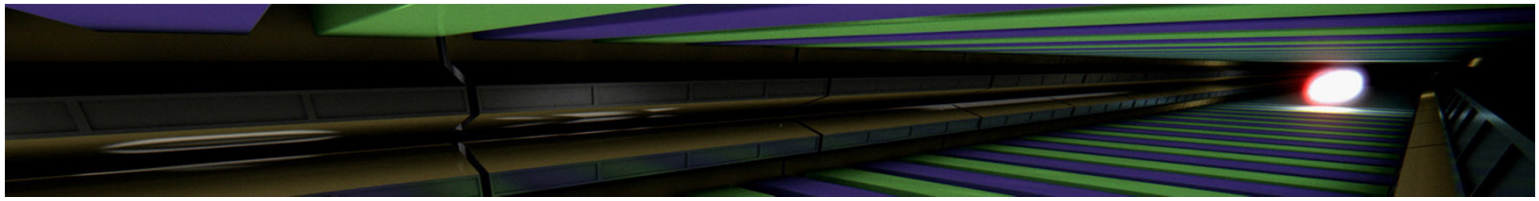
European XFEL



# FXE Instrument

Femtosecond X-Ray Experiments

Christian Bressler

March 12, 2012

# XAS/XES/XRD at the FXE instrument



- Dynamics of Solids and Liquids
- Combine versatile structural tools into one single setup
  - x-ray absorption (XANES, EXAFS)
  - x-ray emission (XES, RXES, …)
  - x-ray scattering (XRD, diffuse scattering)

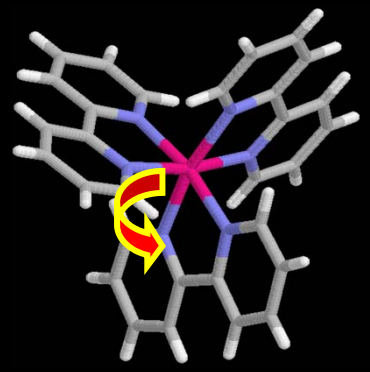
→ Obtain new information during the dynamics

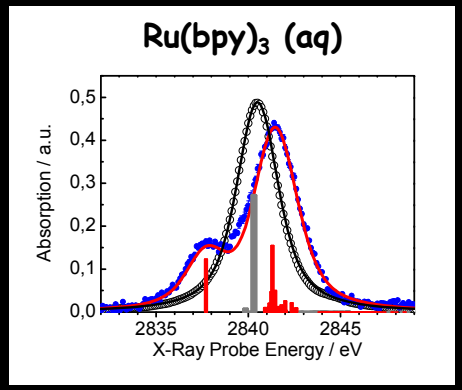
- Maintain both ambient and vacuum options
  - ambient conditions for liquids, solids, …
  - vacuum chamber for surfaces, cryogenic samples, …

- Exploit the highest possible time resolution (≤25 fs)
  …include as much flux as possible (≥ 120 pulses)

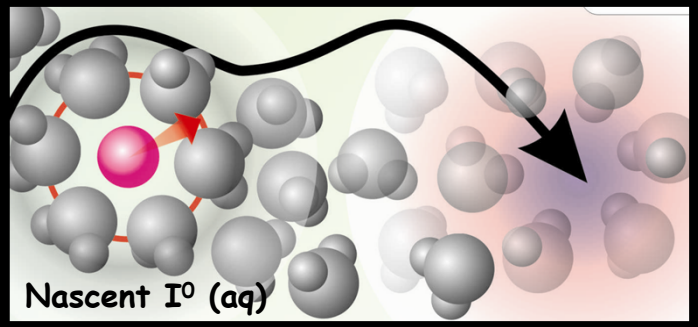
# Dynamic Studies in Photochemistry

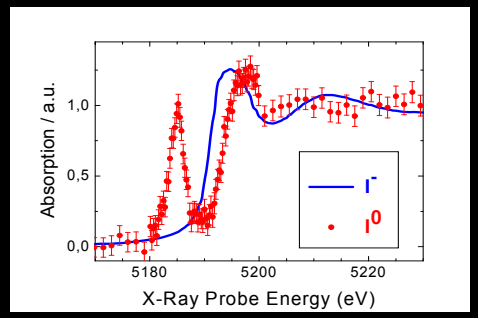
1. Intramolecular Charge Transfer (ps)






2. Towards Solvation Dynamics (ps, fs)



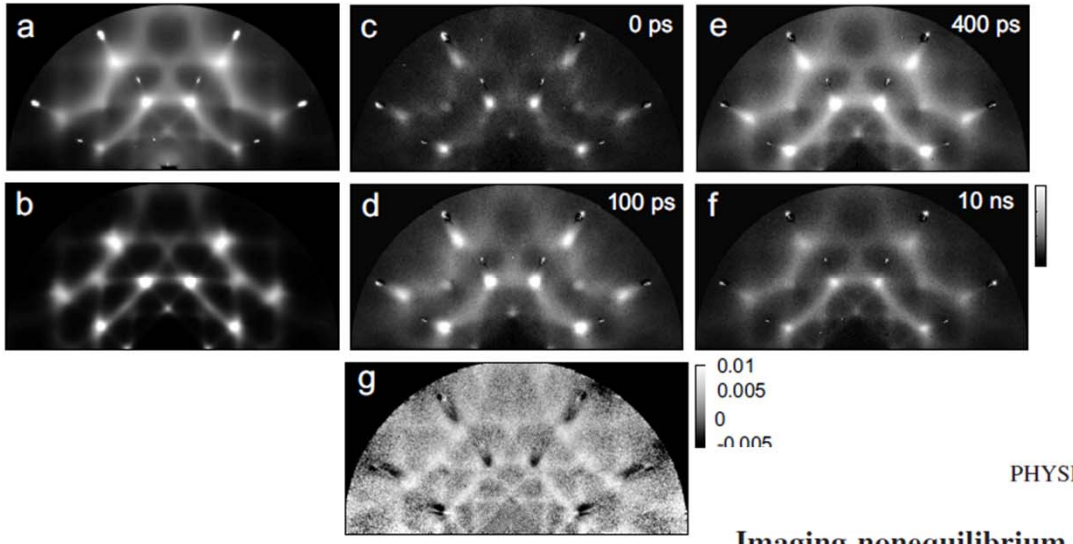



# Science Case



## Solid state phenomena

FXE offers new opportunities to study mechanisms that create or destroy long and short range symmetries of the lattice, charge, orbital, and spin degrees of freedom in a solid. These mechanisms are a key factor in understanding many cooperative phenomena in complex solids. The tools to study this include XRD, RXRD, and GID.

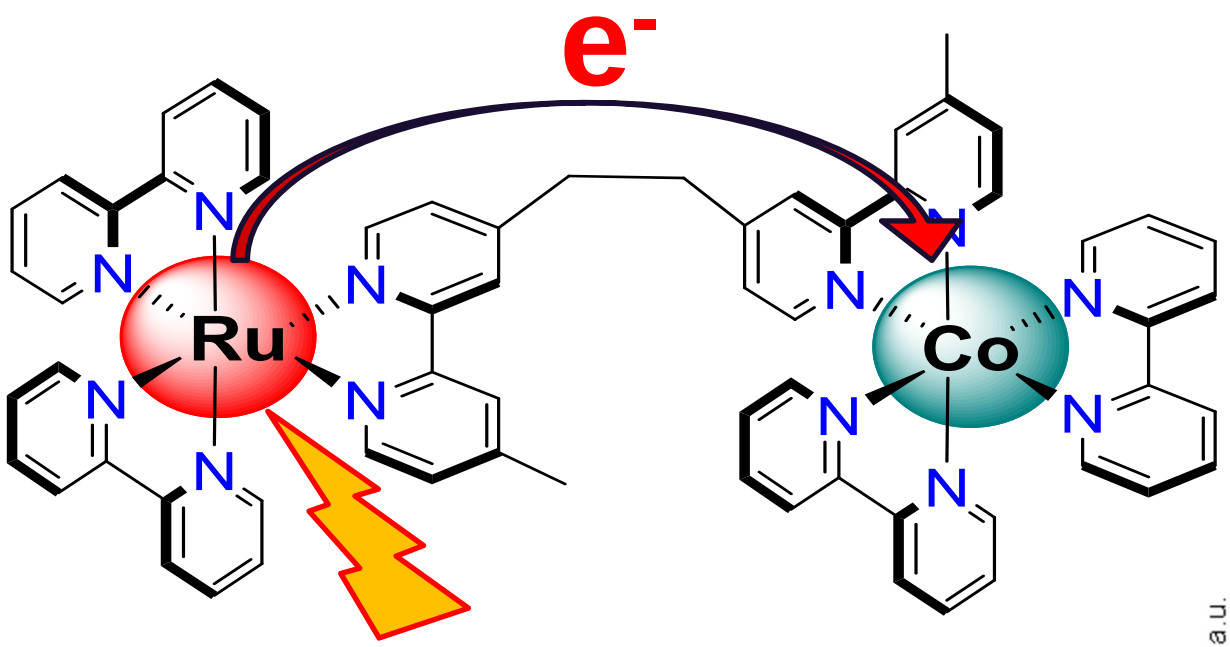



PHYSICAL REVIEW B 82, 235205 (2010)

**Imaging nonequilibrium atomic vibrations with x-ray diffuse scattering**

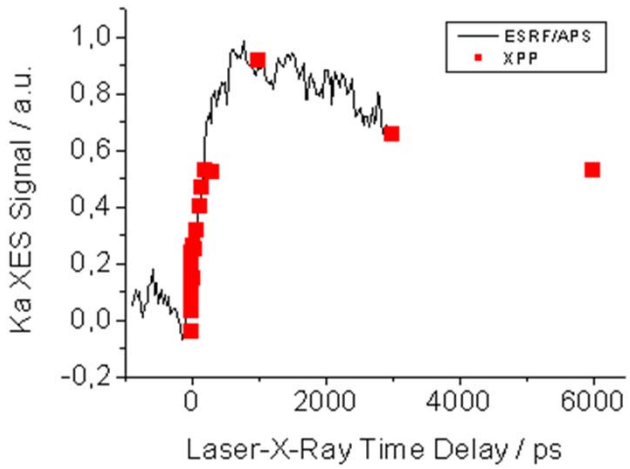
# Chemistry: Complementary Tools Desired





