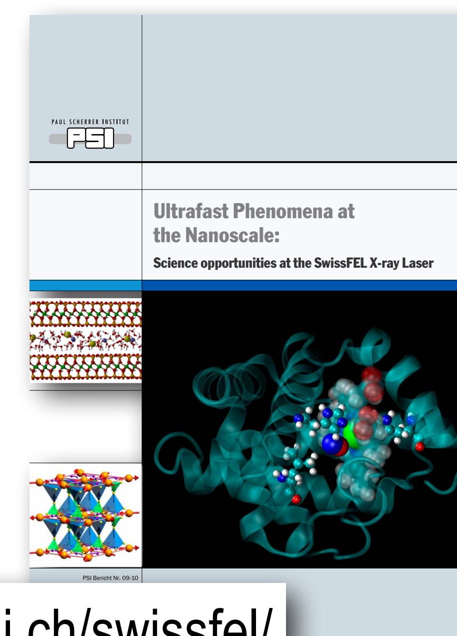
B. Patterson et. al., *CHIMIA* **68**, 73 (2014)

## 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

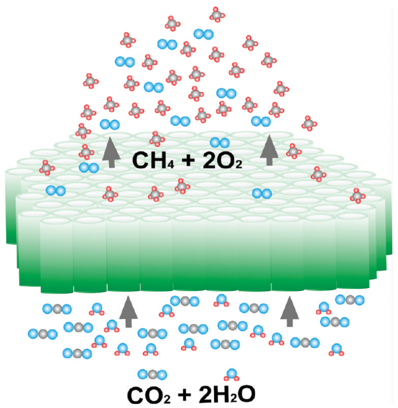
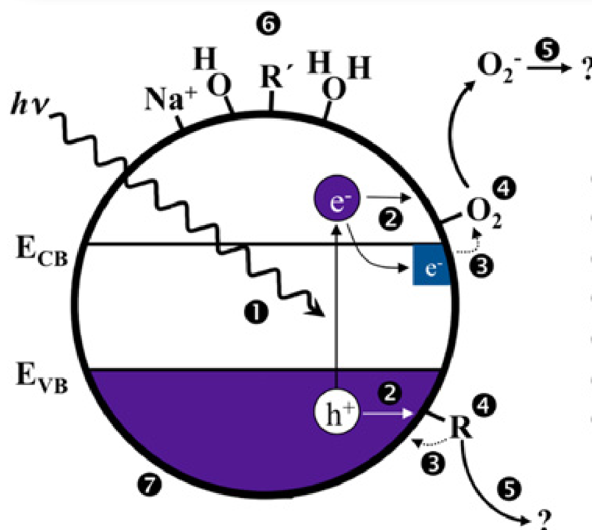



Figure 16. Depiction of flow-through photocatalytic membrane for $CO_2$ conversion.

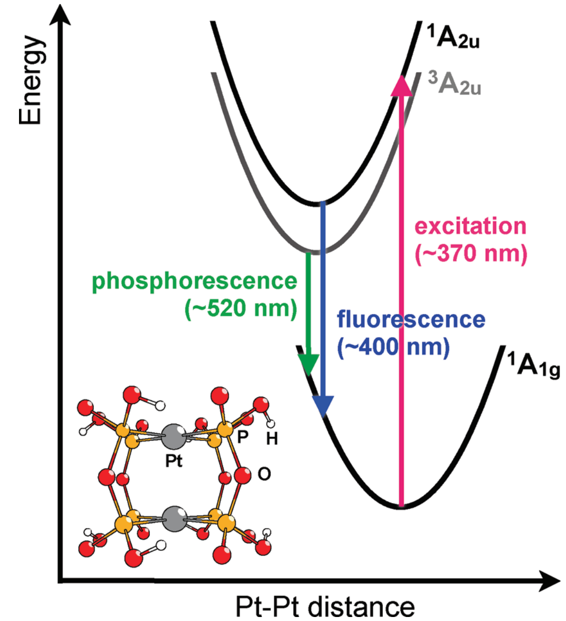
## Electronic relaxation in nanoparticles

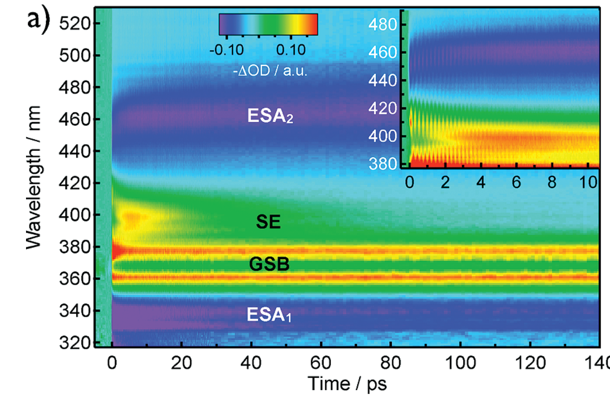


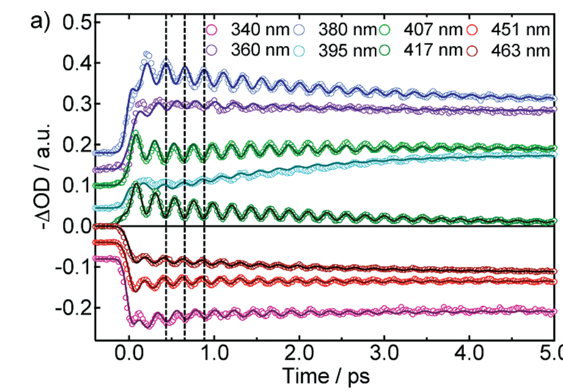

Important issues
❶ excitation
❷ charge transport and trapping
❸ charge transfer
❹ molecular adsorption
❺ reaction mechanisms
❻ poisons and promoters
❼ surface and material structure

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



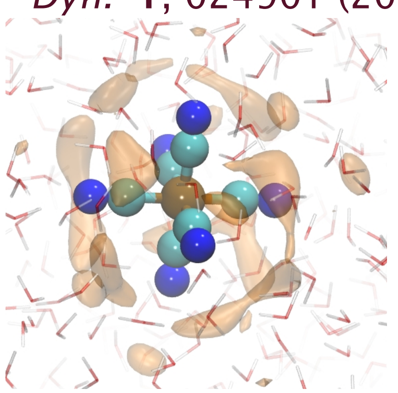



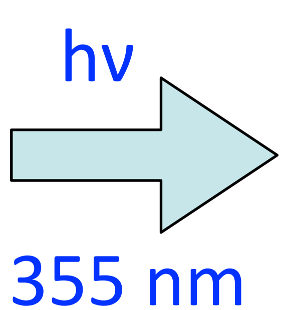

R. van der Veen et al. *JACS* **133**, 305 (2011)

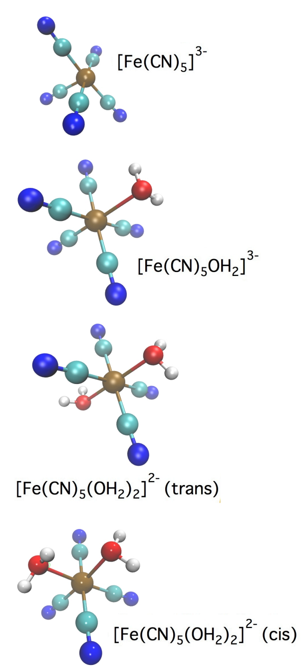
## Bond breaking and bond making

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



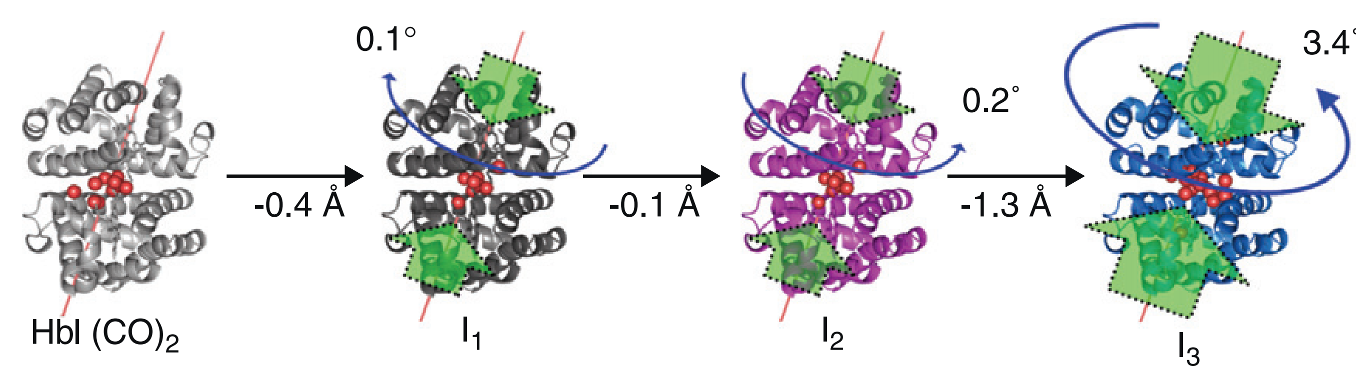
$[Fe(CN)_6]^{4-}$




## Protein function

Intermediate states of homodimeric hemoglobin (HbI) ligated with CO

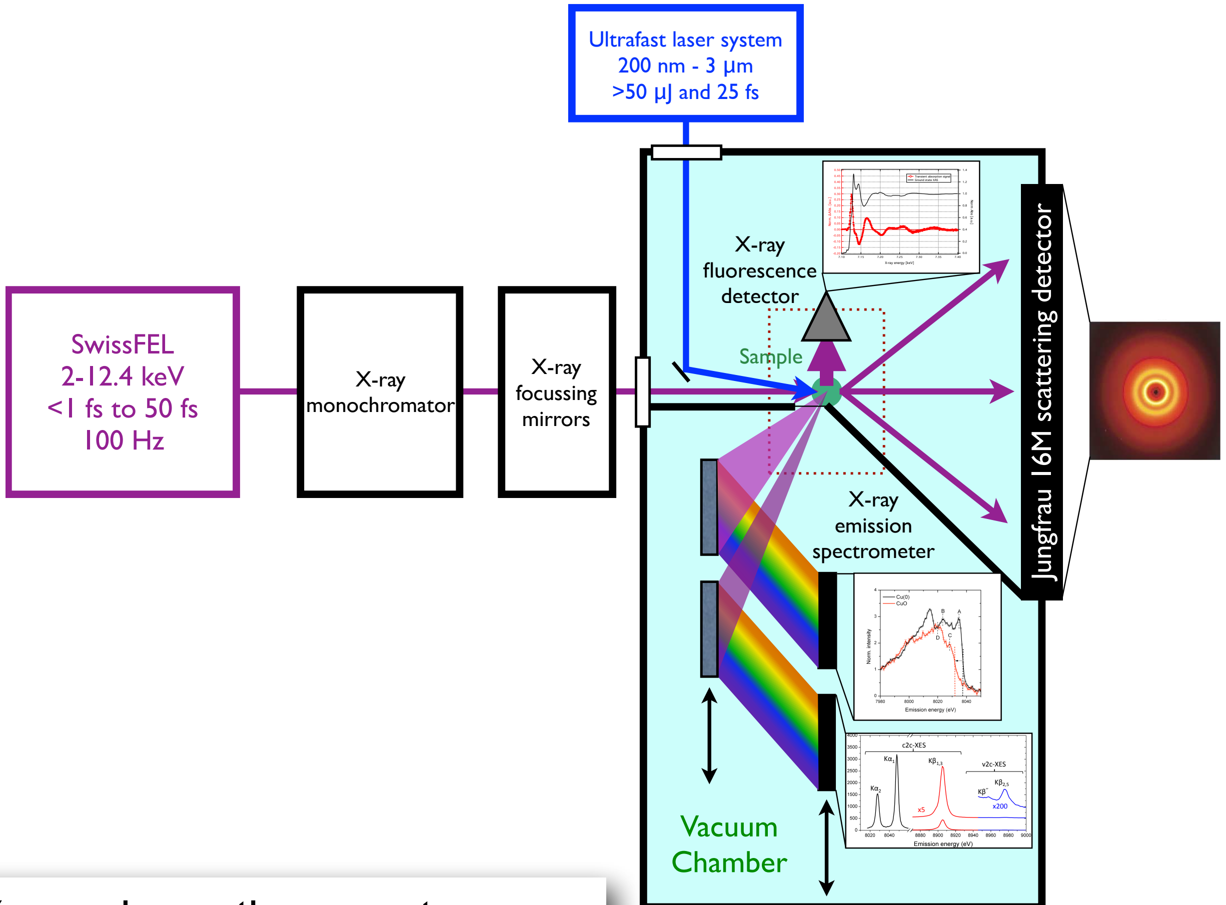



R. Neutze and K. Moffat *Curr. Op. Struc. Bio.* **22**, 651 (2012)

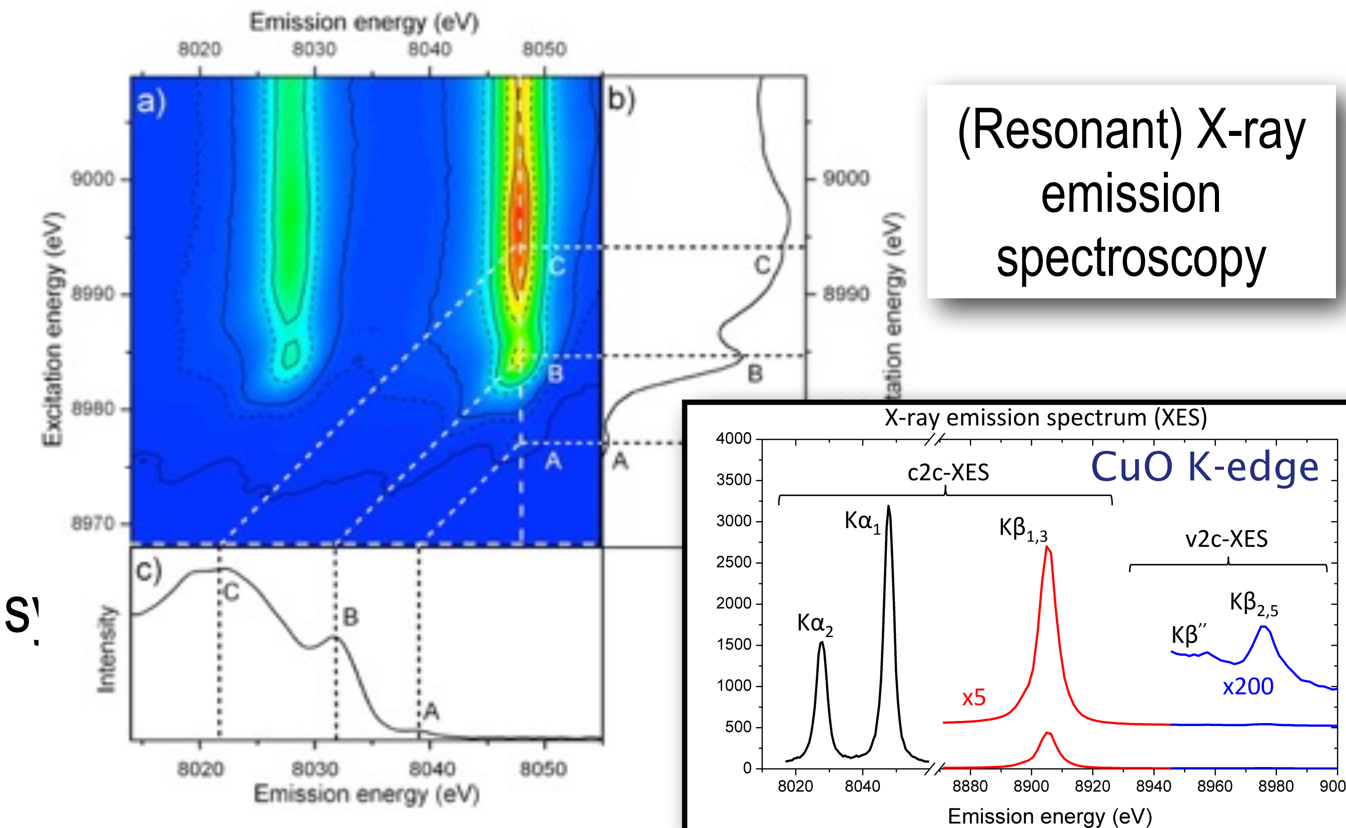
**We want time-resolved electronic and structural information on these systems as they evolve**