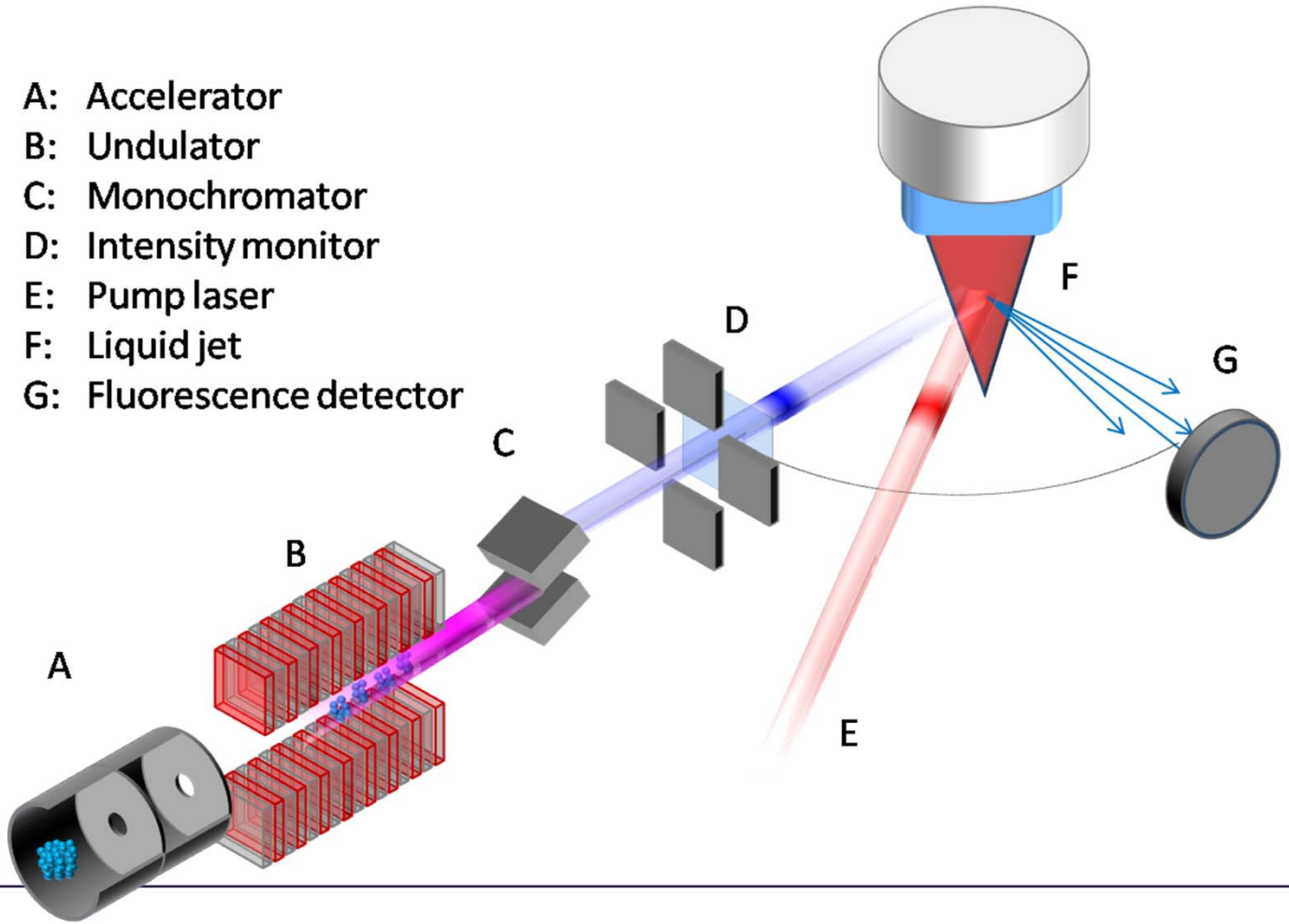

XES: occupied DOS (spin)
XAS: empty DOS (orbitals)
XRD: geometric structures

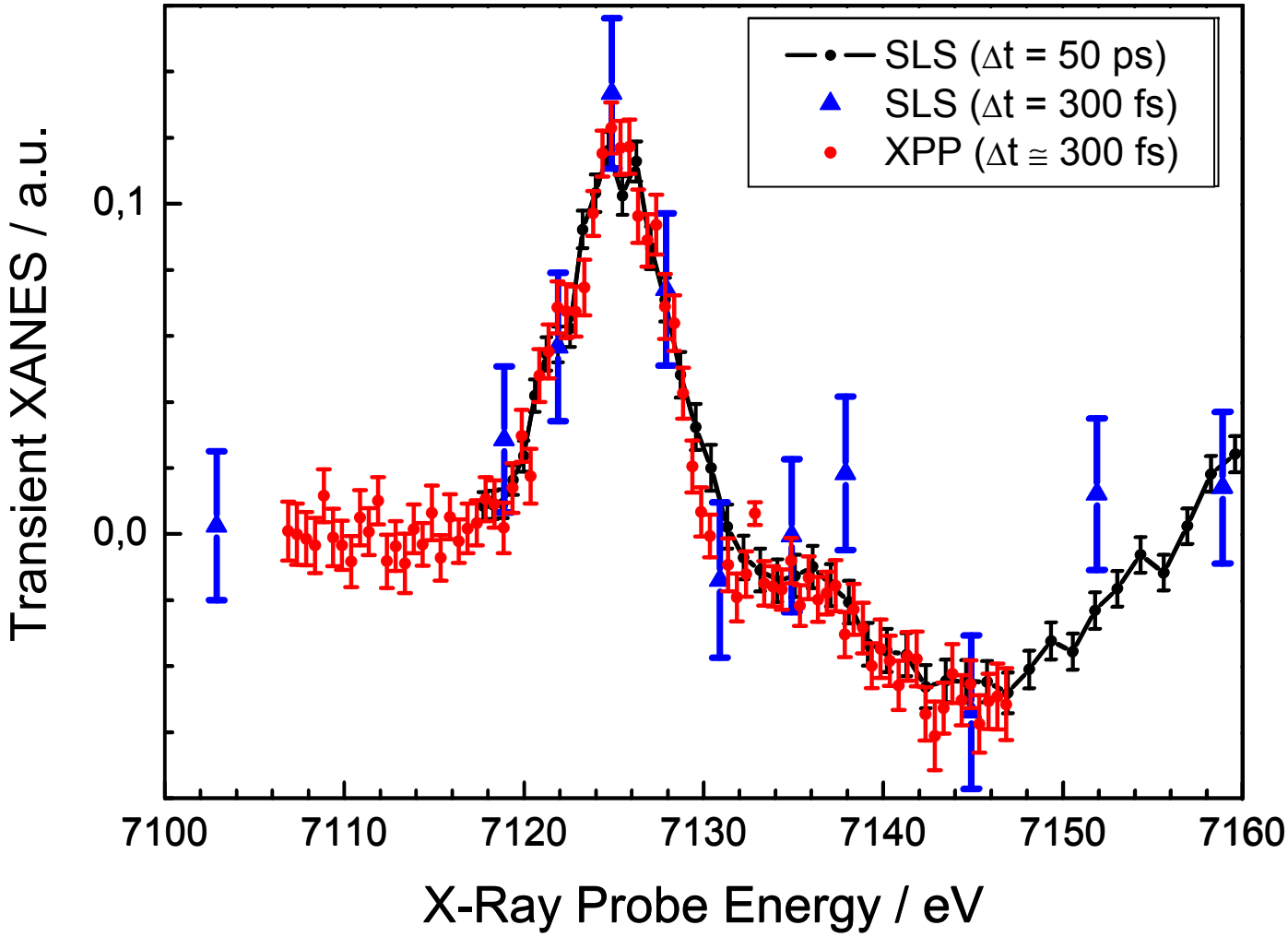
1) Ru(II) → Ru(III) (**XAS**, XES, optical)
2) IVR + e-transport (**XRD, optical**)
3) Co(III) → Co(II) (**XAS**, XES, optical)
4) Co(II) LS→HS (XAS, **XES**)



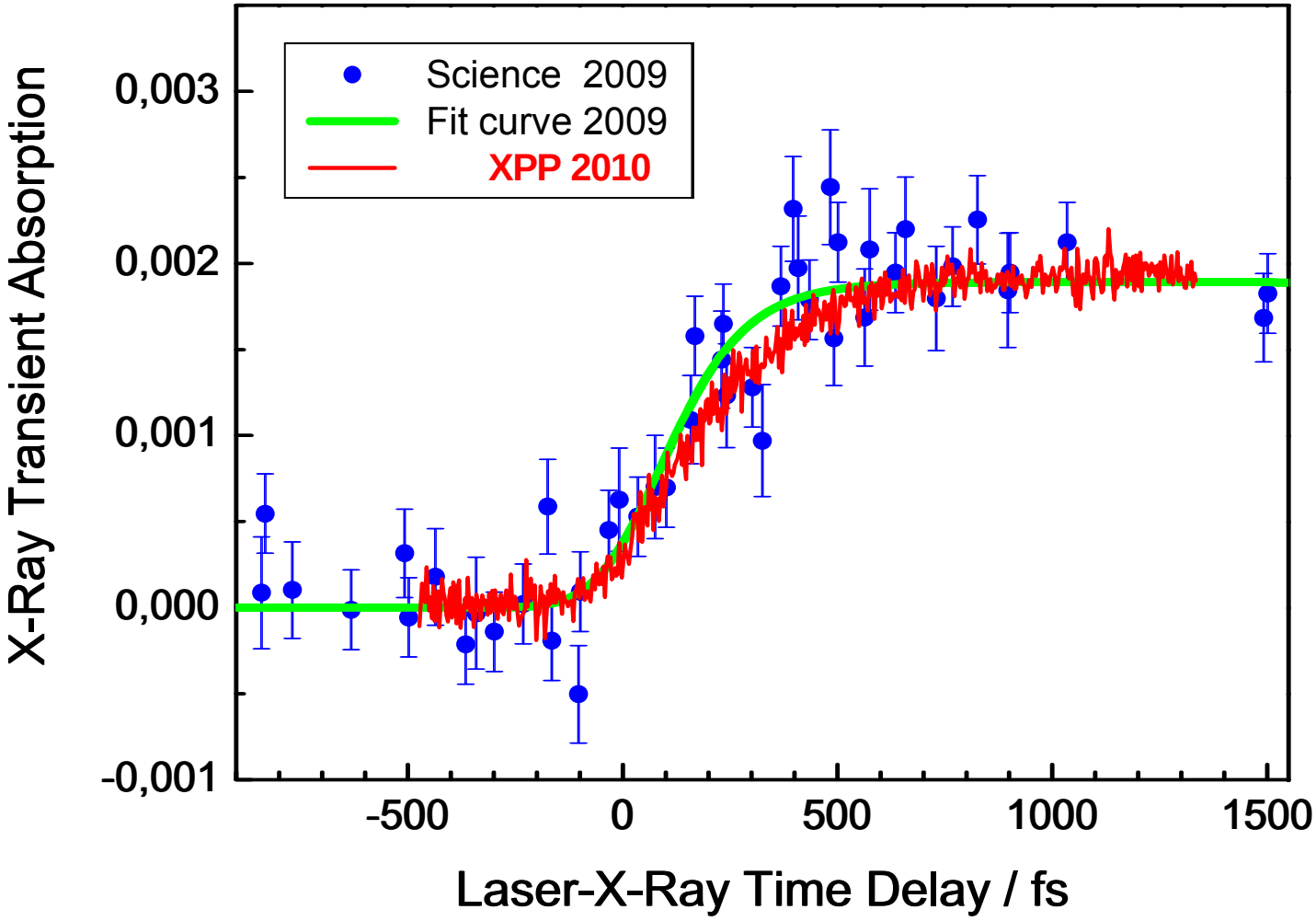
# XPP Commissioning (LCLS, Oct 2010) (L806)

- Entering the femtosecond time scale
- Credits: M. Cammarata, D. Fritz (SLAC)



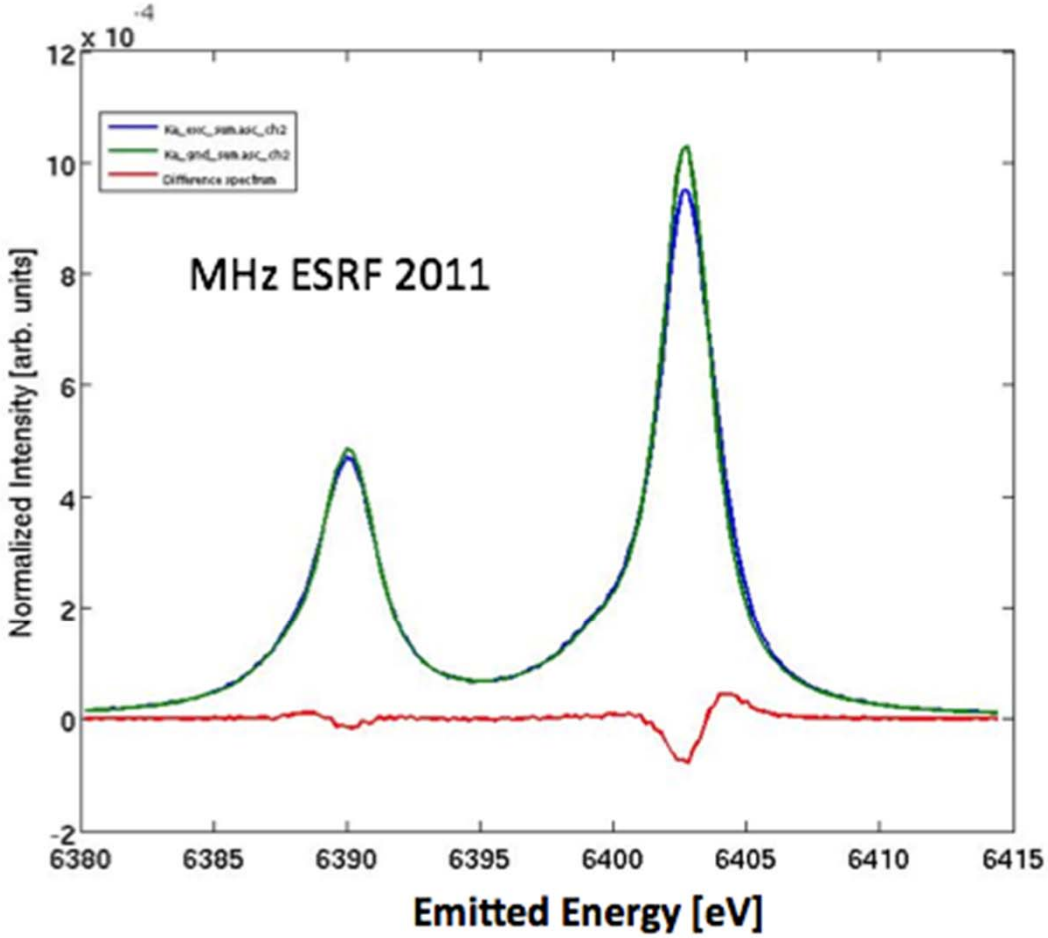

SLS (Δt = 50 ps)
SLS (Δt = 300 fs)
XPP (Δt ≅ 300 fs)
Transient XANES / a.u.
0,1
0,0
7100
7110
7120
7130
7140
7150
7160
X-Ray Probe Energy / eV