# ESA: The X-ray probe techniques

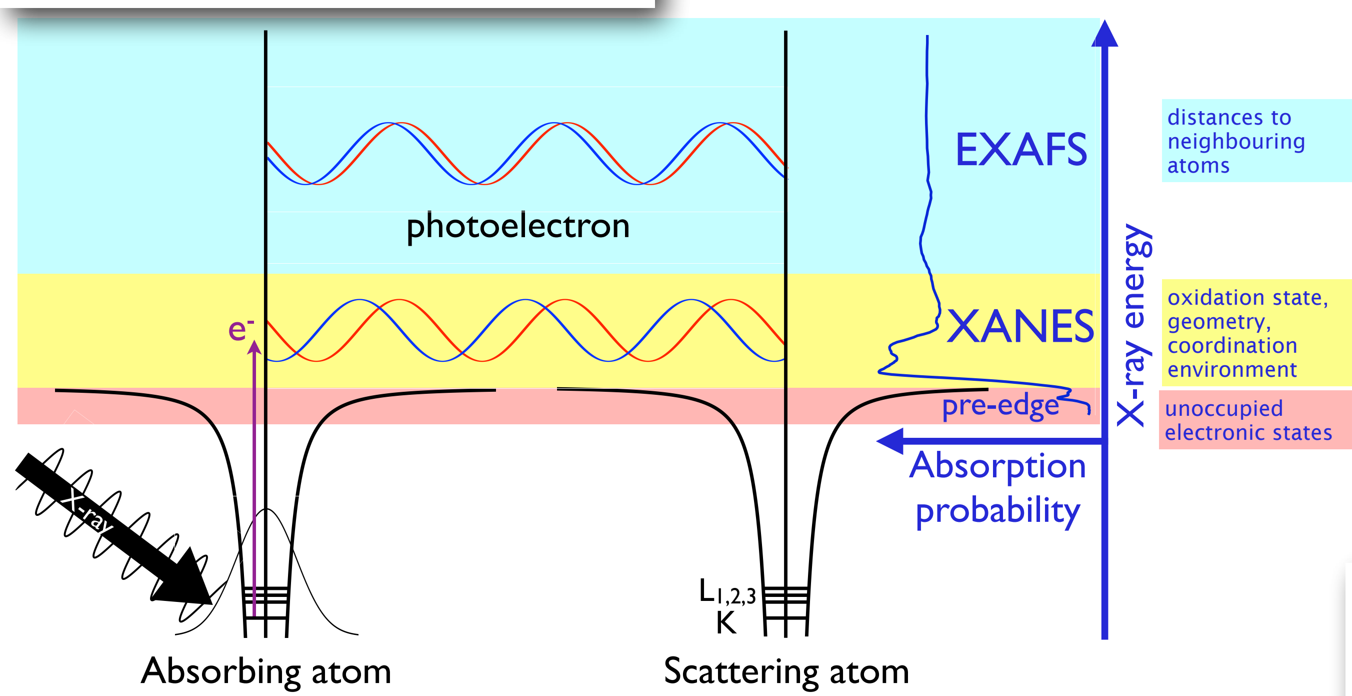
C. Milne,
J. Szlachetko
and G. Knopp




## (Resonant) X-ray emission spectroscopy

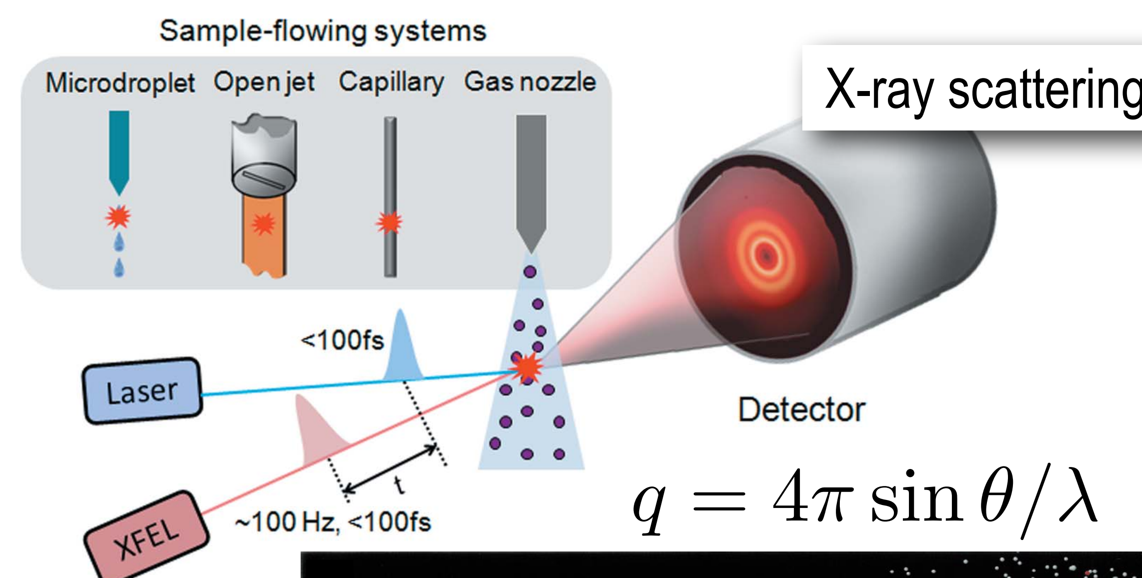



## X-ray absorption spectroscopy



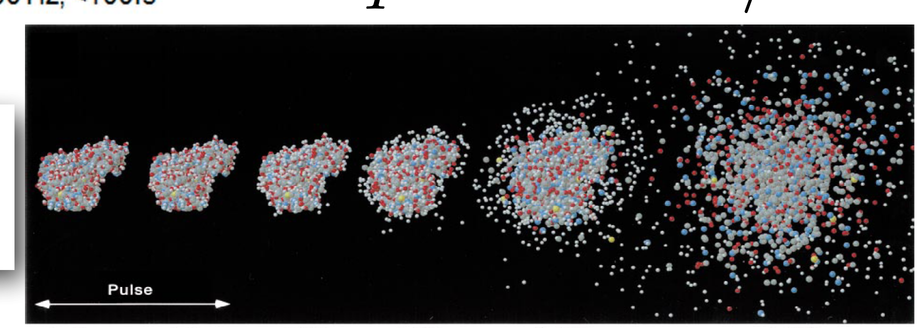

C.J. Milne et al. *Coord. Chem. Rev.* **277** 44 (2014)

## X-ray scattering



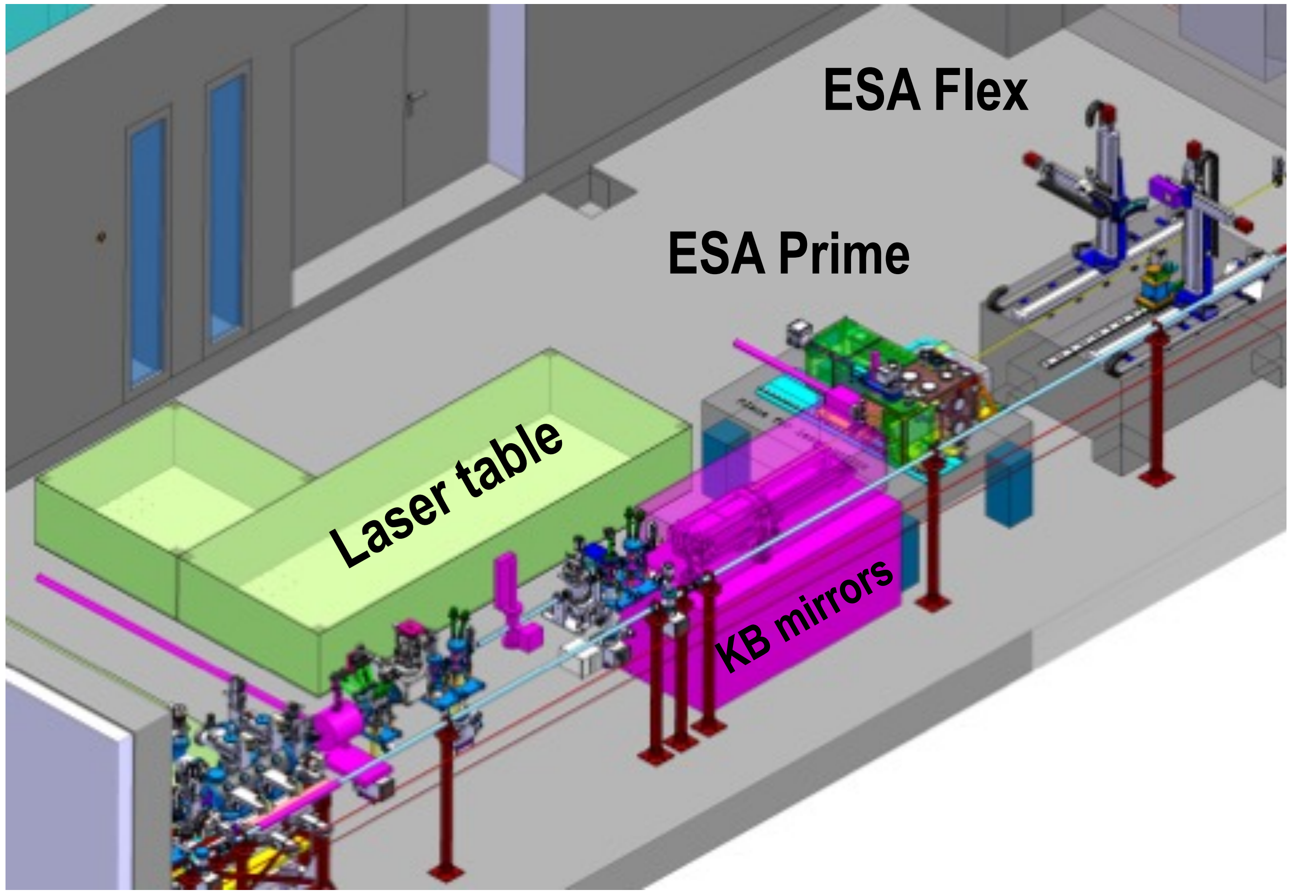

$$q = 4\pi \sin\theta / \lambda$$

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



# The ESA Instruments: Prime and Flex

C. Milne,
J. Szlachetko
and G. Knopp

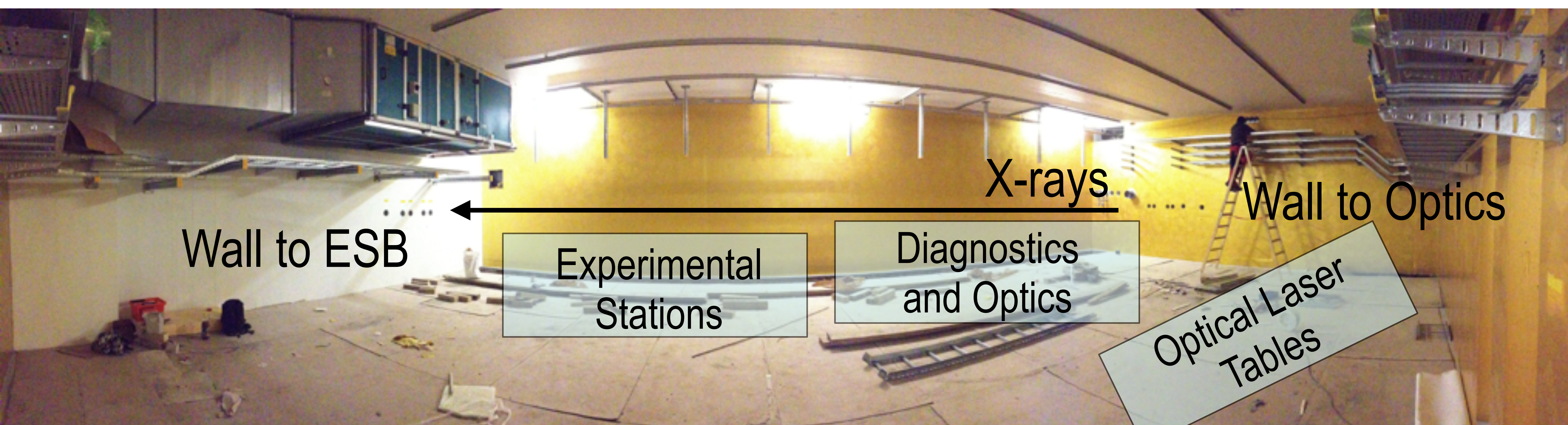



**ESA Prime**

- 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**

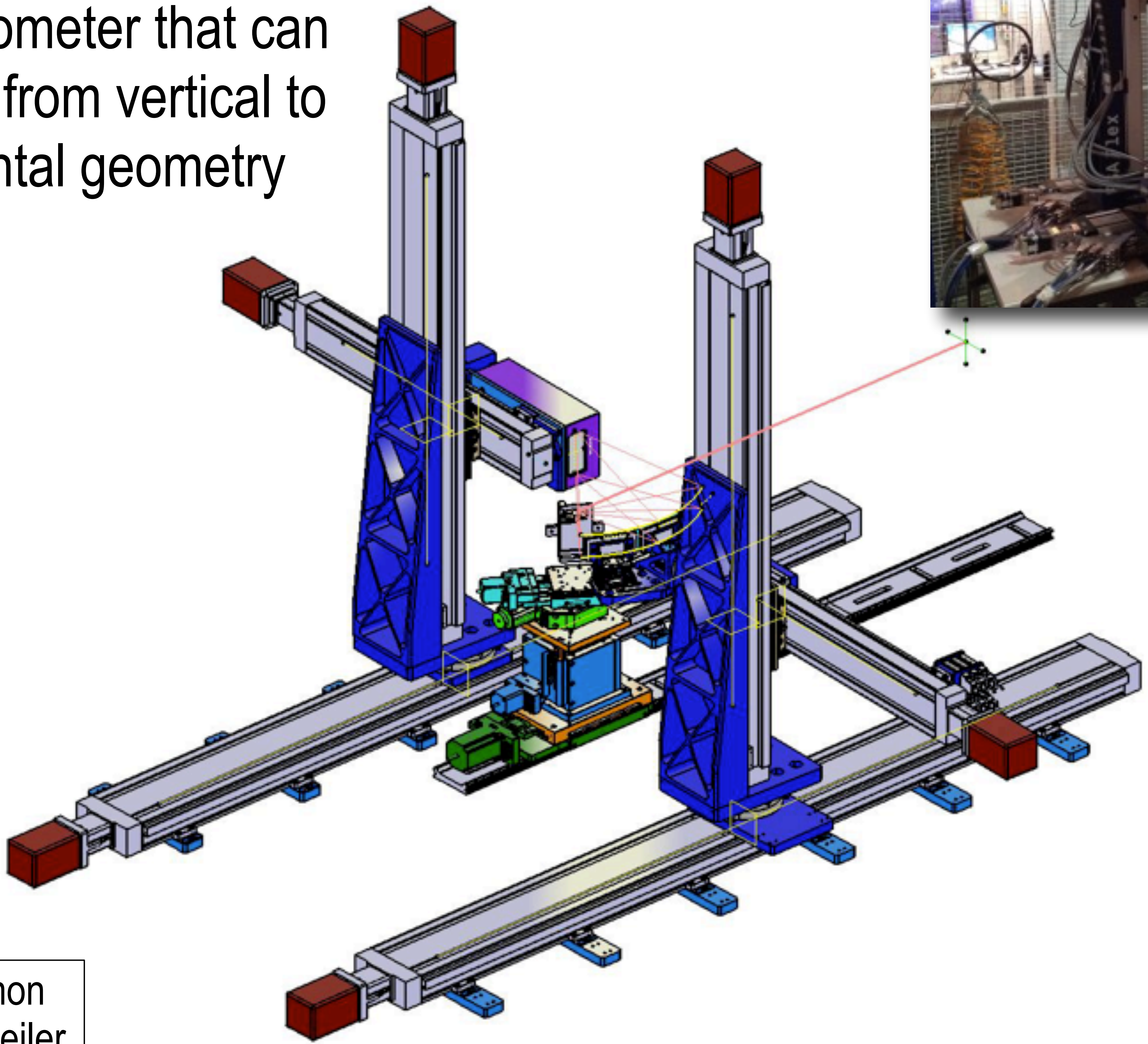
**ESA Flex**

- **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

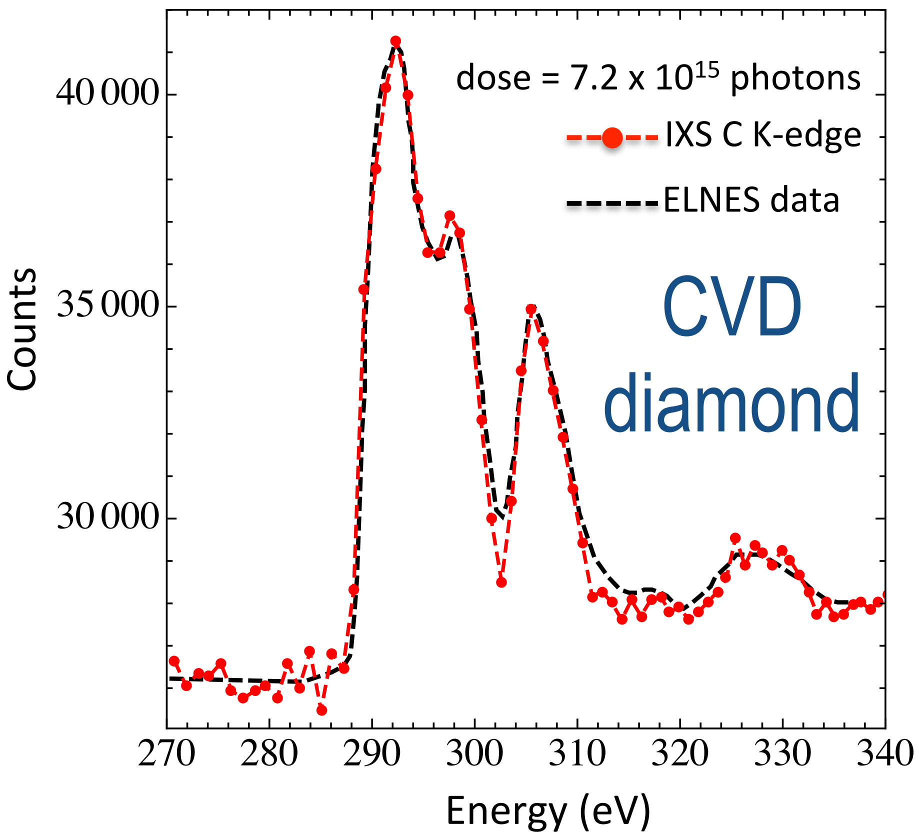


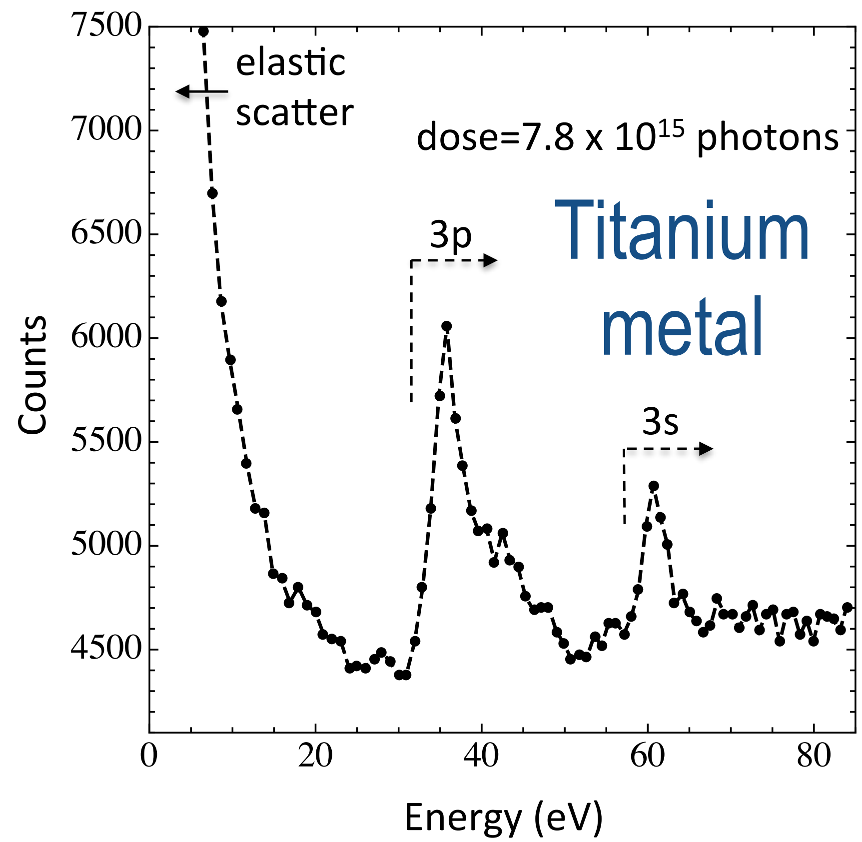
A. Ammon and C. Seiler

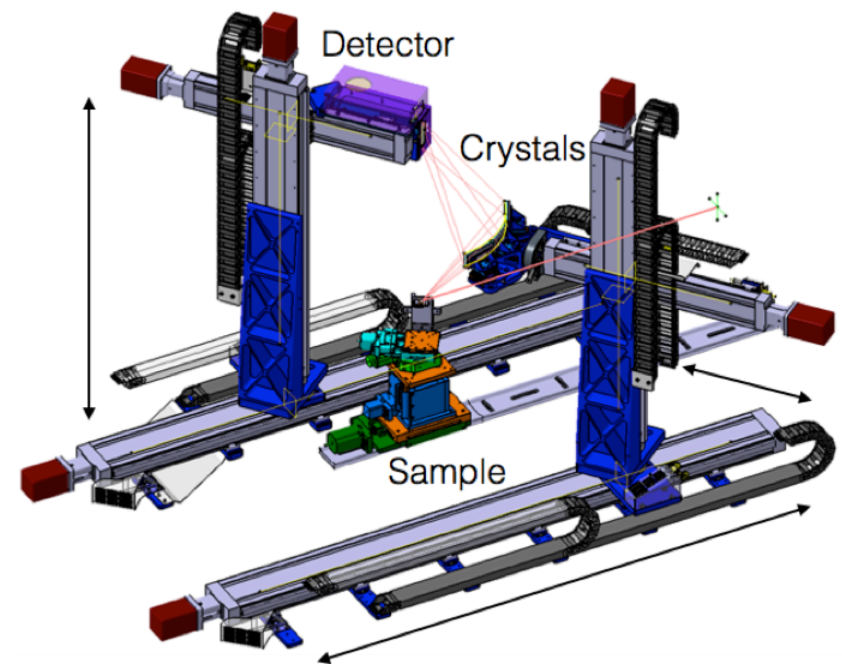
Commissioned at the SLS May 5-12

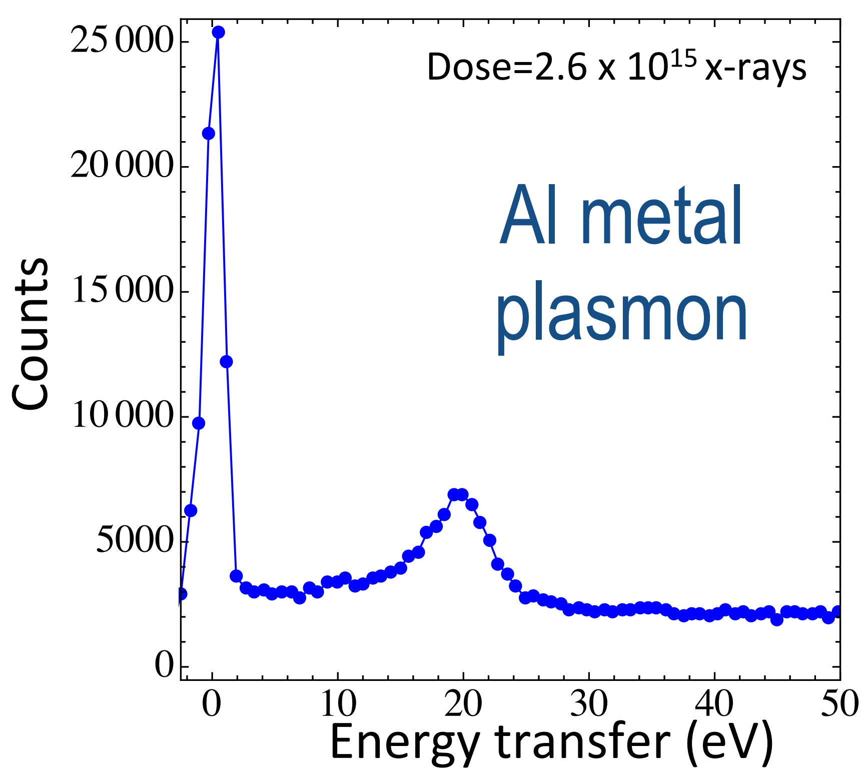
# Inelastic X-ray Scattering at ESA Flex