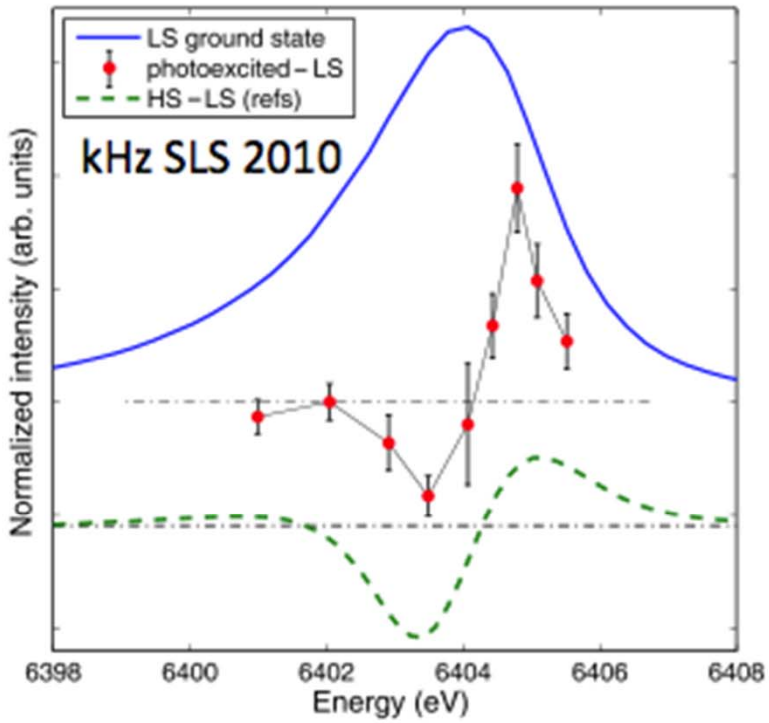
# Real-Time Traces



# Dramatic increase in Signal to Noise



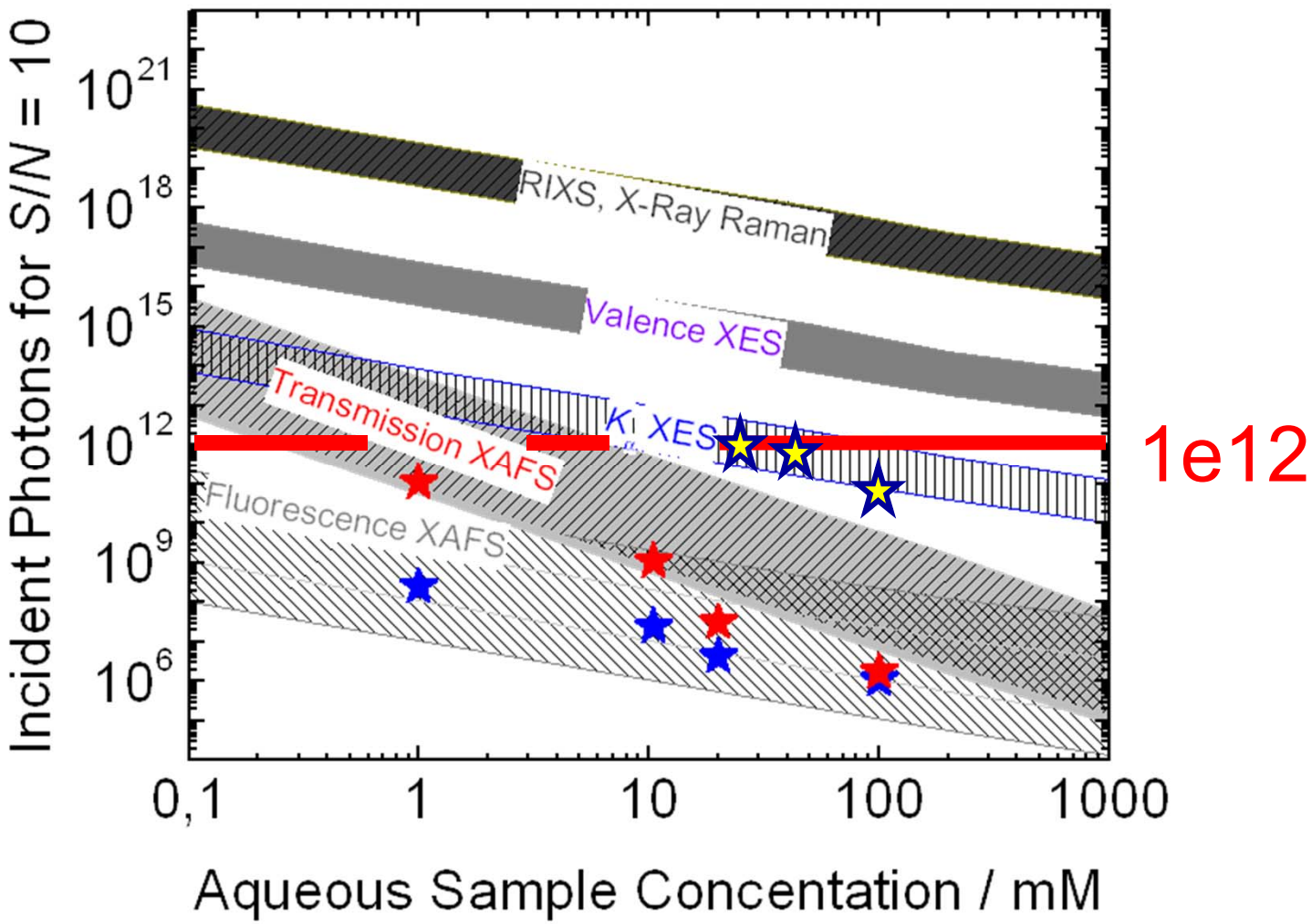



G. Vanko *et al.*, *Angew. Chem. Int. Ed.* (2010)

# Time-Resolved X-Ray Spectroscopies

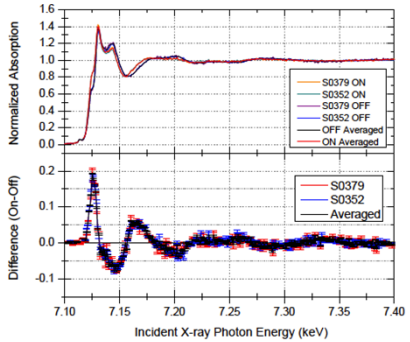


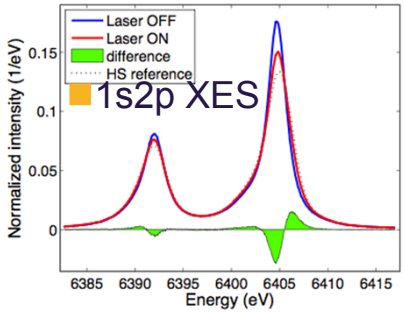


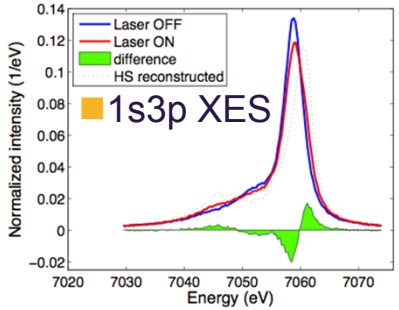
# Exploiting complementary techniques (ESRF, APS)

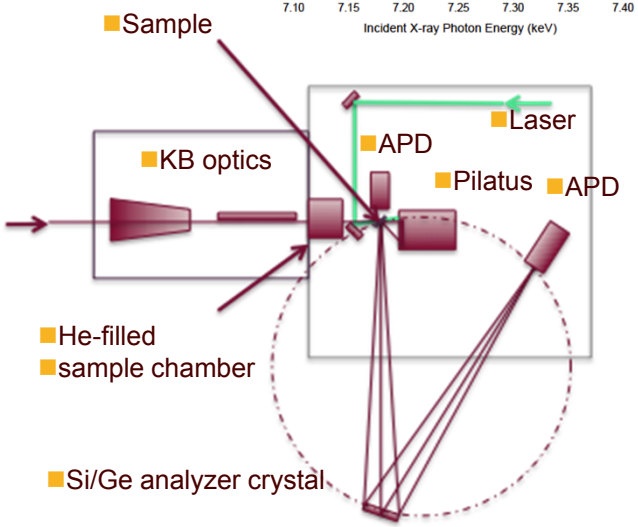


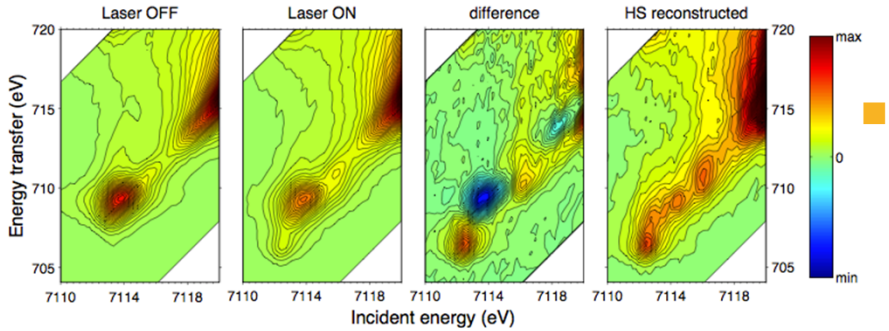
- XANES
- EXAFS



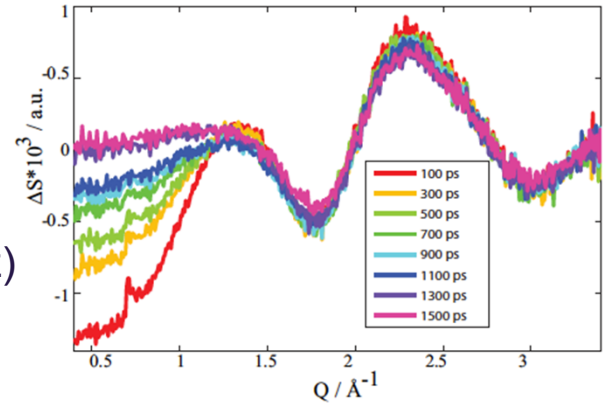




- 1s2p RXES

- UDECS collaboration at work!
- Sector 7ID @ APS, Argonne (3.36 MHz)