Collaboration with SuperXAS beamline

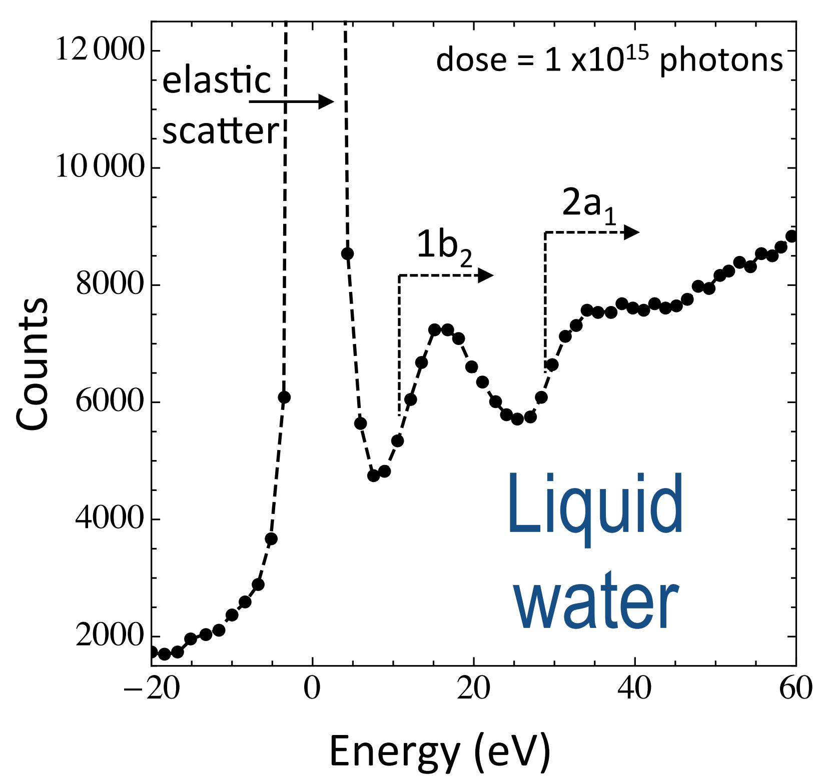


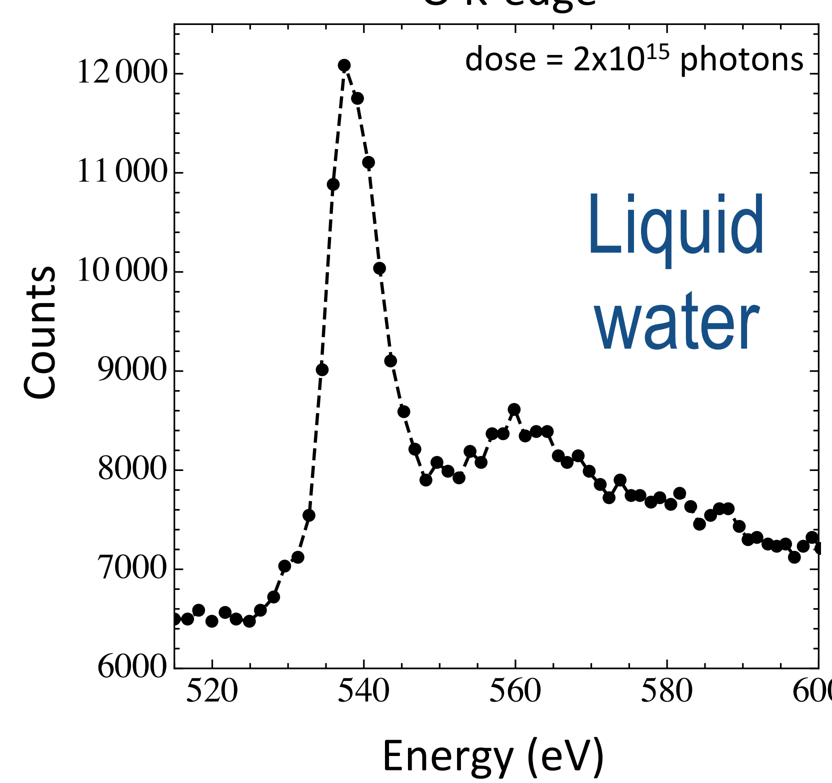




O valence excitations

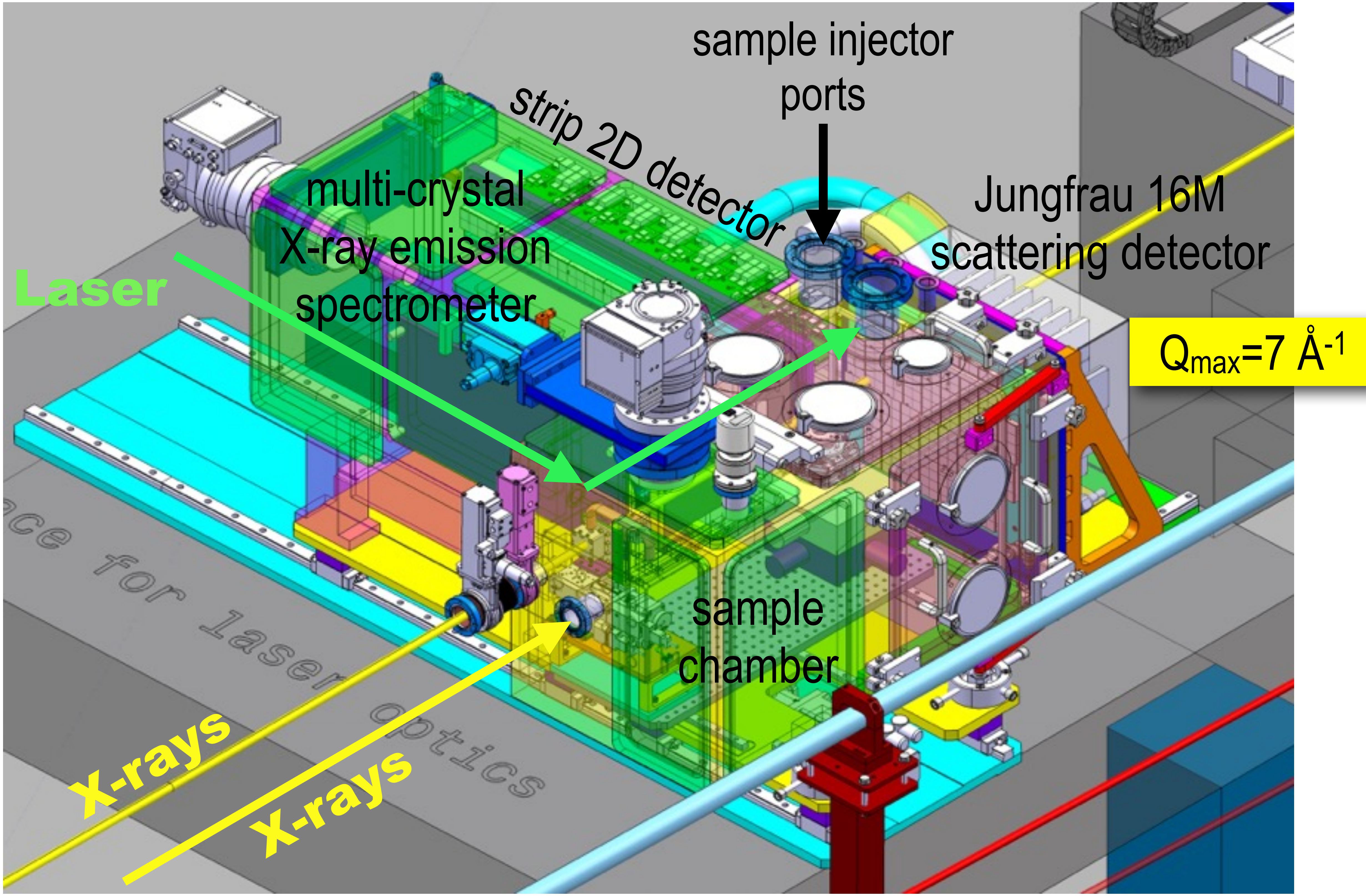



O K-edge



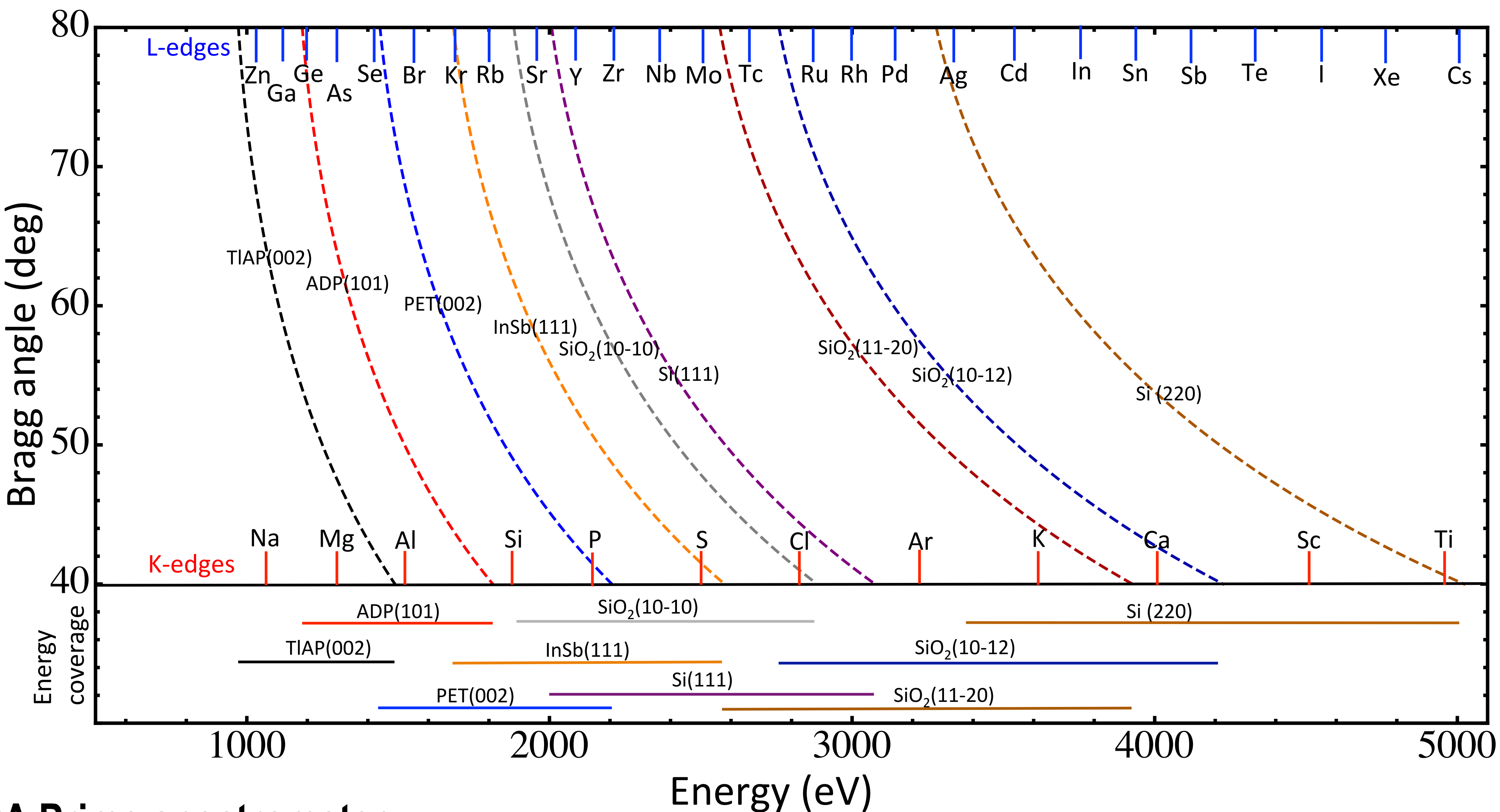
# ESA Prime: Pre-final design

Markus Vitins and Jérome Stettler




**ESA Prime status:** design completion goal July 2015

# ESA Prime: 'Tender' X-ray von Hamos spectrometer

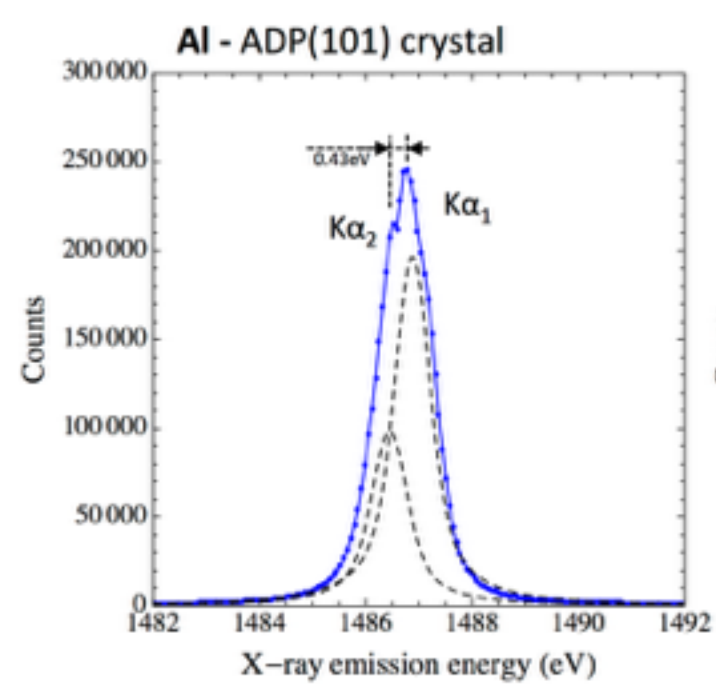


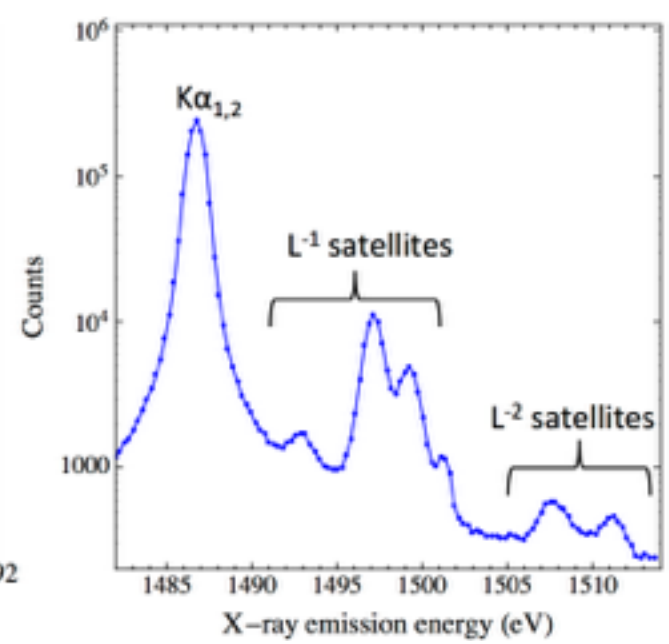

**Tender X-ray crystals tested:**

- ADP
- PET
- InSb

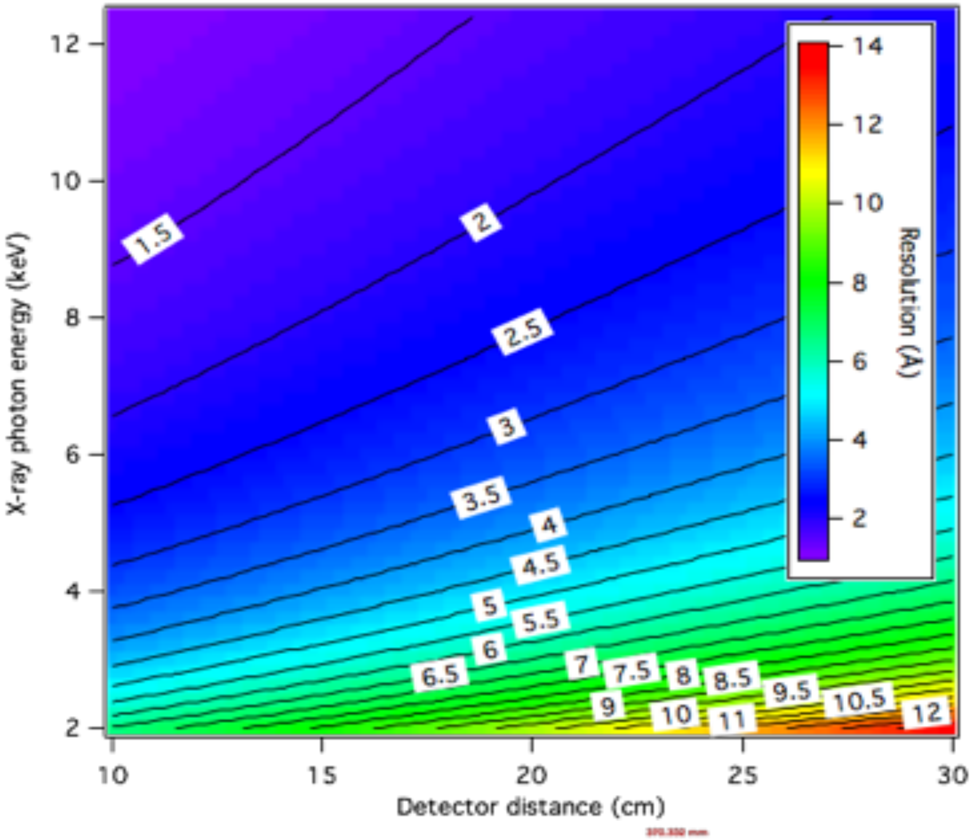
## ESA Prime spectrometer

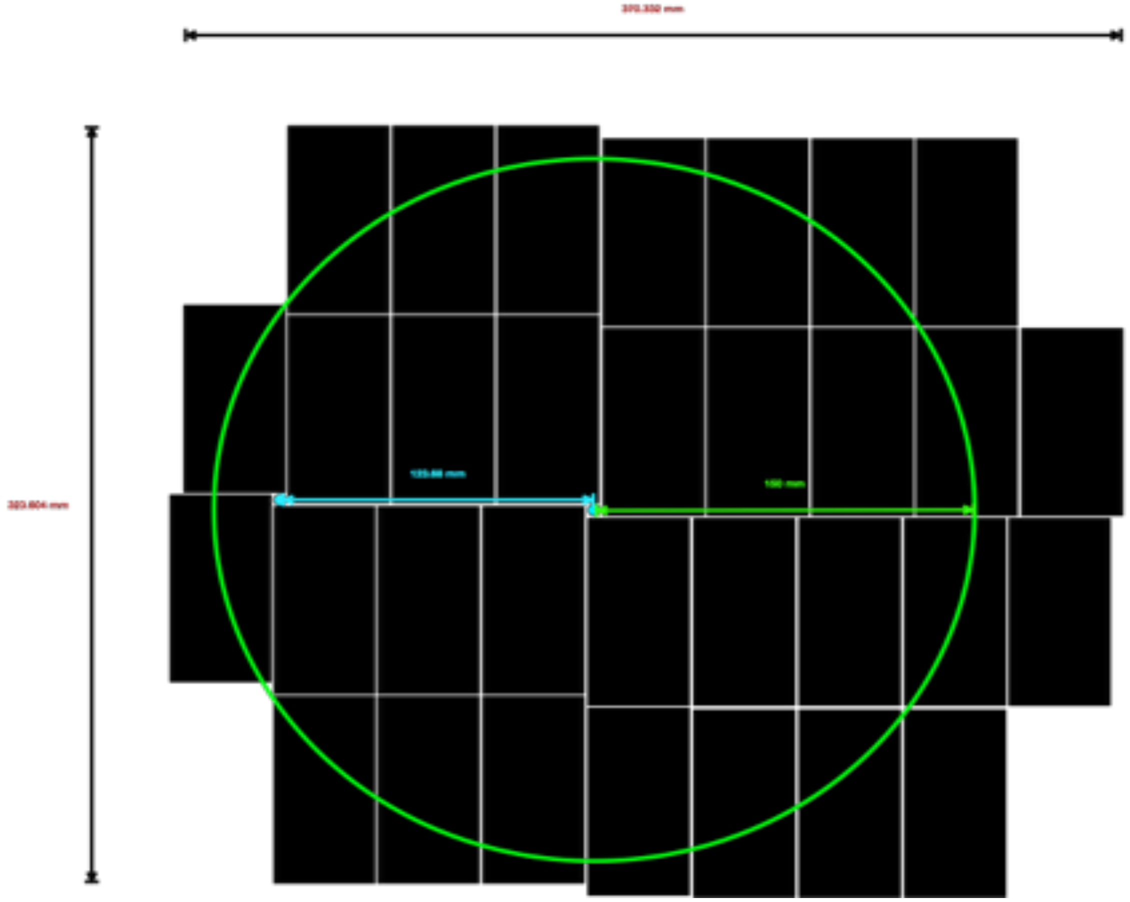
- To cover 1-5 keV X-ray emission energies we need exotic crystals
- Needs to operate in vacuum to avoid X-ray loss
- Spectrometer compartment should be isolated from sample compartment
- Crystals and detectors need some travel range to cover the desired X-ray energies
- This X-ray energy range is a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



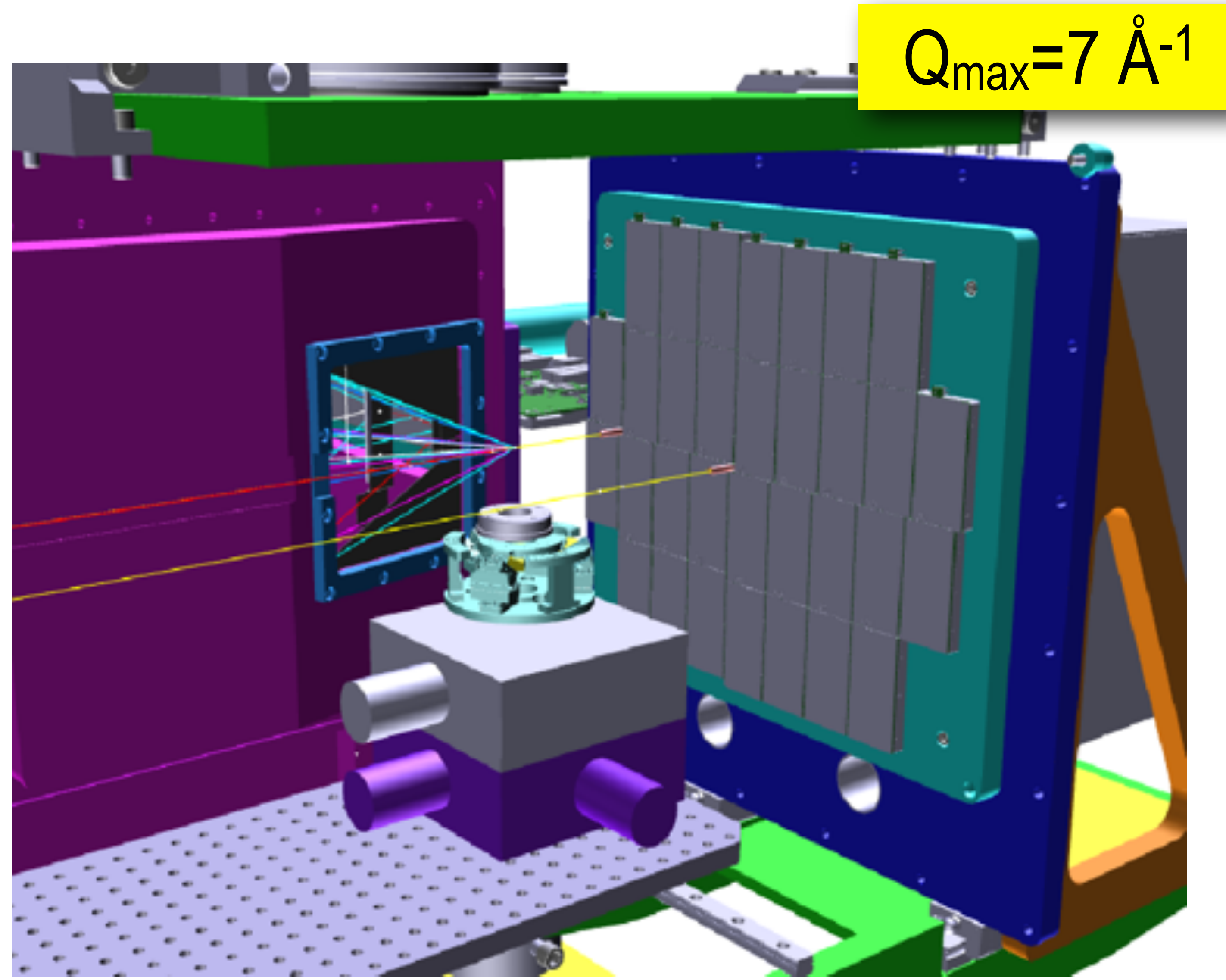
# ESA Prime: Scattering experiments



**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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BIOLOGY | MEDICINE

Received 16 October 2014
Accepted 1 December 2014

**Lipidic cubic phase serial millisecond crystallography using synchrotron radiation**

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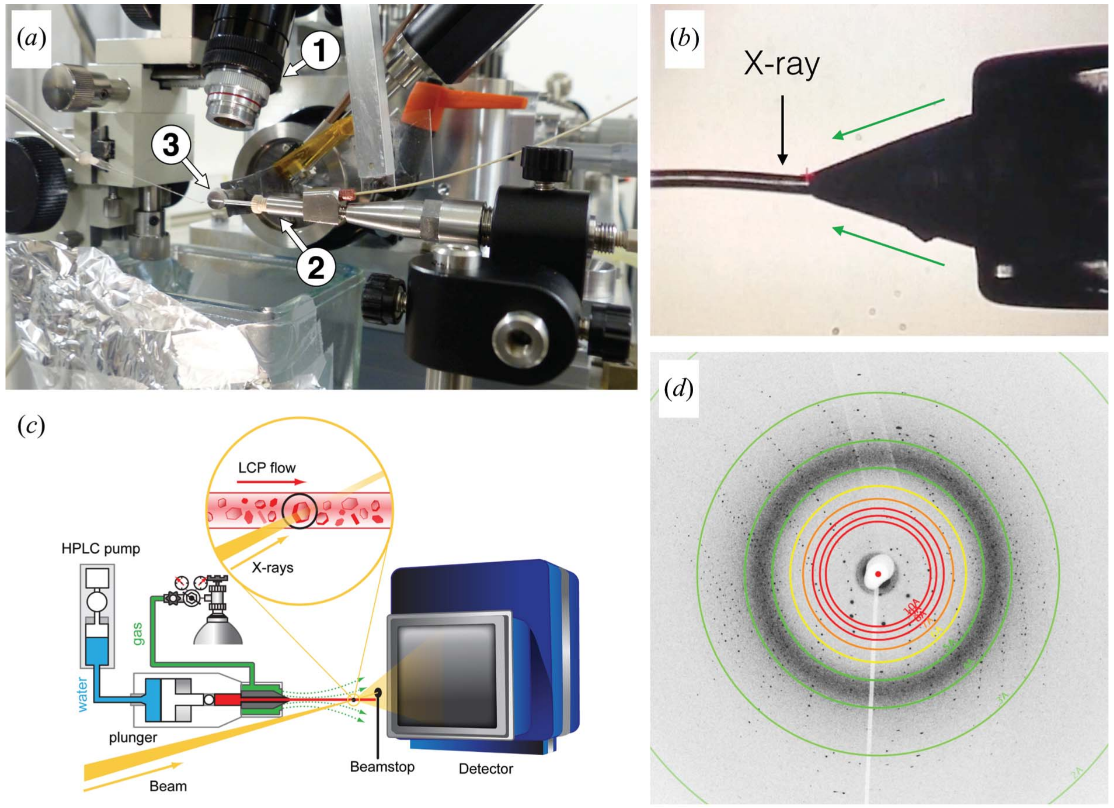
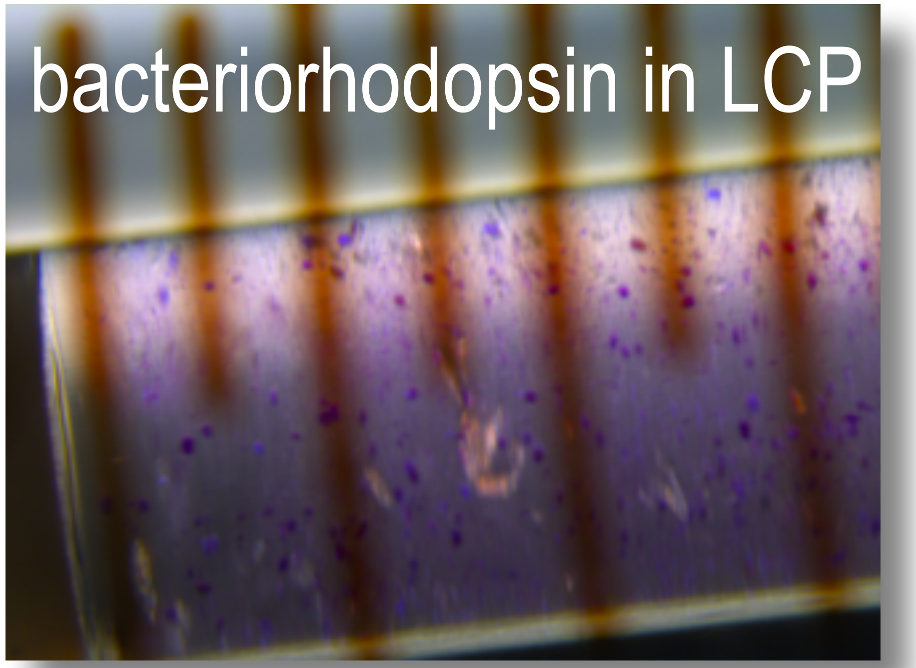
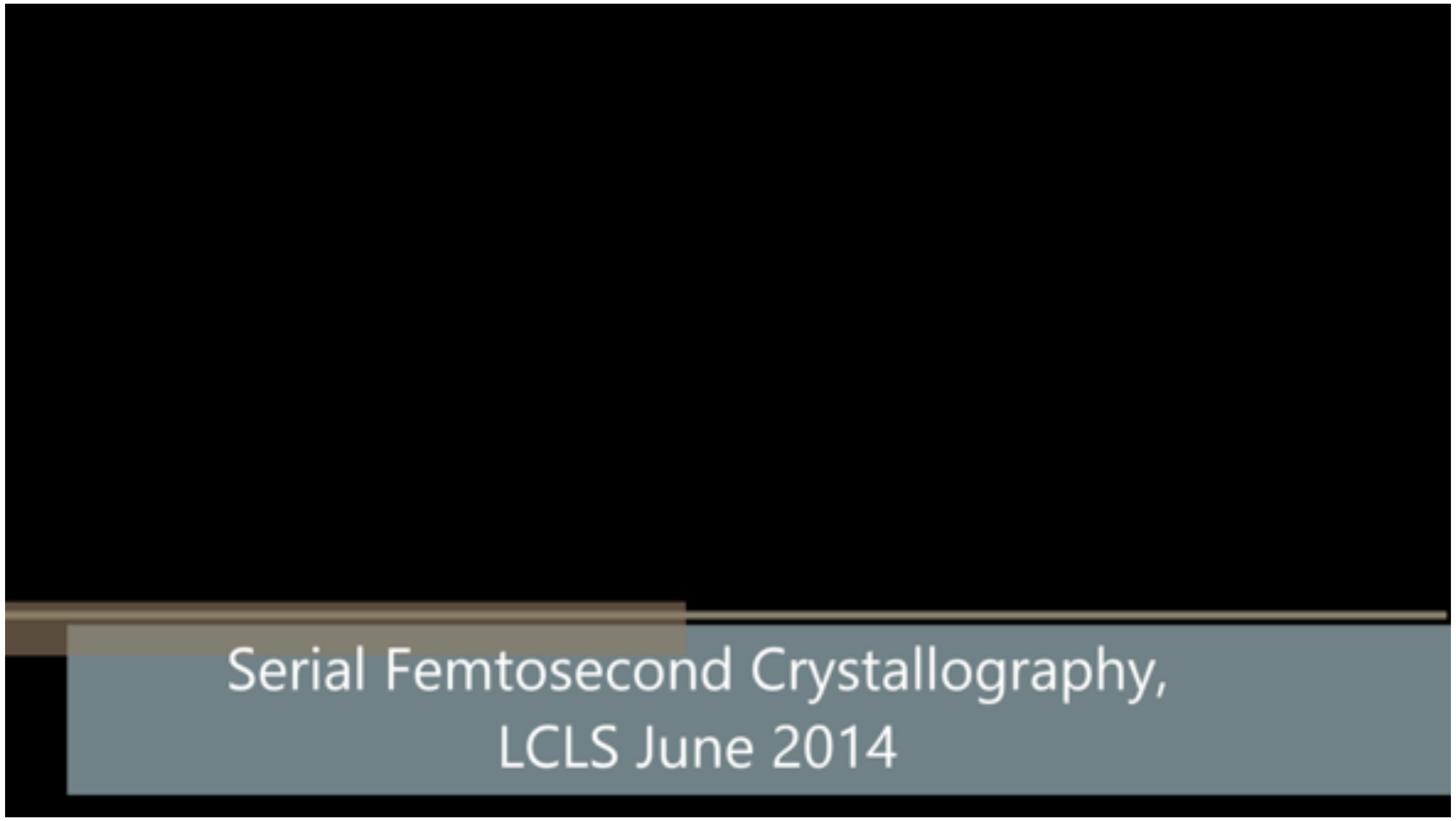


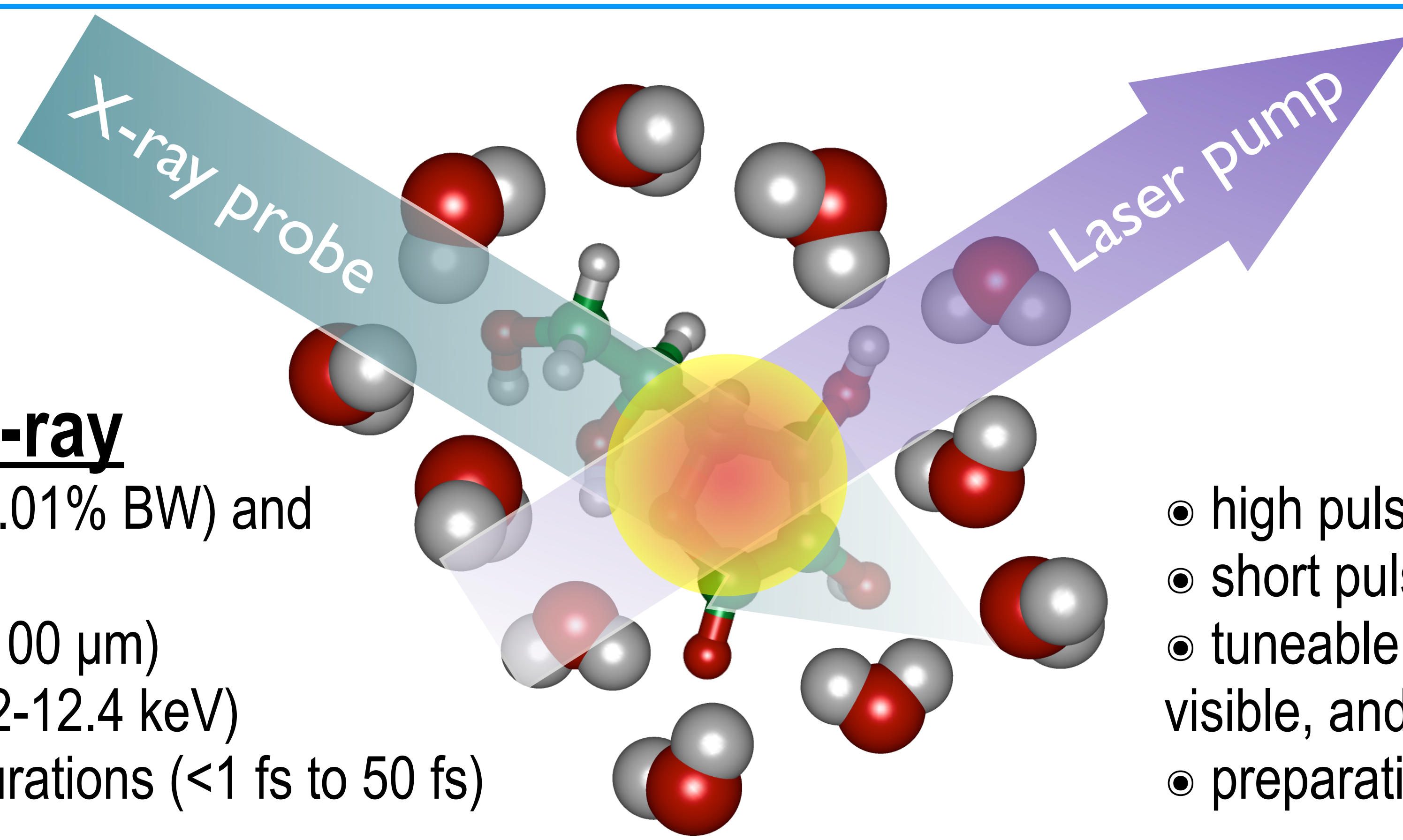




media courtesy of Przemek Nogly



# SwissFEL Experimental Station A

**Goal:** To have this ready by 2017




## X-ray

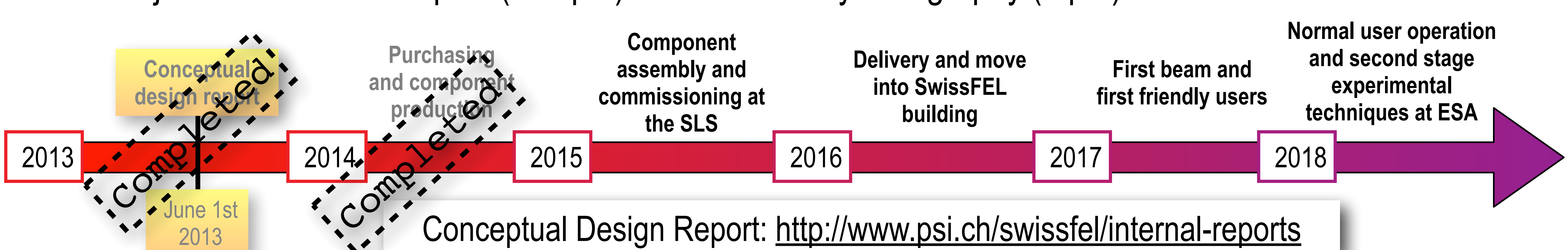
- monochromatic (0.01% BW) and broadband (1-4%)
- variable focus (1-100 μm)
- tuneable energy (2-12.4 keV)
- ultrashort pulse durations (<1 fs to 50 fs)