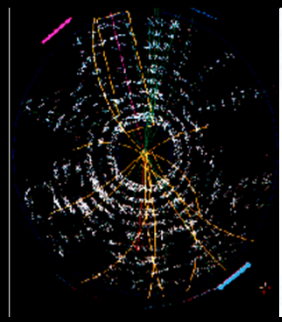


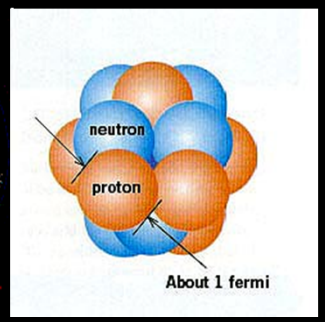

- X-ray Diffuse Scattering (XDS)
- To be submitted 2012

# What are the fundamental timescales?

Chemistry and Biochemistry

Solid State Dynamics

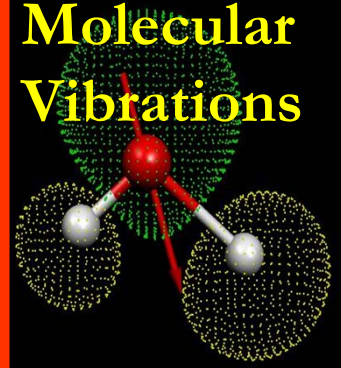





Photosynthesis

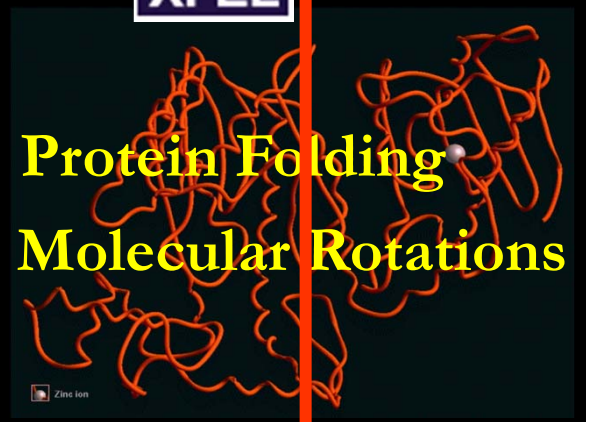
Vision

Molecular Vibrations



Protein Folding

Molecular Rotations



Strings, Cosmology

Particle Collisions

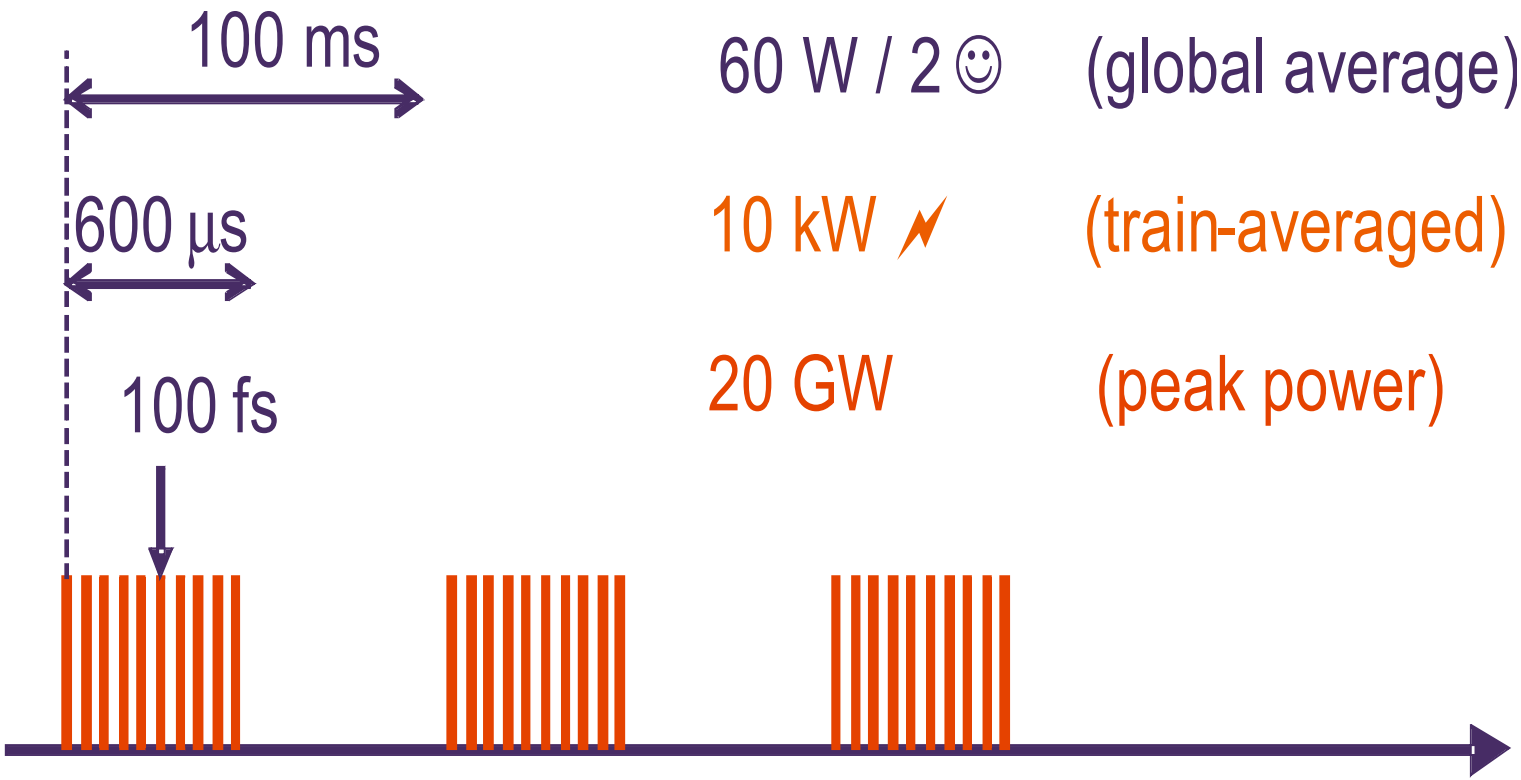
Electron dynamics

| harpo | yacto | zepto | atto | femto | pico | nano | micro | milli |
|---|---|---|---|---|---|---|---|---|
| $10^{-27}$ | $10^{-24}$ | $10^{-21}$ | $10^{-18}$ | $10^{-15}$ | $10^{-12}$ | $10^{-9}$ | $10^{-6}$ | $10^{-3}$ |

Time /seconds

# Time and Power Scales






60 W / 2 ☺ (global average)

10 kW (train-averaged)

20 GW (peak power)

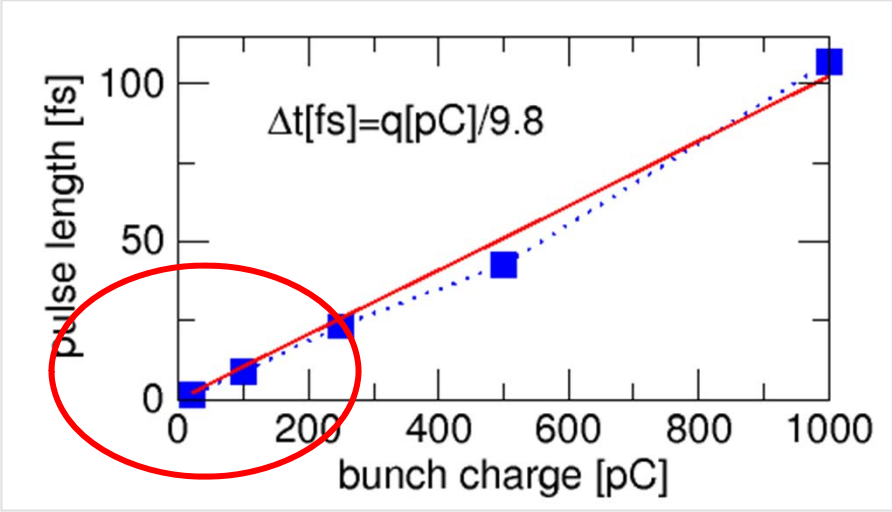
2700 pulses
(2 mJ/pulse)

# FXE Overview Specifications



- 5 – 20 keV (24), 0.1 % bw
  → > 10 A-1 q-range possible (WAXS)
- 1e-4 (Si-111) – XANES, XES, XRD
- 1e-5 (Si-311, 333) – RIXS
(primary monochromator)

- Low-Charge Mode (< 250 pC)!
  < 25 fs pulse width !
- 120 pulses/burst, up to 2700
- Flexible Spot Size (< 1 mm)
  (line, spot)



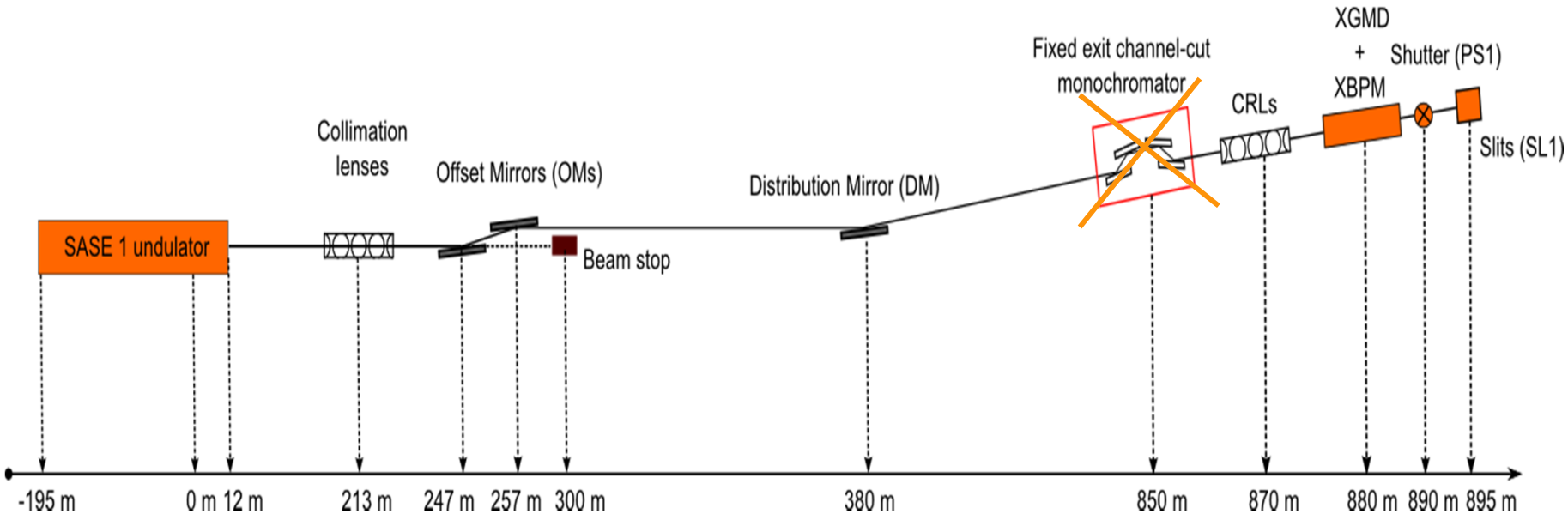
# Overview

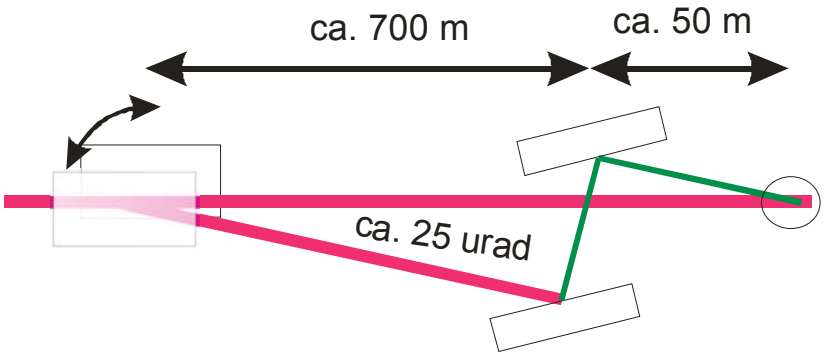


- From/since FXE Workshop (12/2009)
  - Emphasis on secondary spectrometers
  - Diffraction capability
  - Ultrahigh time Resolution (1st goal: <30 fs cc)
- Users want
  - variable pulse patterns (1-10 Hz, 1-1000 pulses/burst)
  - small foci (SAXS nano, Protein XRD)
  - large spots (solid PT, Protein XRD, surface refl, …)
  - < 0.5 mrad divergence
  - < 1e-3 energy bw (down to e-5)
  - usual laser conditions (<25 fs, UV-vis/NIR, THz, …)