## 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)

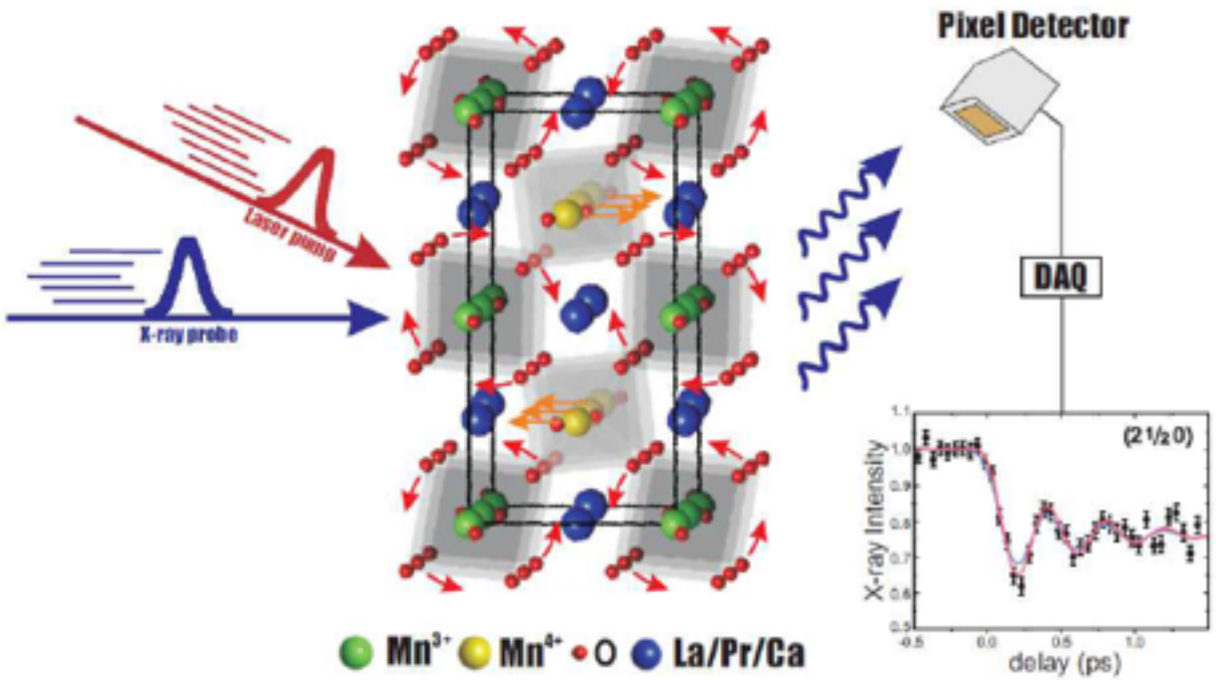


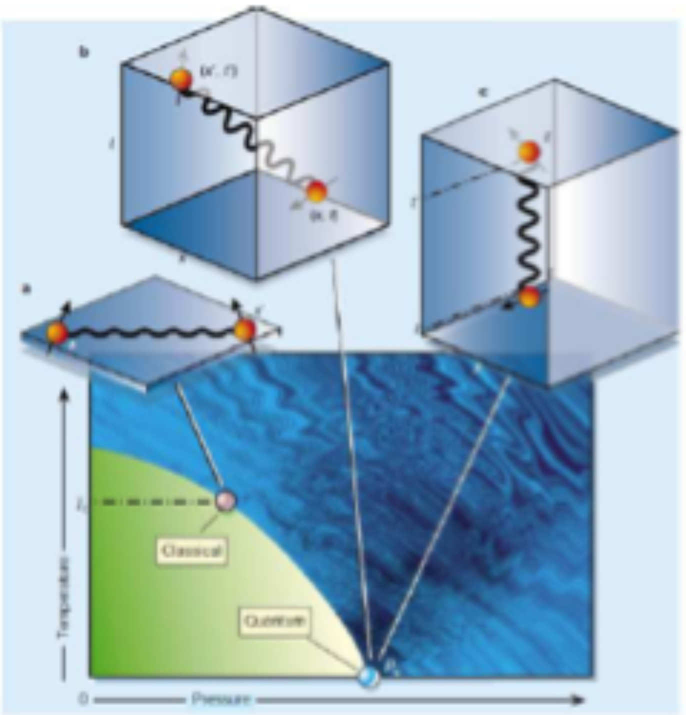

Conceptual Design Report: http://www.psi.ch/swissfel/internal-reports

# 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)]

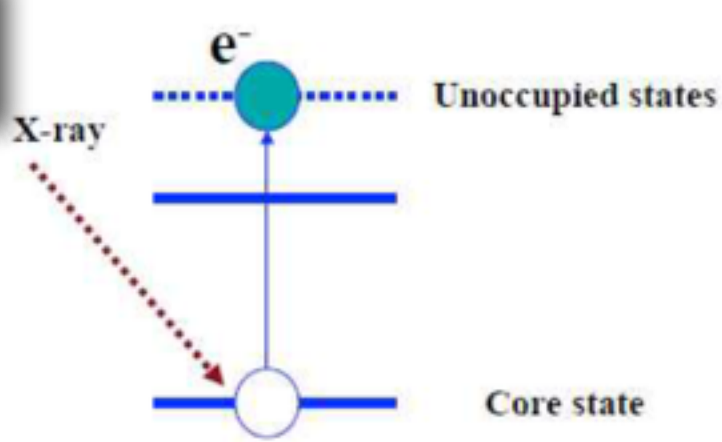
## → X-ray probe: how does the (coherent) excitation evolve in time ?

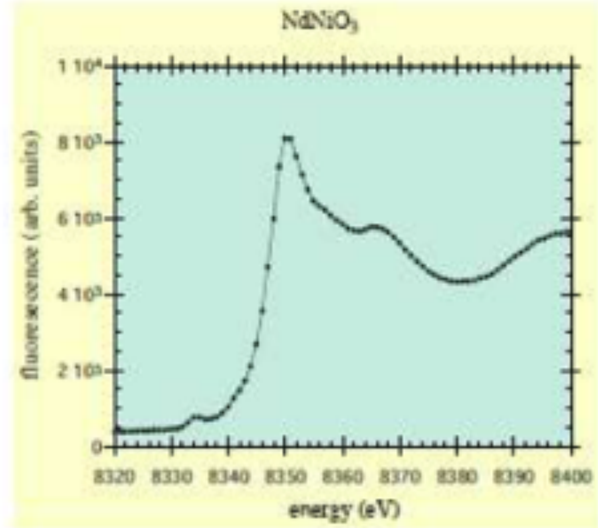
↔ tr-XRD: measures changes in lattice constants & symmetry
↔ tr-RXRD: sensitive to coupling of charge-, orbital- and spin-order (↔ polarization)
↔ tr-(N)TDS: measures $S(\mathbf{q},\omega = 0)$ & fluctuating coherence length $\xi_F$
↔ tr-(R)IXS: measures $S(\mathbf{q},\omega)$ & change of momentum dispersion

# ESB: The X-ray probe techniques

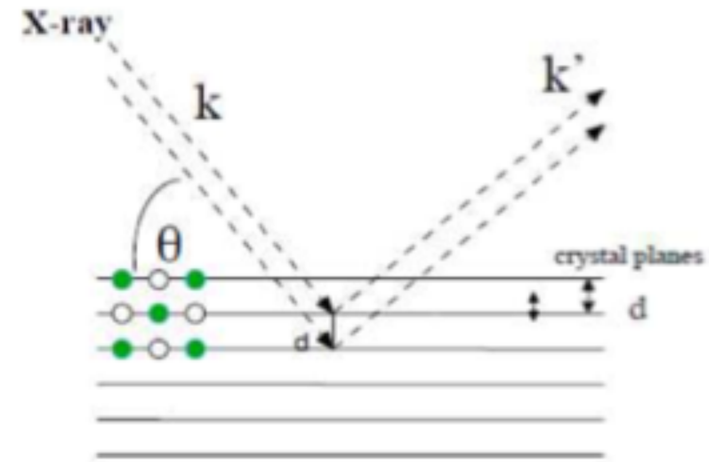
Gerhard Ingold,
Henrik Lemke and
Paul Beaud

## Resonant X-ray Diffraction



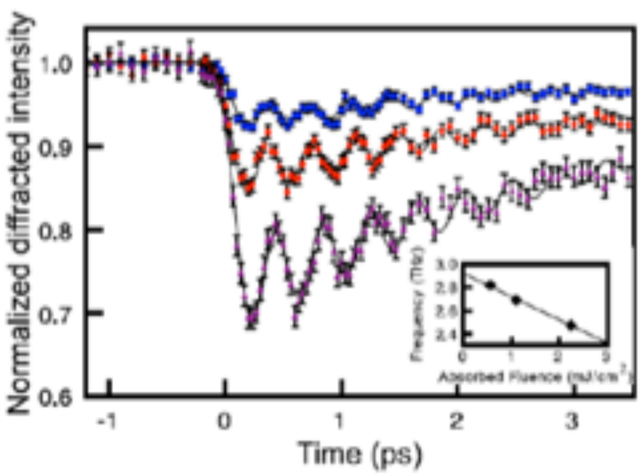




+



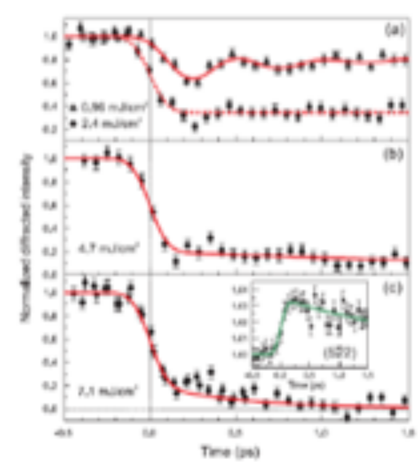

## X-ray Diffraction

Peierls system: coherent phonons (Bi)



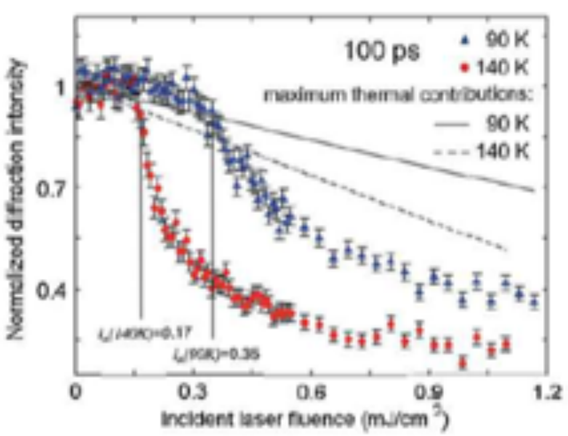

[ Johnson PRL 2008 ]

Jahn-Teller dynamics (LCMO)



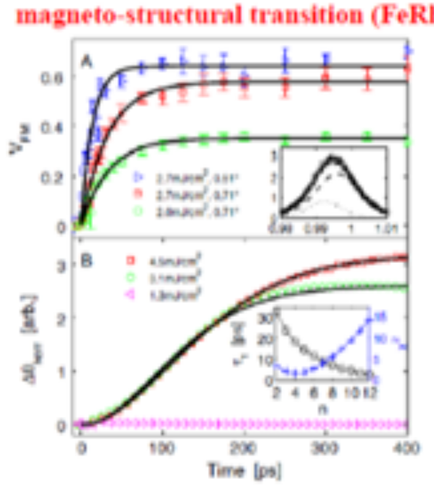
[ Beaud PRL 2009 ]

excitonic CDW system ($TiSe_2$)



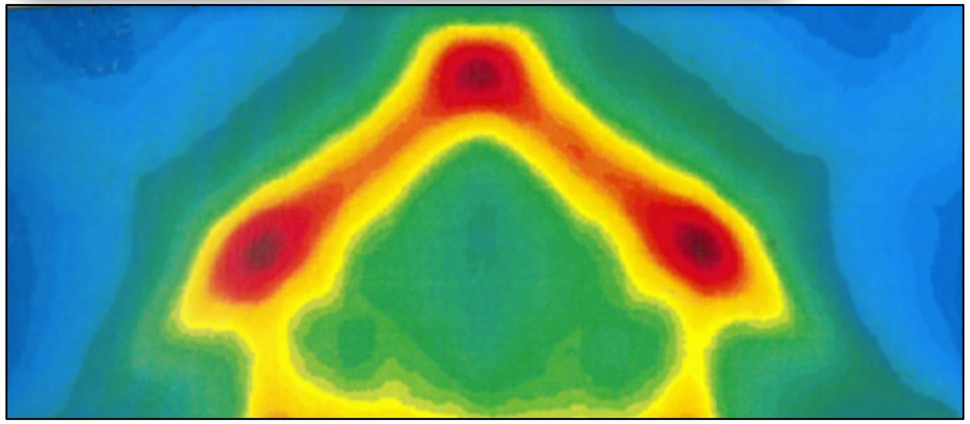

[ Vorobeva PRL 2011 ]

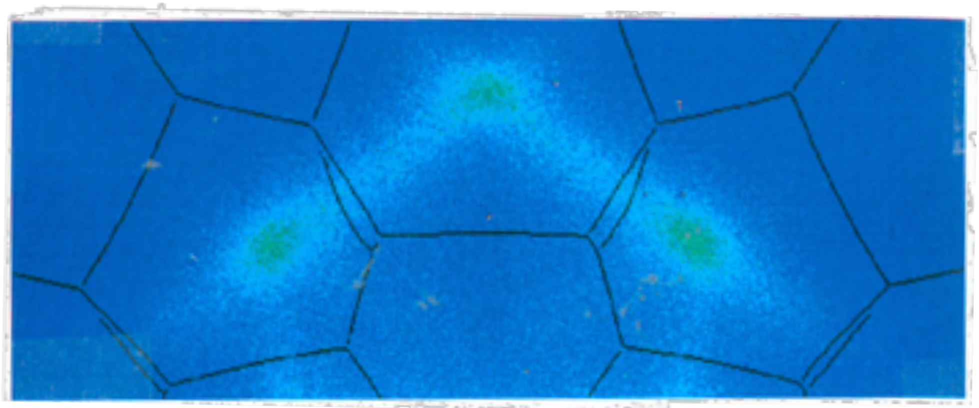
magneto-structural transition (FeRh)




[ Mariager PRL 2012]

## Elastic X-ray Diffuse Scattering

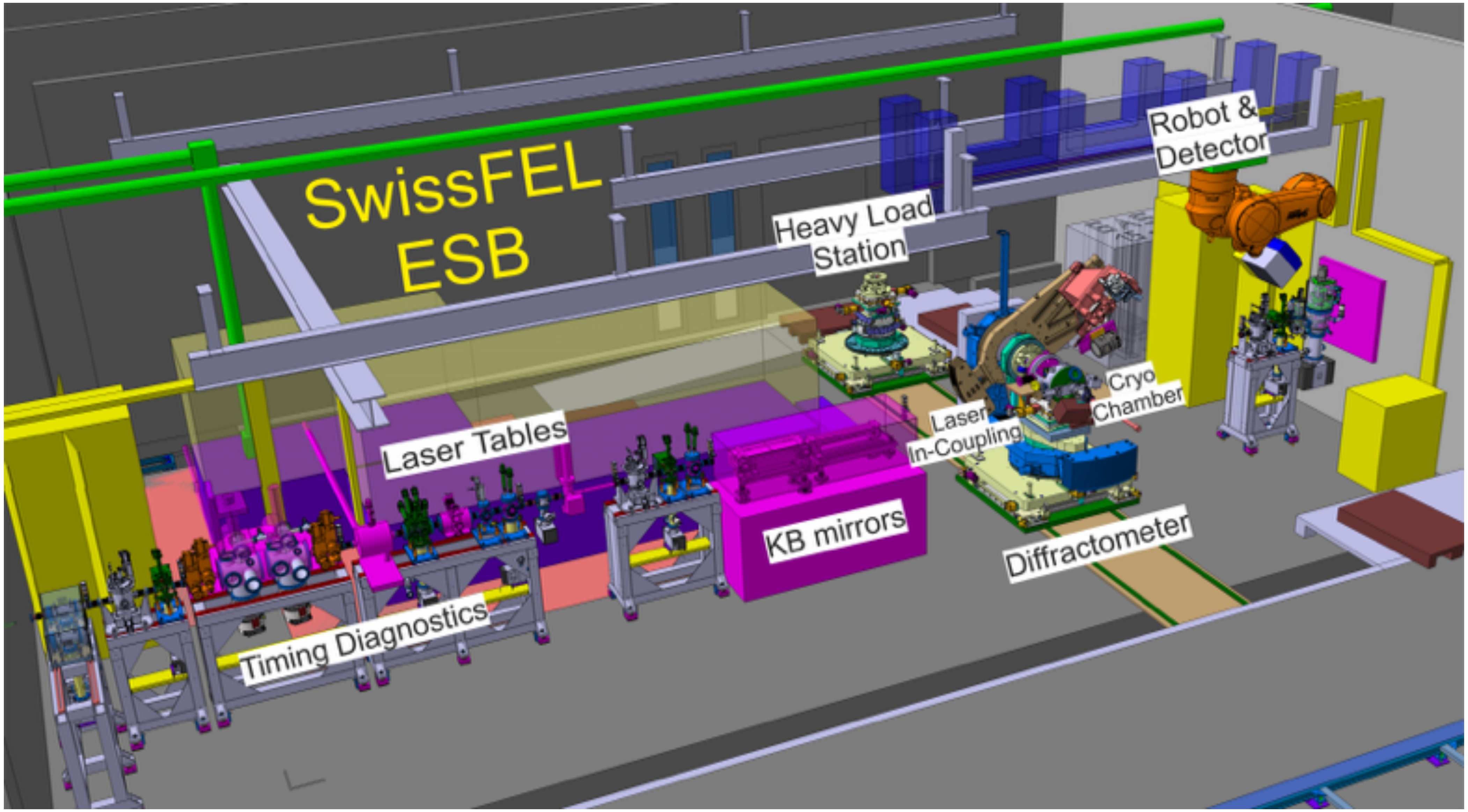




TDS from Si(100) measured at the SLS (courtesy J. Johnson)

# 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 $\mu$m**

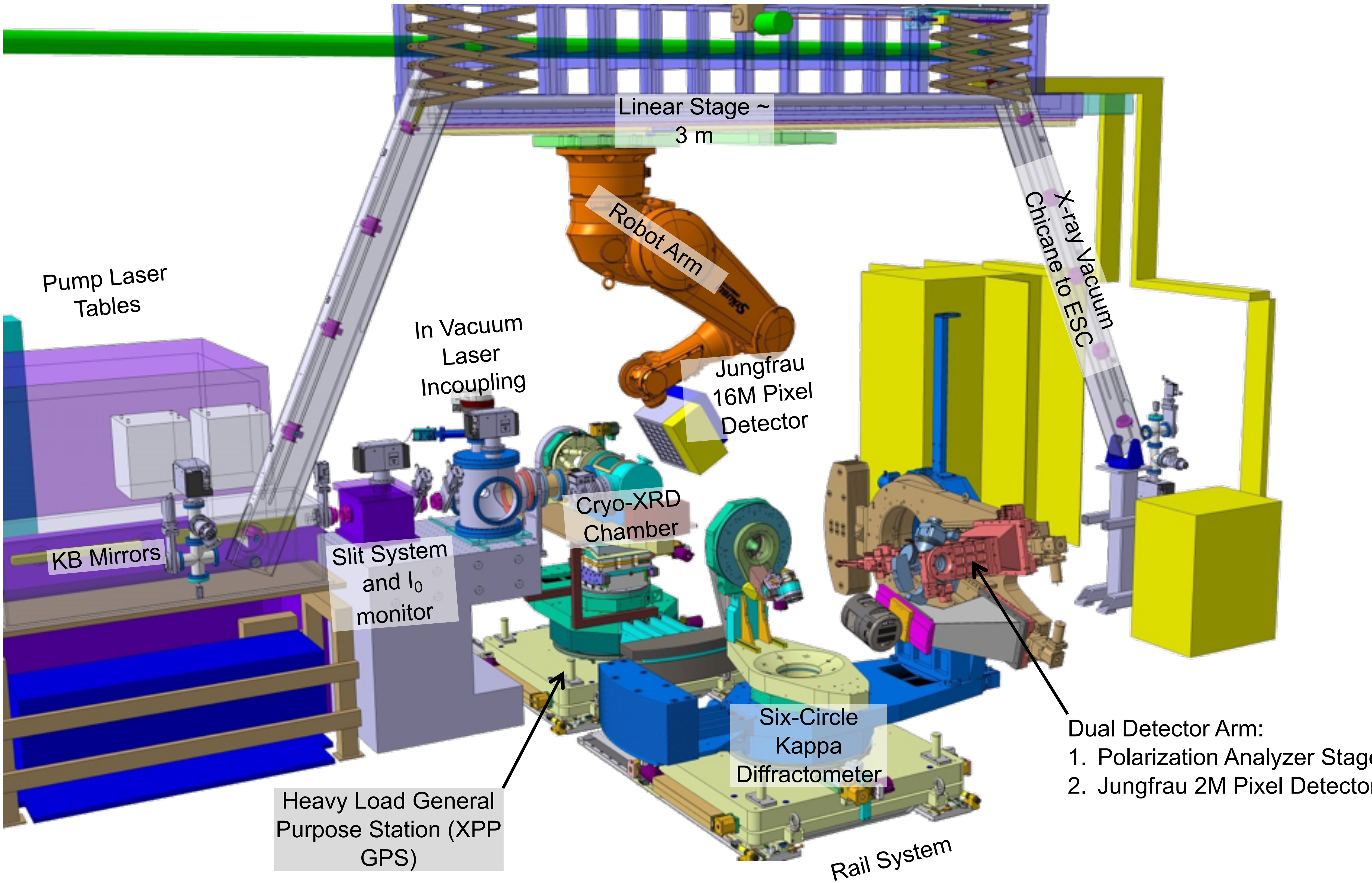



**Single X-ray focus position – two Endstations:**

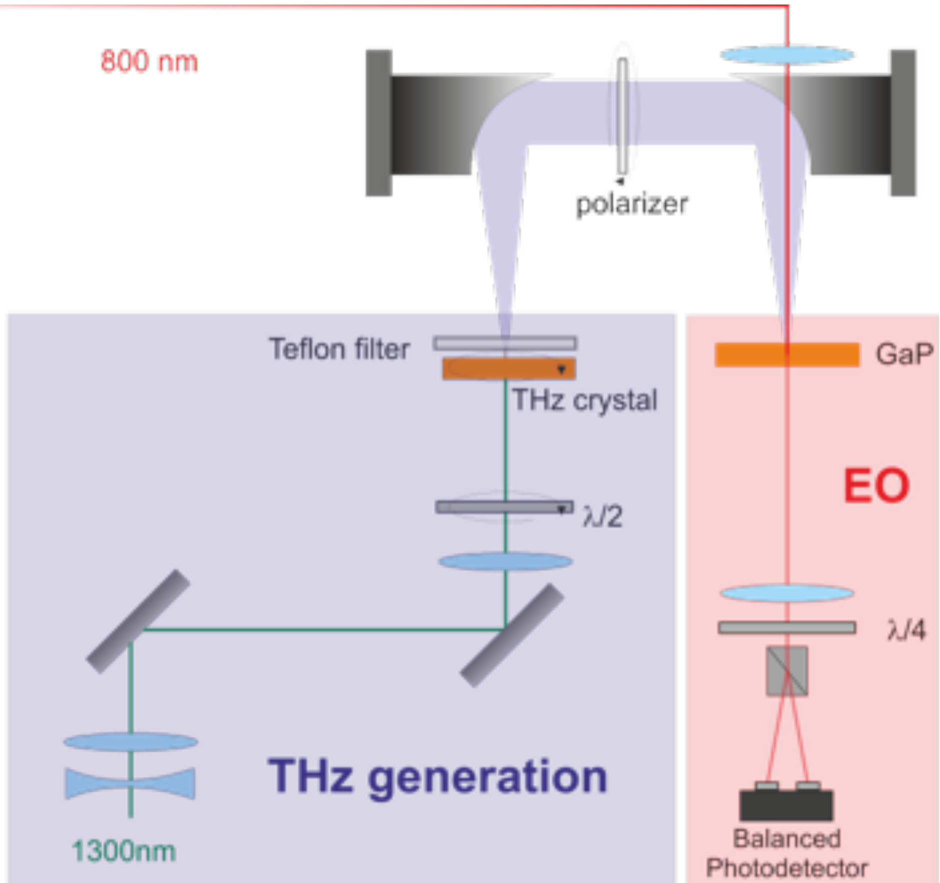
- **Pump-Probe General Purpose Station: XPP GPS (Heavy Load Station + Robot Detector Arm)**
- **Pump-Probe (Resonant) Diffraction: XPP XRD (Six-Circle Kappa Diffractometer)**

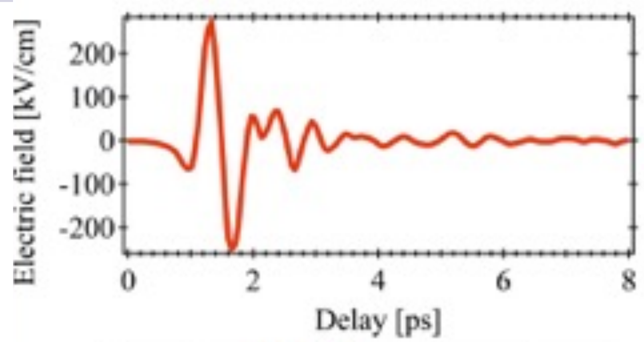
**(Cryo Diffraction Chambers mounted on both stations)**

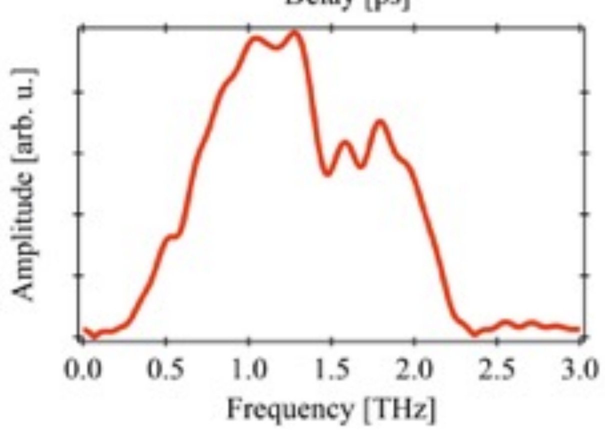
# SwissFEL ESB: Two Endstations



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

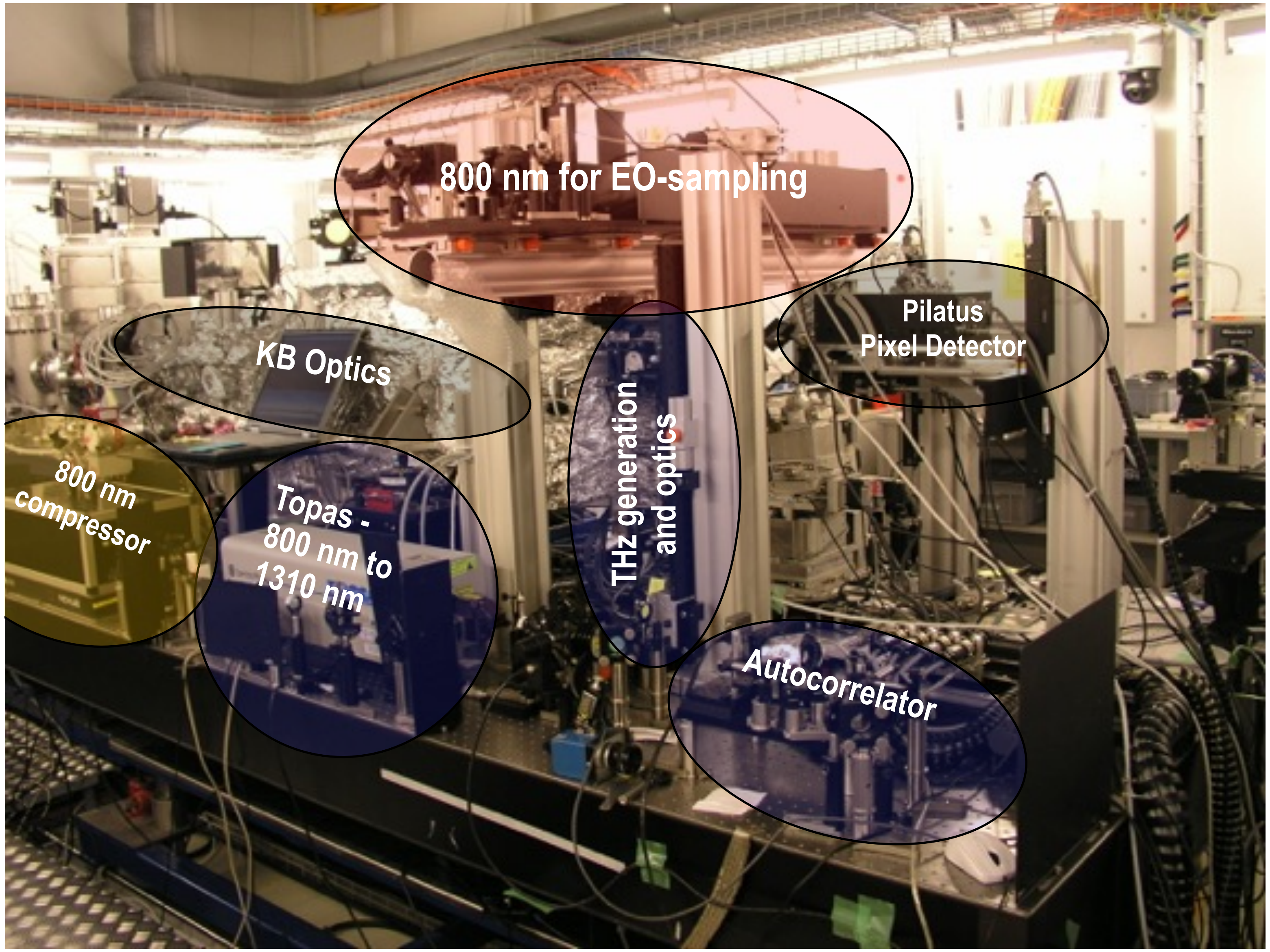


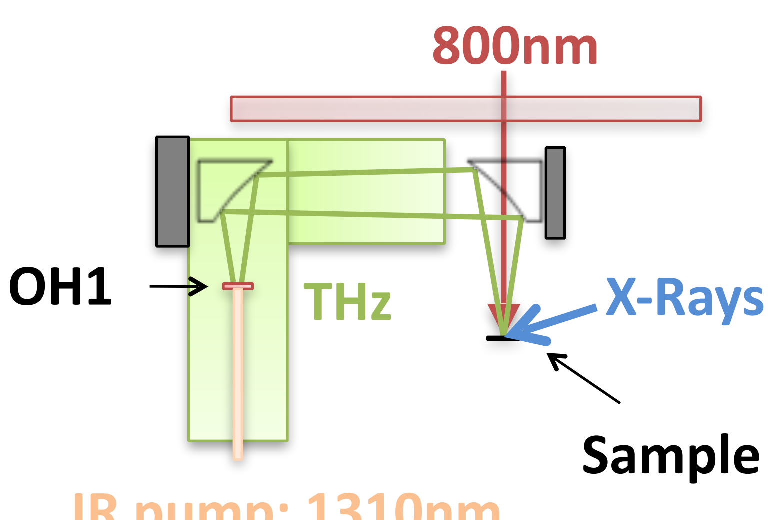



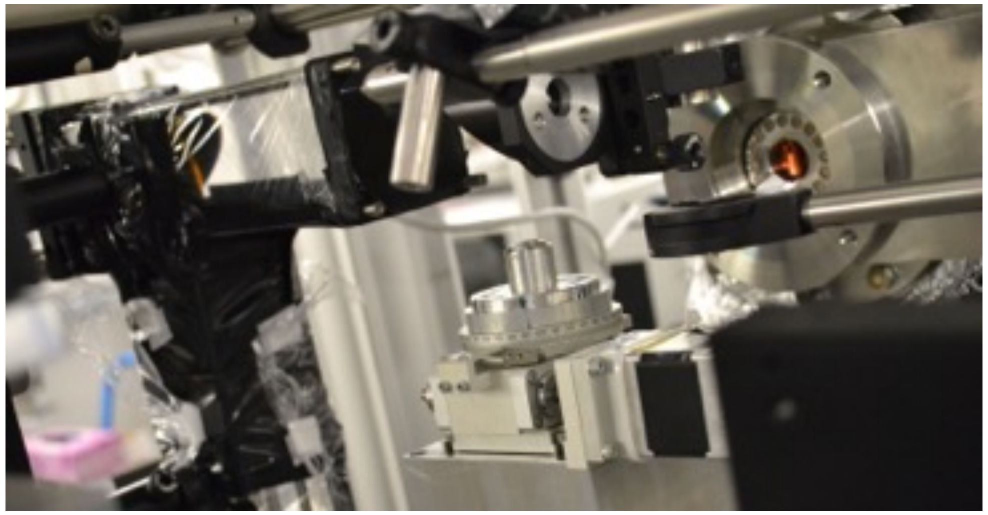




**Structural Order in $Sn_2P_2S_6$: Ferroelectric Polarization**

Grübel et. al. (in preparation)