# X-Ray Beam Transport (5-20 keV), top view





# Natural Divergence (urad) and spot sizes

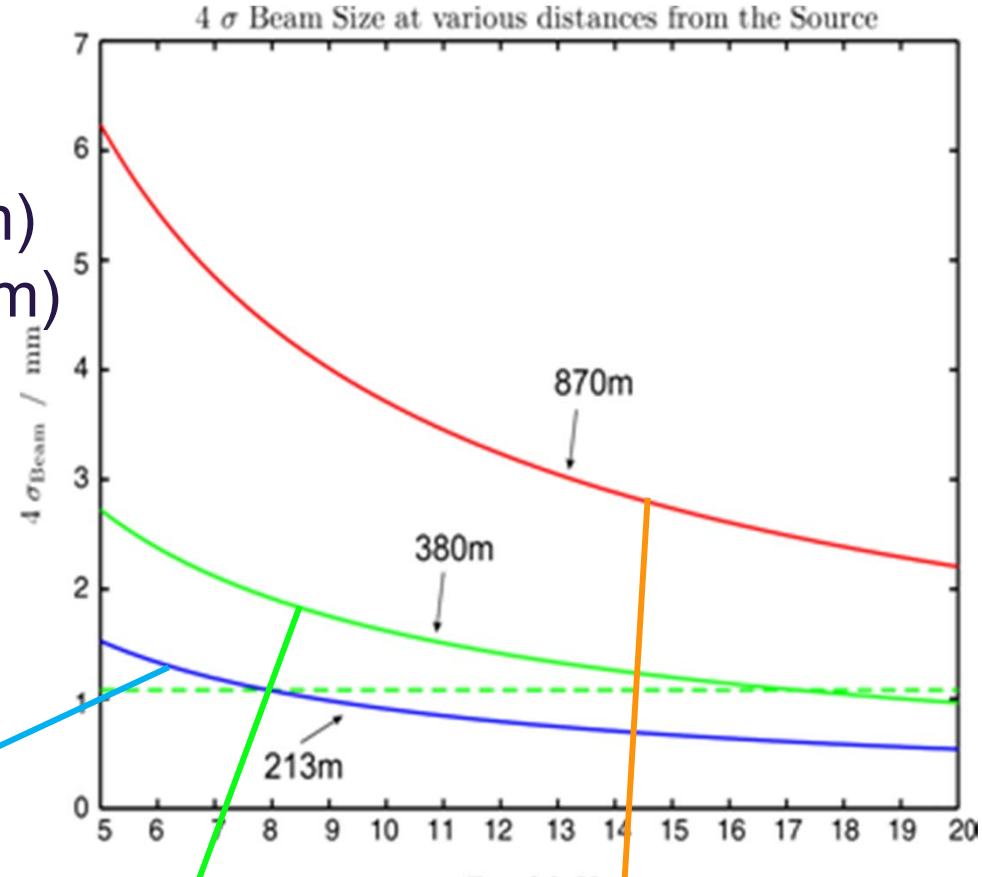


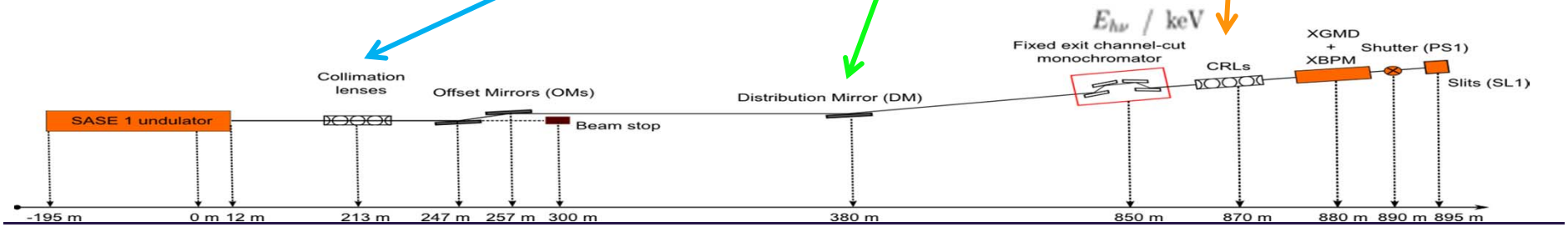
- Beam on DM (380 m):

- horizontally bend OM (250 m) (intermediate focus near 600 m)

- collimate beam at 213 m (CRL collection)