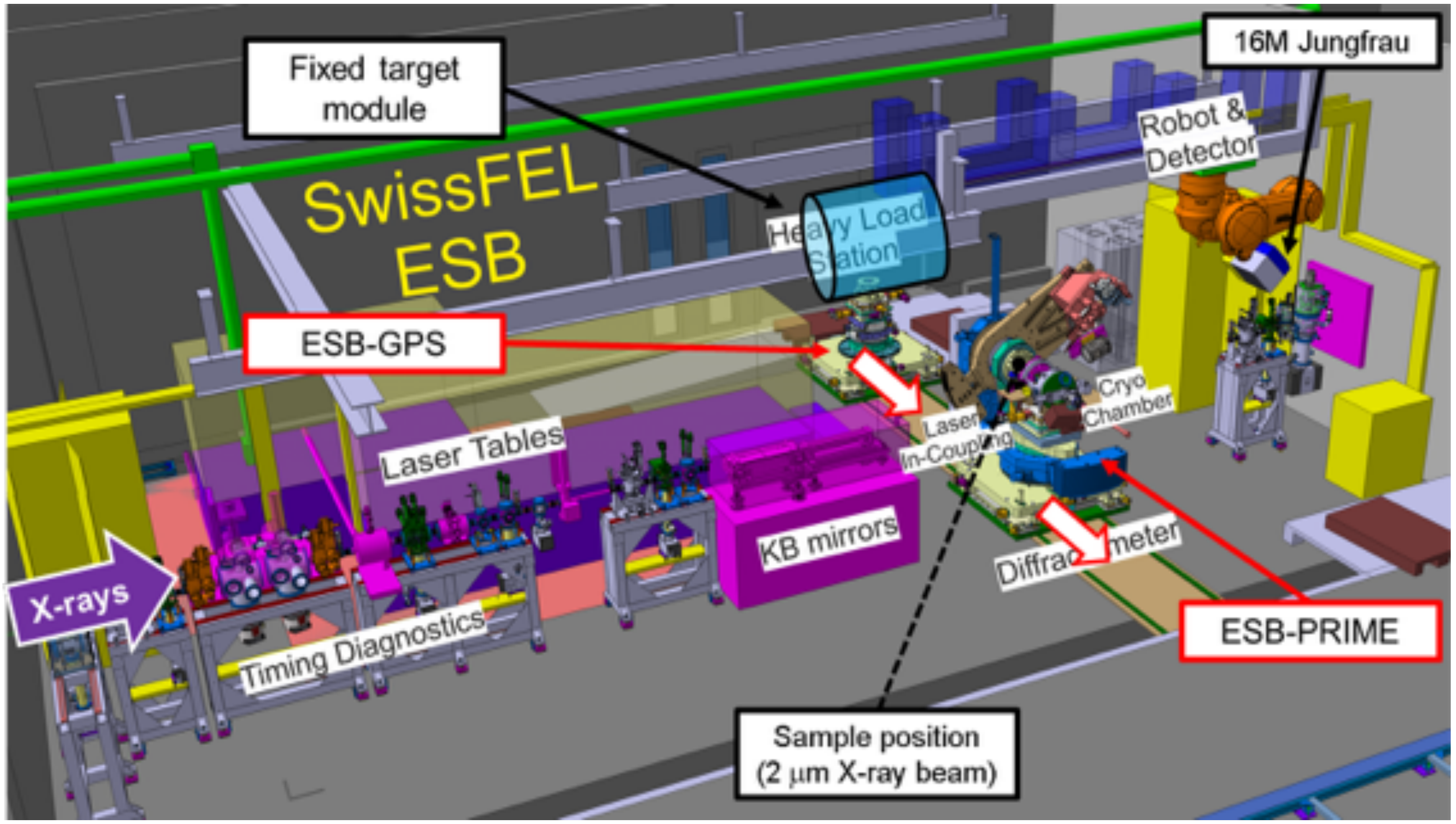


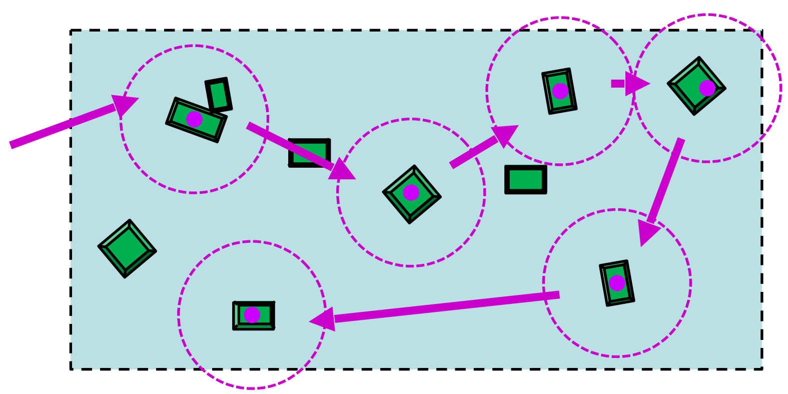



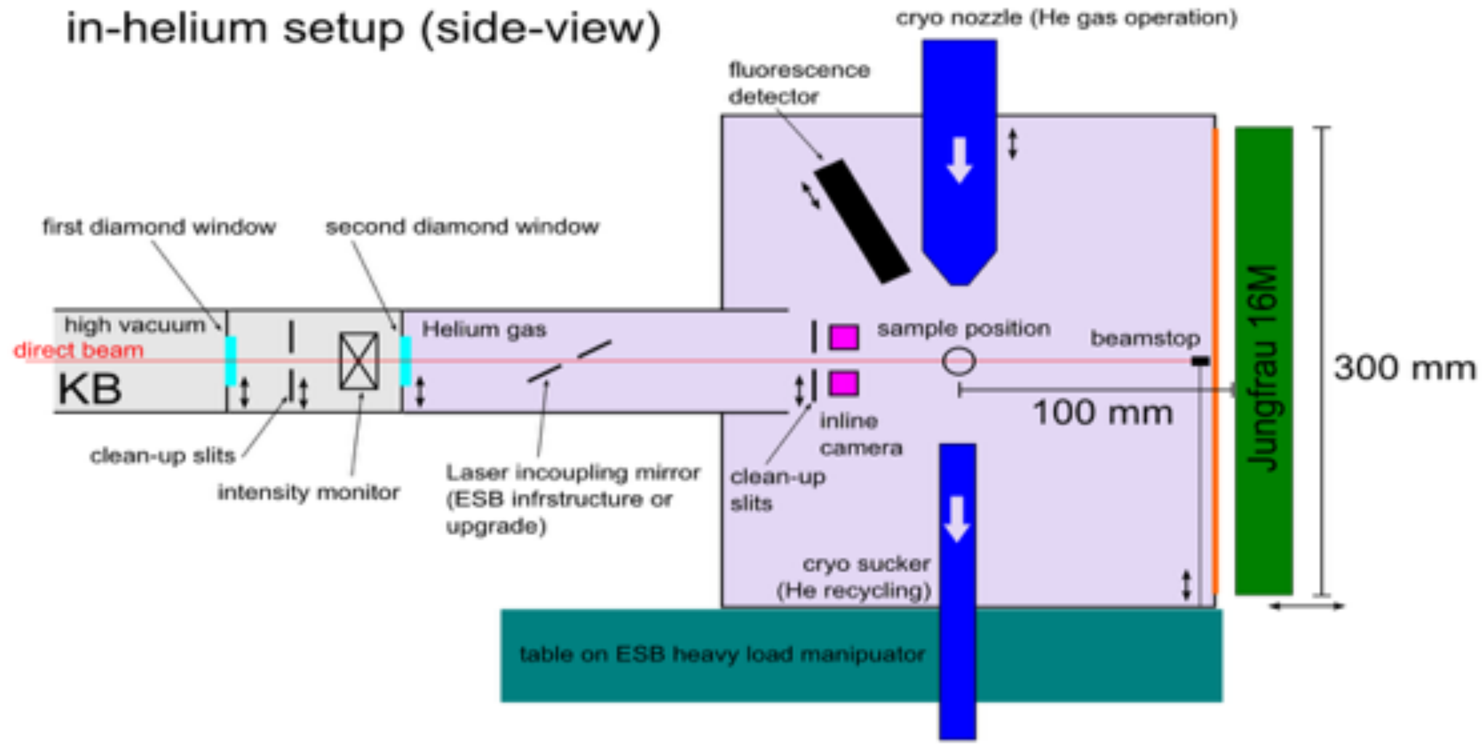
# Fixed target protein crystallography module at ESB-GPS

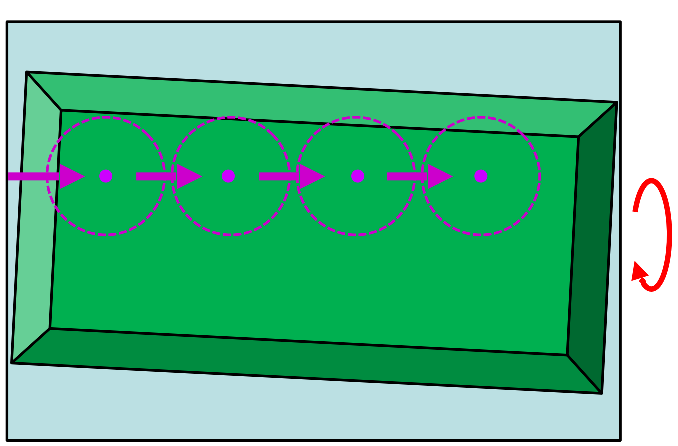
- Movable, suitable for ESB-GPS
- Room temperature AND Cryo
- In-air AND In-helium
- 100 Hz serial (scanning) femtosecond crystallography (< 5 μm xtals)
- Synchrotron-like femtosecond crystallography (> 5 μm xtals)




**Serial (scanning) femtosecond crystallography**



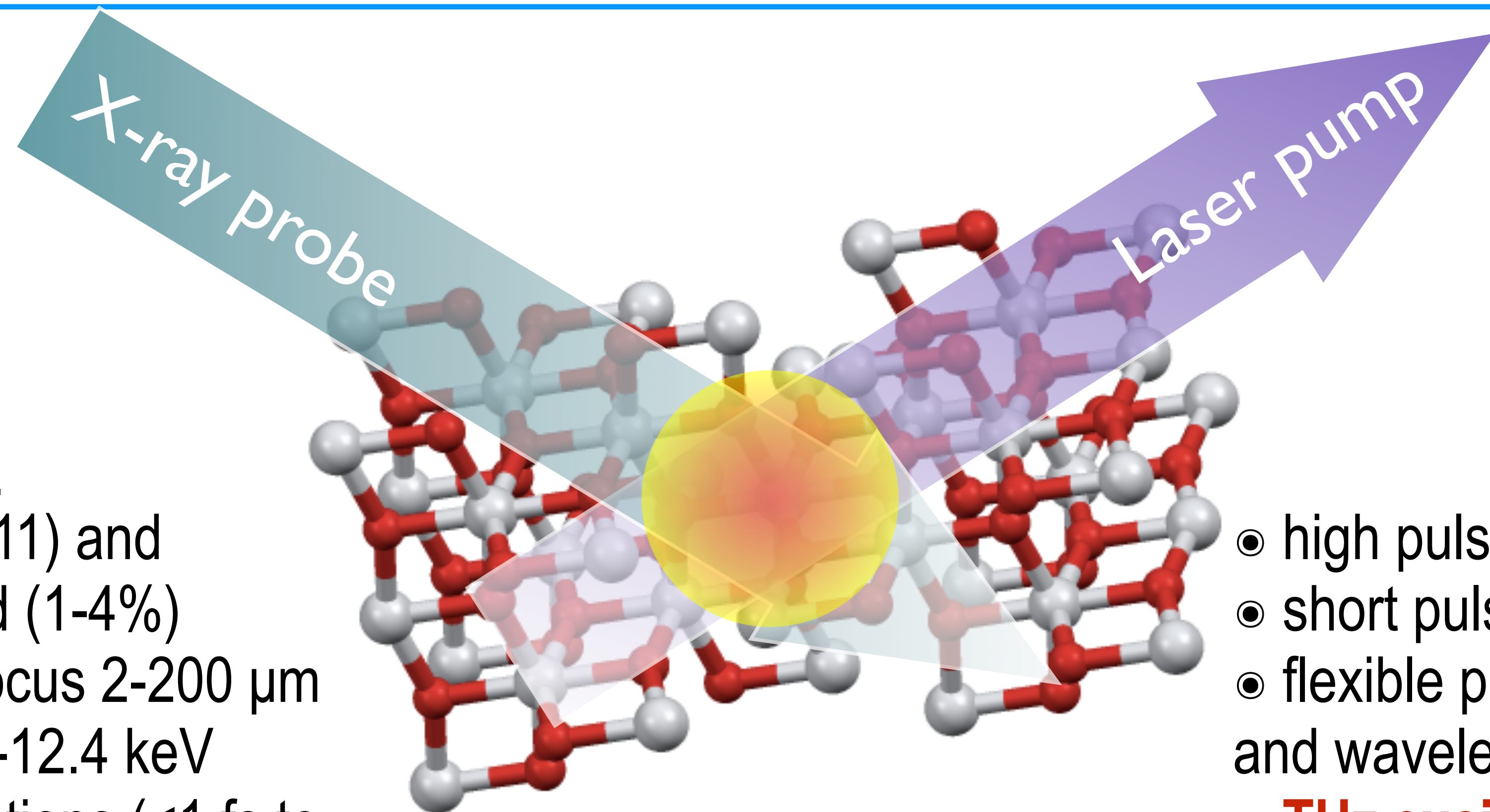


**Synchrotron-like femtosecond crystallography**

# SwissFEL Experimental Station B

**Goal:** To have this ready by 2017




## X-ray

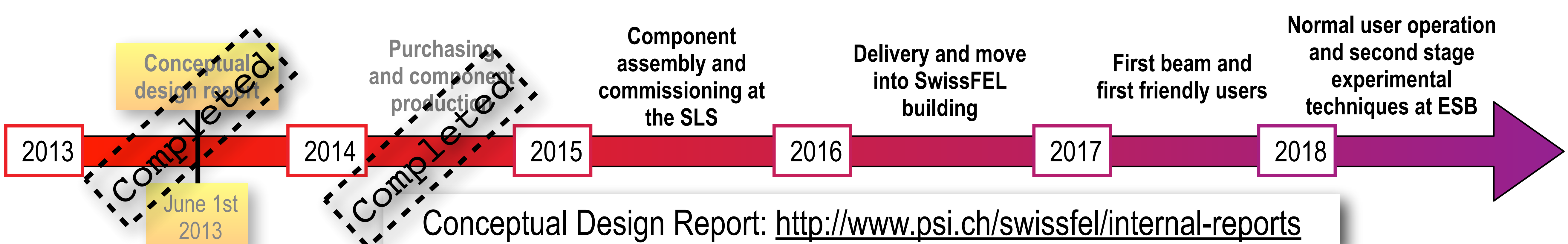
- monochromatic Si(111) and Si(311) and broadband (1-4%)
- variable KB mirror focus 2-200 µm
- tuneable energy 4.5-12.4 keV
- ultrashort pulse durations (<1 fs to 50 fs)

## 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

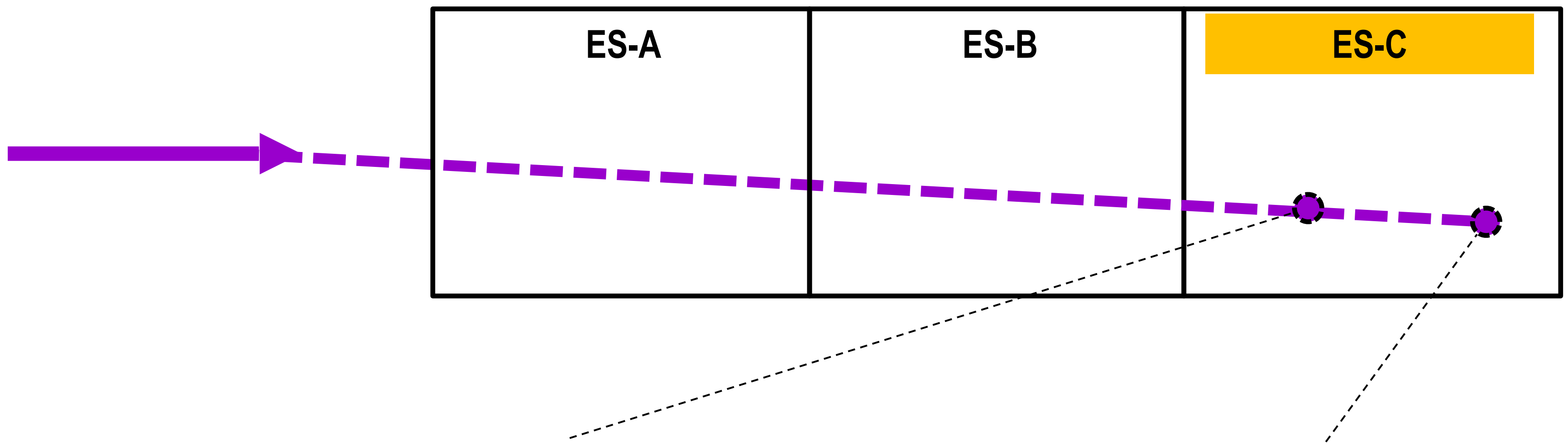
- 6-circle diffractometer
- 2D scattering detector (PSI 16M Jungfrau, 75 µm pixels, $10^4$ dynamic range)
- **HV/UHV diffraction chamber with cryo cooling (10-700 K)**
- Time arrival monitor <10 fs  P. Juranić et. al., Opt. Expt. **22**, 30004 (2014).
- General-purpose station for hosting user setups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

# Acknowledgements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**Rennes:** M. Lorenc;

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