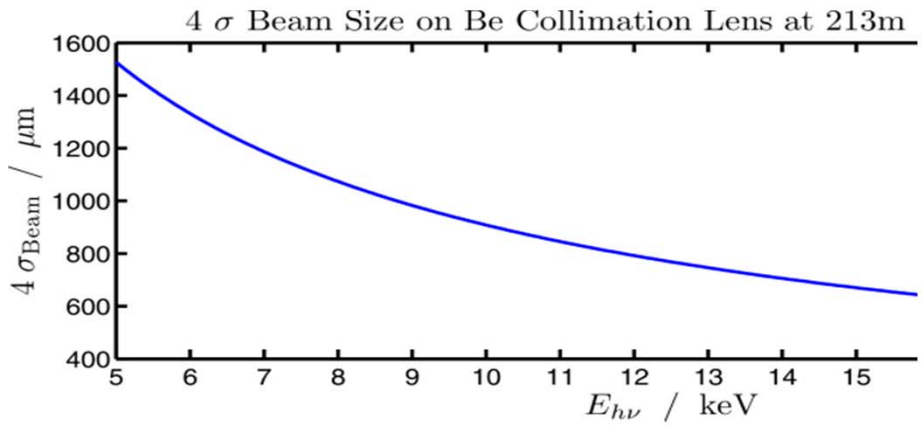
- combination of both

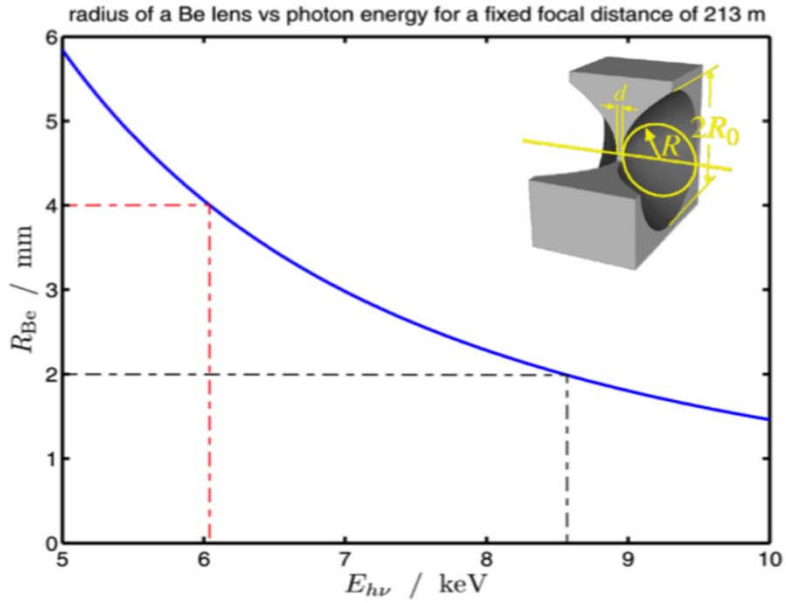


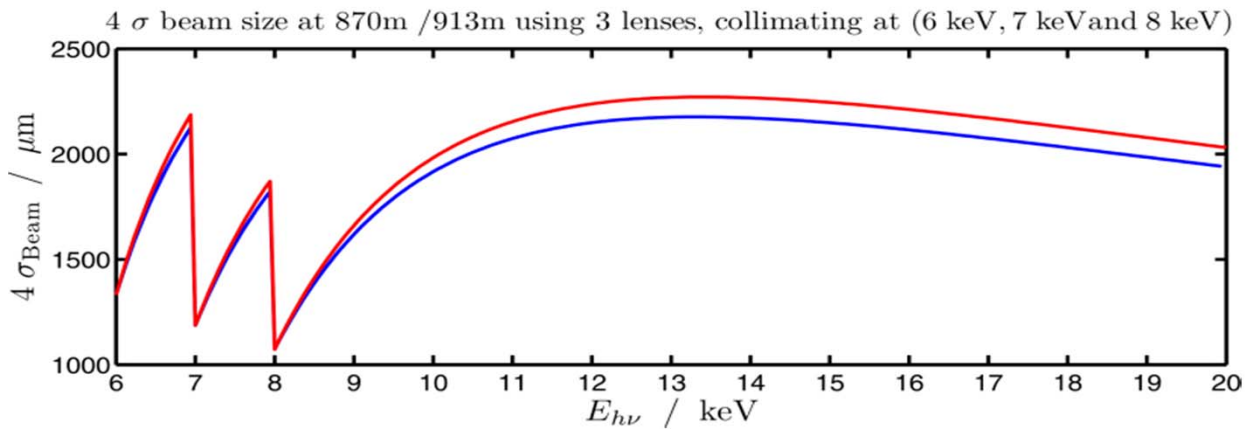



# Be lenses (CRL) at 213 m: Spot Sizes



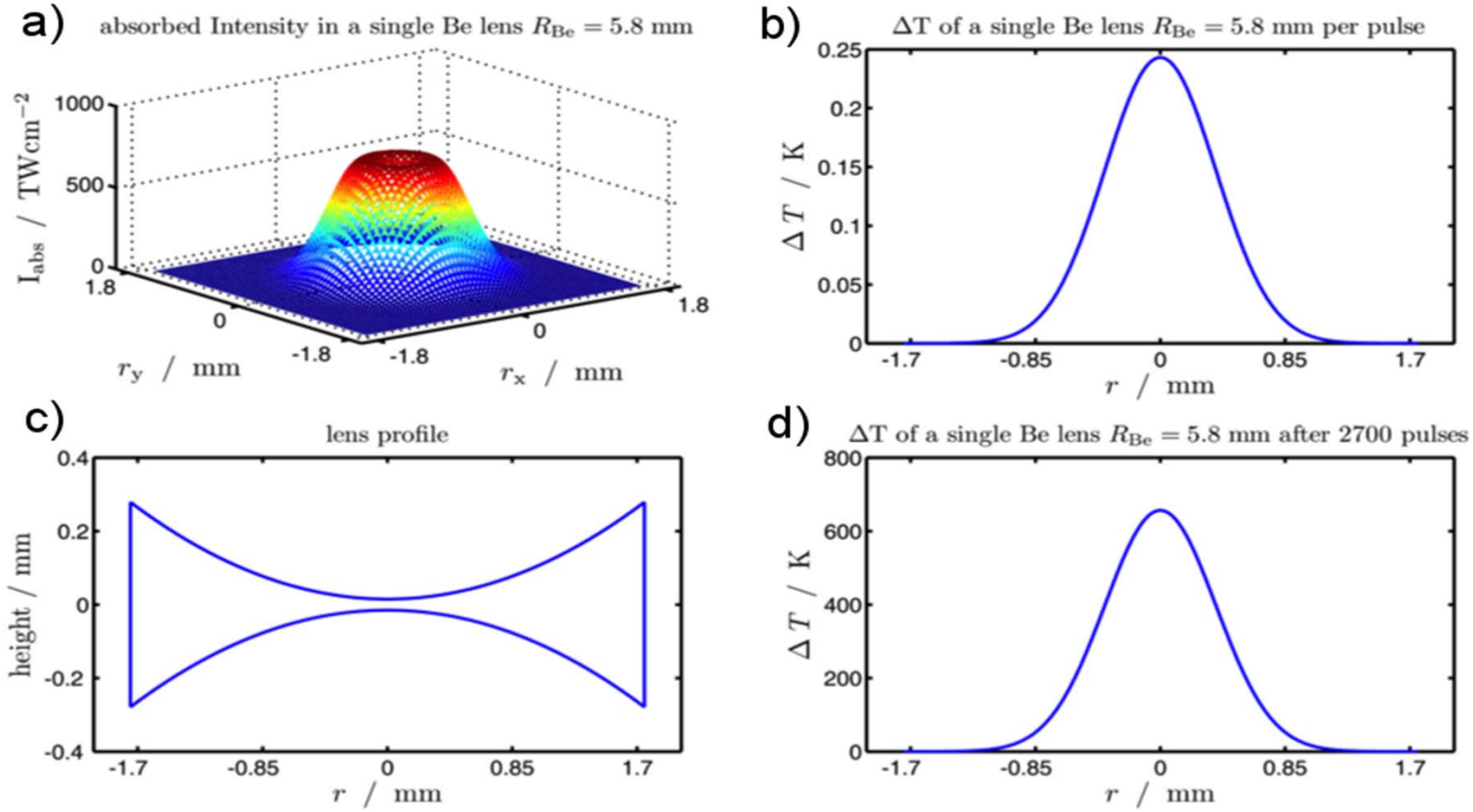


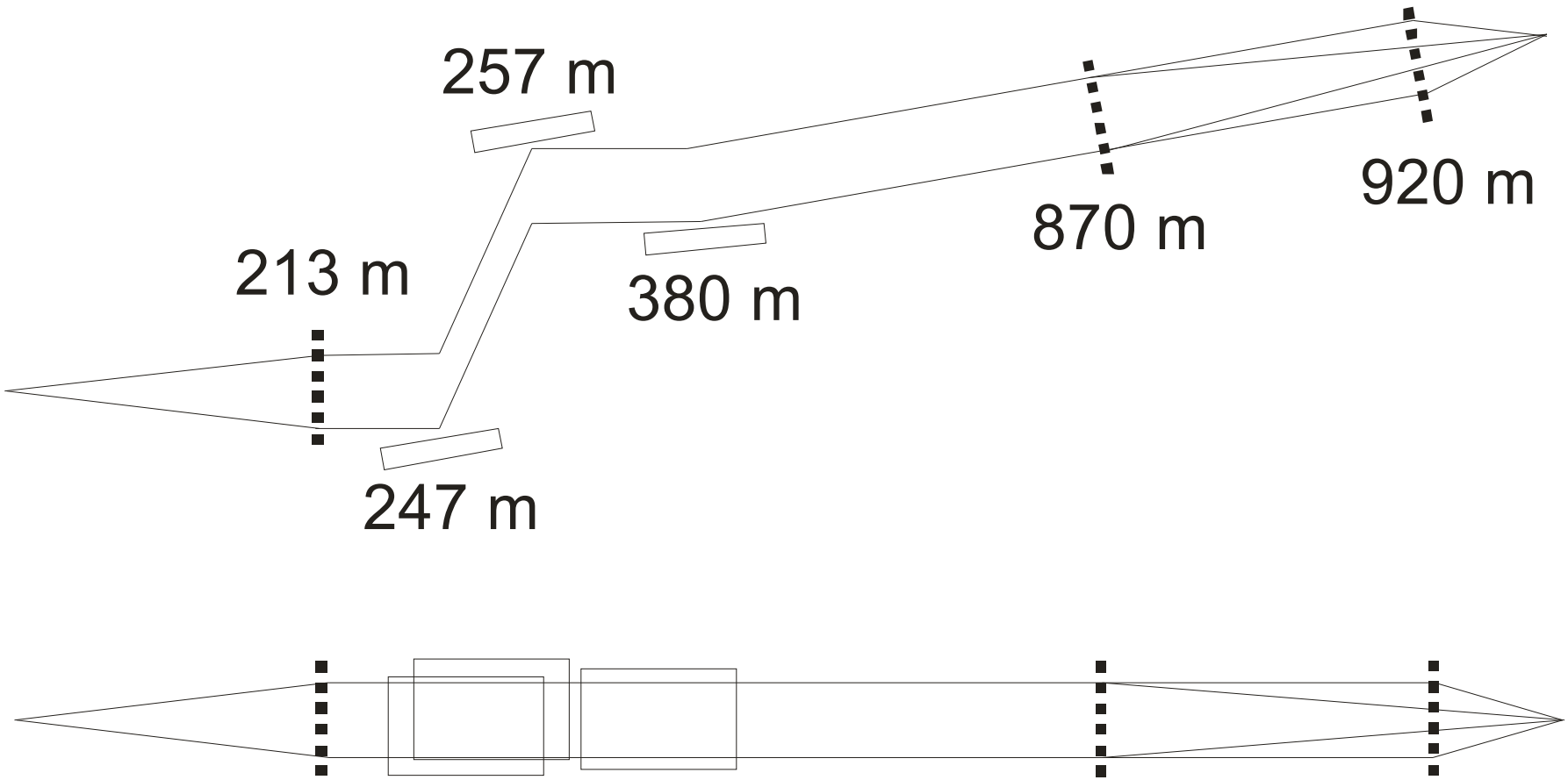
# Heat Load on Be lens (213 m), 5 keV/0.25 nC





# Beam Transport Concept: < 250 pC CRLs ok





# Refocussing lenses: 870 m, 913 m



**Table 1:** *Relevant beam parameters (divergences, focal sizes, etc.) for selected x-ray energies at the FXE instrument using CRL stacks for focusing and beam collimation*

| X-ray energy /keV | Source divergence $4\sigma$ / rad | Spot size (213 m) $4\sigma$ /mm | Divergence at 870 m / rad | Focal spot Size FWHM / m (Be stack at 870m) | Focal spot Size FWHM / m (Be stack at 913 m) |
|---|---|---|---|---|---|
| 6 | 6.25 | 1.33 | 0 | 5.6 (f = 48m, N = 2) | 0.6 (f = 5m, N = 16) |
| 7 | 5.57 | 1.19 | 0 | 5.4 (f = 48m, N = 2) | 0.6 (f = 5m, N = 21) |
| 8 | 5.04 | 1.07 | 0 | 5.2 (f = 48m, N = 3) | 0.5 (f = 5m, N = 28) |
| 9 | 4.61 | 0.98 | 0.57 | 5.1 (f = 46.3m, N = 4) | 0.5 (f = 5m, N = 35) |
| 12.4 | 3.63 | 0.77 | 1.25 | 4.7 (f = 42.5m, N = 8) | 0.5 (f = 5m, N = 67) |
| 18 | 2.74 | 0.58 | 1.30 | 4.3 (f = 41.8m, N = 17) | 0.5 (f = 5m, N = 142) |

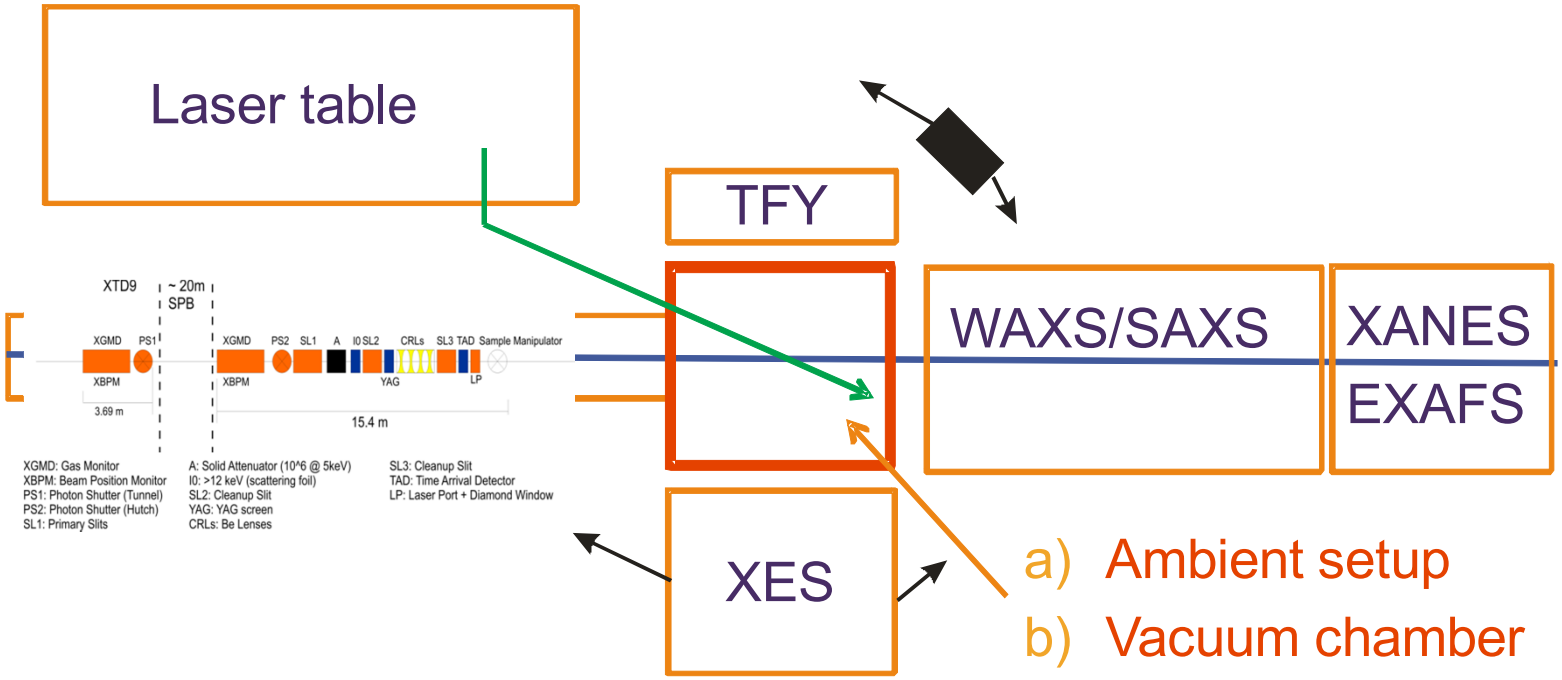
870 m: 5 um focus

913 m: 0.6 um focus

- Additional Option: smaller KB system (913 m)

# FXE basic design





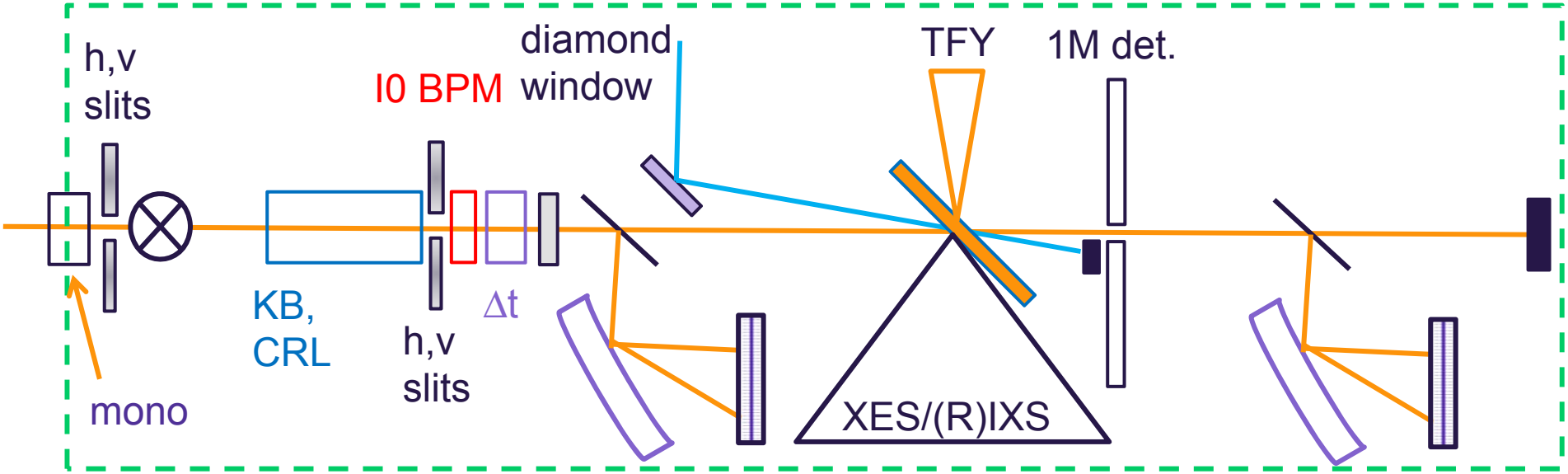
# Maintaining Options for 5 – 600 um Spots Sizes



- Ambient Experimental Station
  - 50 – 600 um spot sizes (line, spot)
  - **flexible He environment**
  - → rotatable XES/RIXS spectrometer
  - divergence adjustable (0 – 70 urad)
  - samples can survive beam in low-charge mode
- Add-on Equipment: Vacuum Chamber
  - small foci possibility
  - **vacuum chamber compatible**
  - may even exploit 4.5 MHz (e.g. 10 um/us)
  - divergence ca 120 urad (no hi-res xtallography)

# Dispersive I0 / I1 Spectrometer






- Scatter off foil before sample
- disperse radiation behind sample

→ XANES without primary mono!

single shot spectrum, normalizable

# Laser Parameters



- Burst Mode Laser
  - 800 nm, 15 fs
  - 0.2 mJ (or more), depending on rep-rate
  - OPA for wavelength tuning (UV-NIR), ca 1-10 uJ

Work horse for pp studies

- 4.5 MHz laser system (Tangerine)
  - 1030 nm, 285 fs, 20 W (4 uJ)
  - 515 nm, <220 fs, 10 W (2 uJ)
  - NOPA for short pulses and UV-NIR

„tickle and probe“

Veto laser (interpulse optical pp)

# Laser fluence conditions (rep-rate dependent)

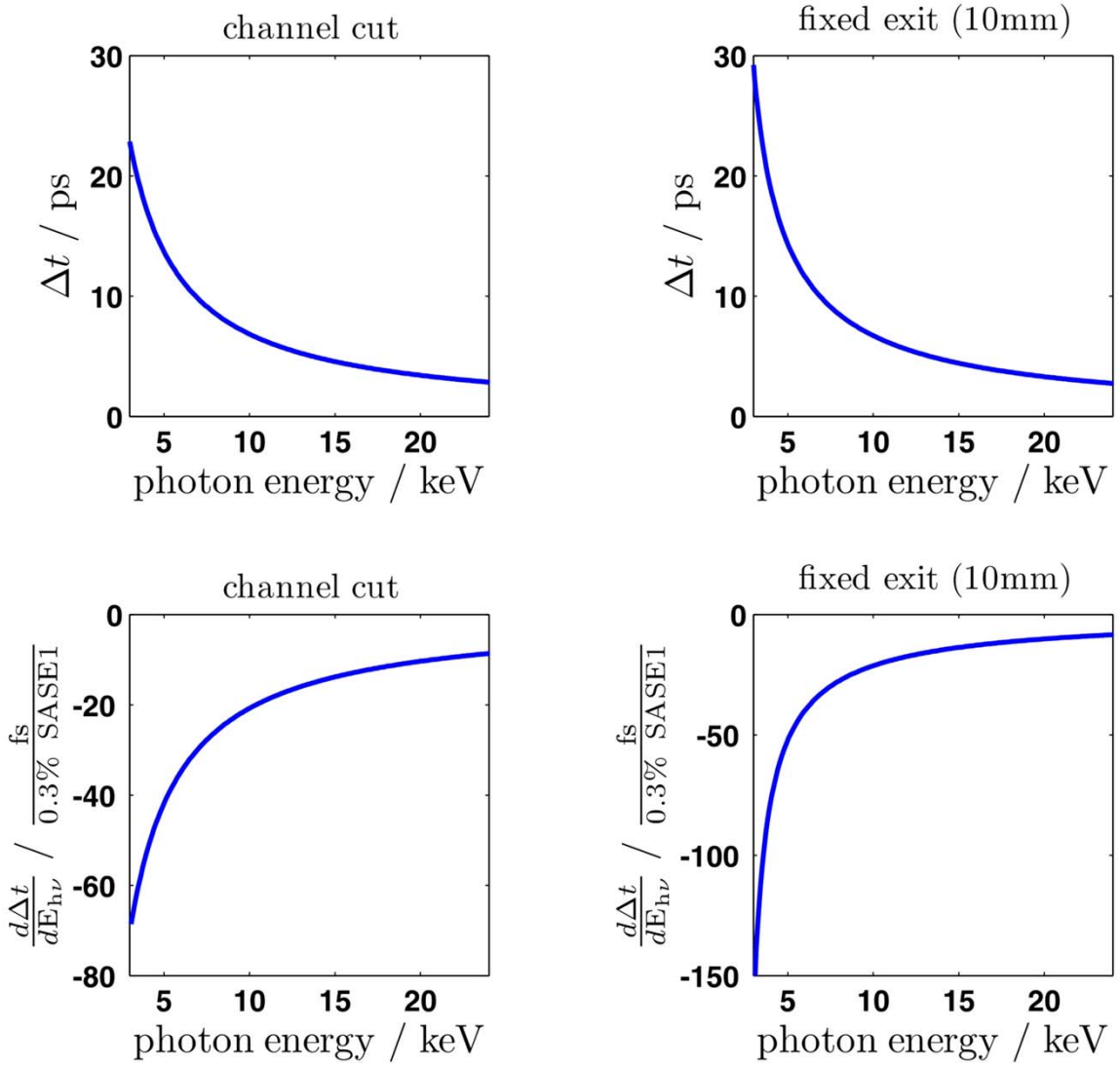


- Solids (e.g., GID)
  - 1-20 mJ/cm2
- Liquids (diffuse scattering, XAS, XES
  - 10-100 mJ/cm2 (10-15 mJ/cm2)
- Molecular Xtals,
  - <5 mJ/cm2 (30 pulses)

- Burst mode strategies
  - small spots/lines (5-20 um) → move to new sample
  - very large spots (500 um) → sample survives

# Si(111): Time arrival shifts (channel-cut)



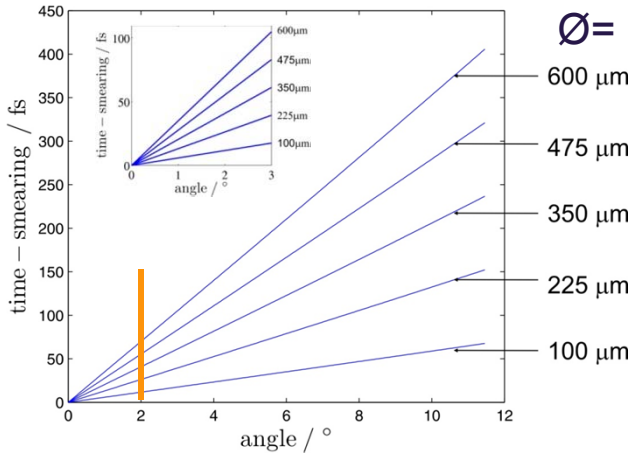



- on-axis mono (4-bounce): x 2

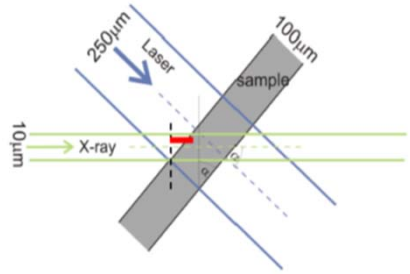
# Femtoseconds: Laser-XFEL Interfacing Issues

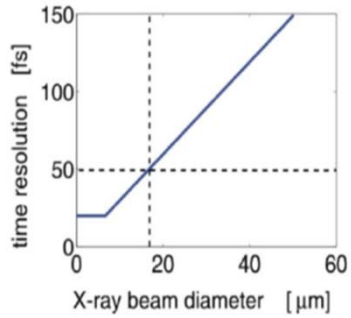


- Time smearing (avoid via wave-front tilt)




- Refractive Index (100 um ←→ 10 um) (167 fs 17fs) can be improved



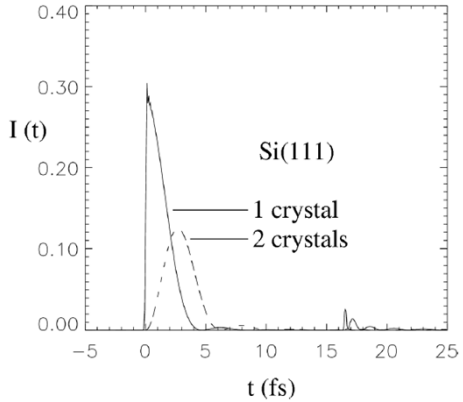



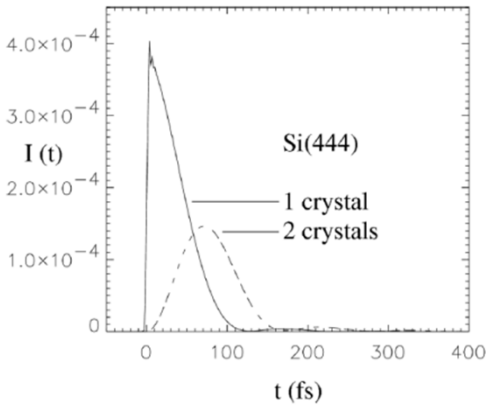

- xray mono effects:

Si(111): ca 3 fs (2e-4)

Si(444): 80 fs (5e-6)

$$\Delta E \Delta t/(2.35)^2 > \hbar/2$$



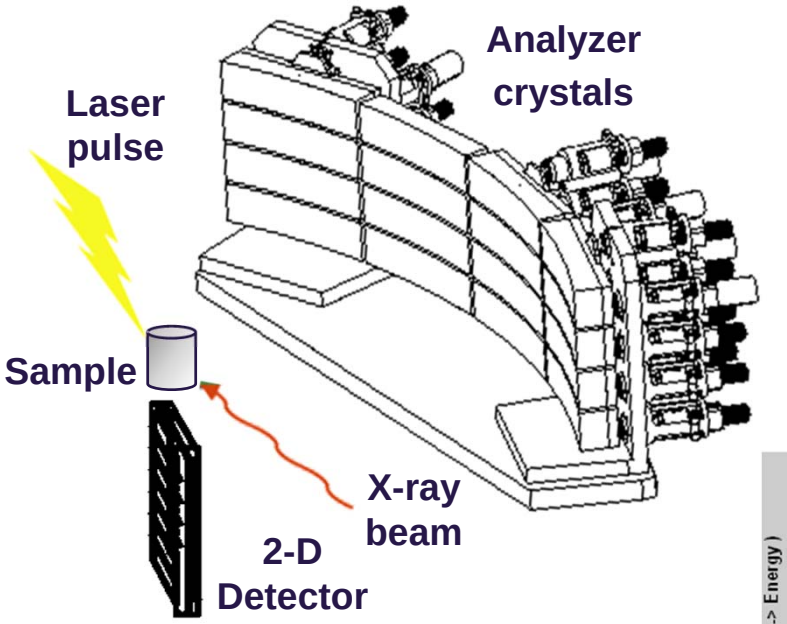



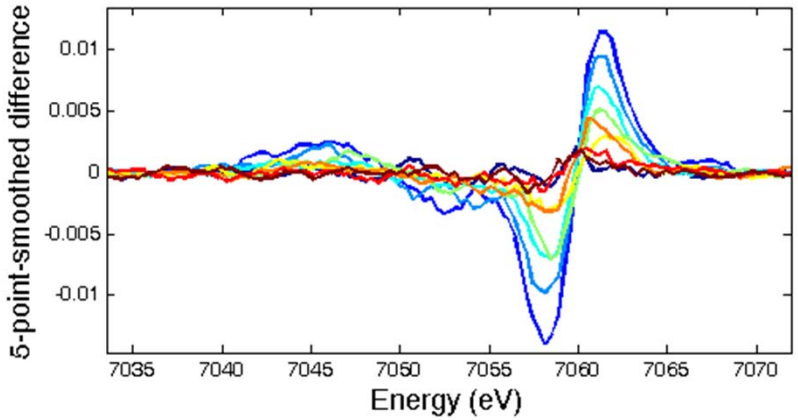


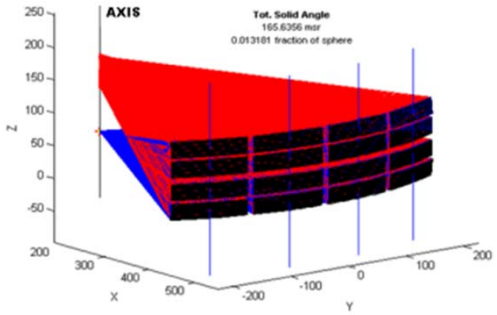

*J. Synchrotron Rad.* (2001). **8**, 1131–1135

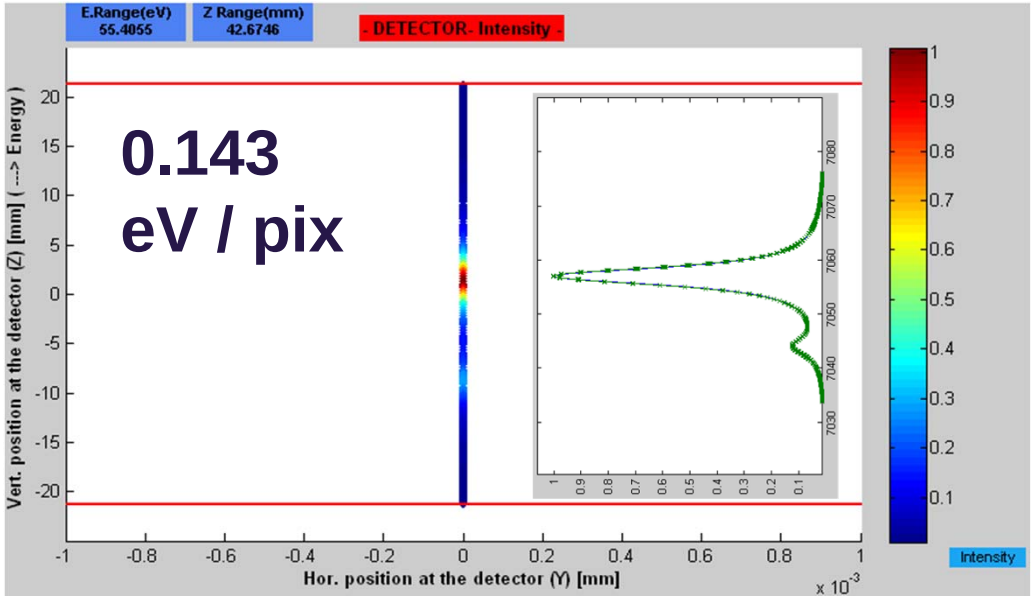
# XES spectrometer: von Hamos (R. Alonso Mori)





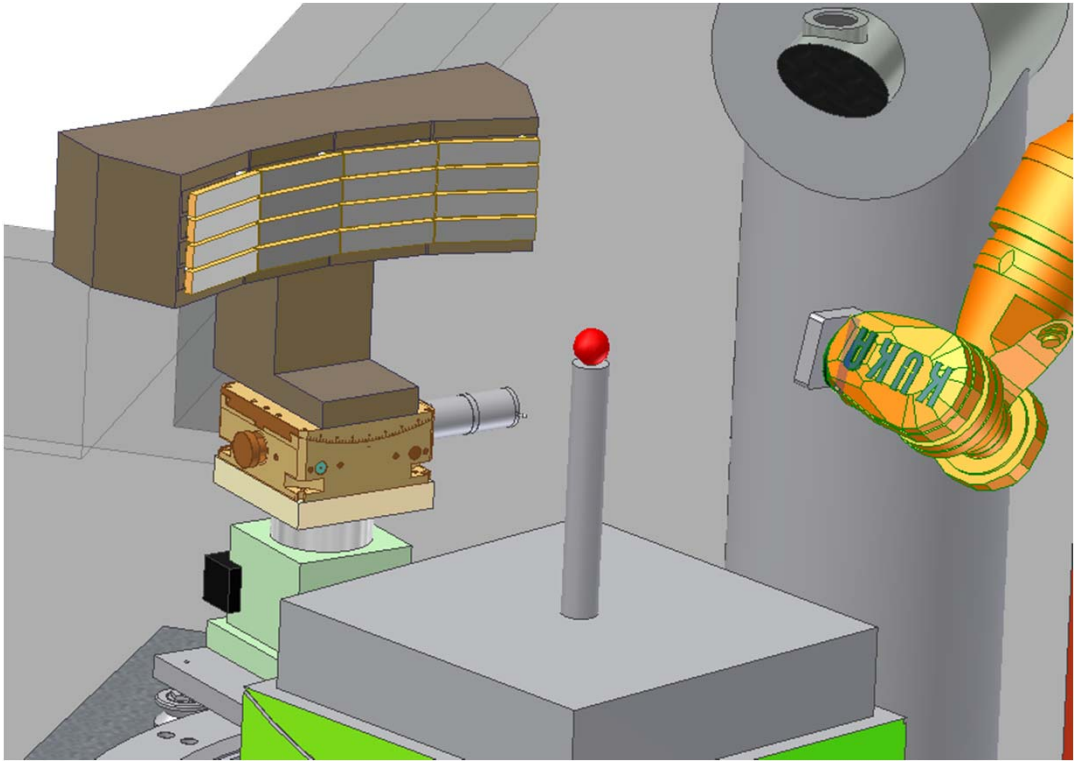



# Von Hamos spectrometer setup





- Each crystal motorized by 3 actuators. Crystal fixture box is also motorized: 2 rotations and 1 translation.

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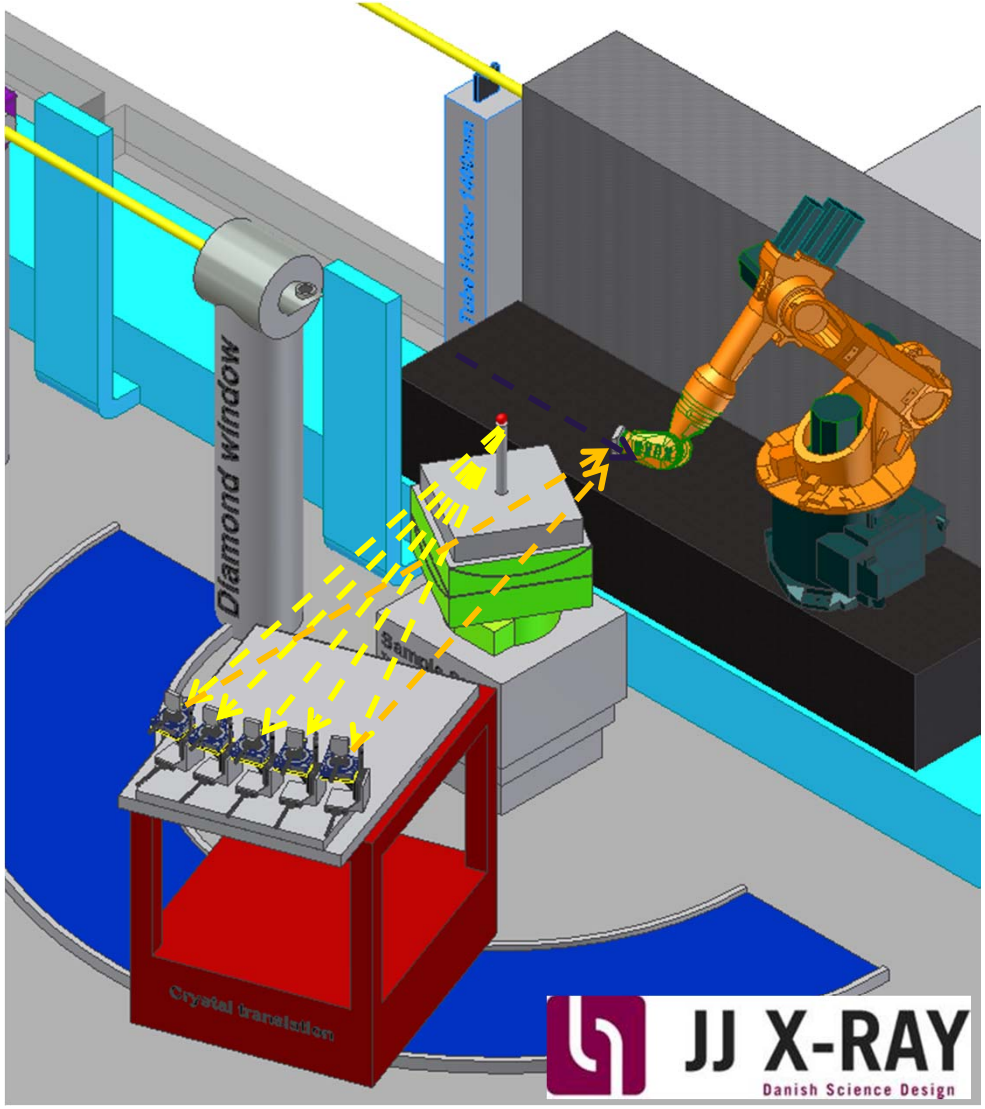
# Five Element Johann Setup



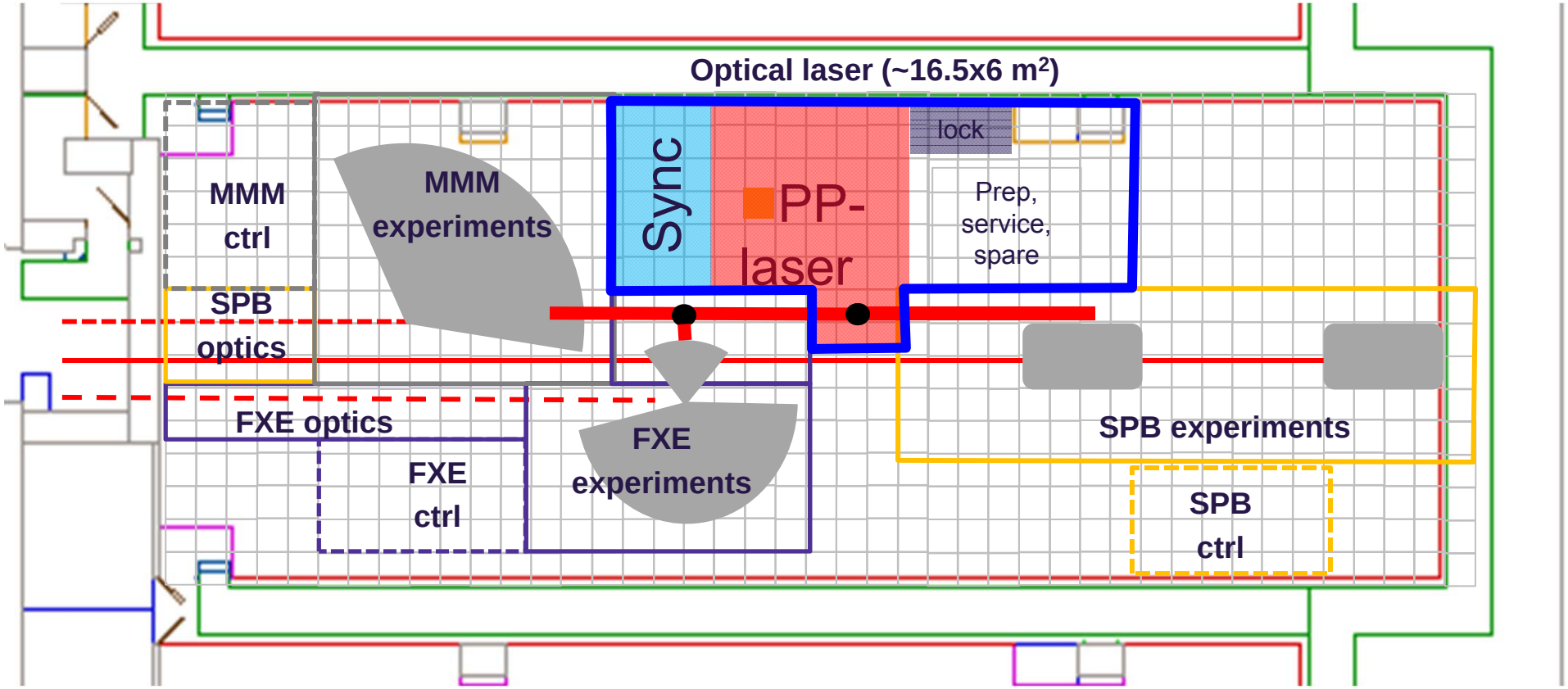

Diamond window:
- 120 pulses/burst
- 0.3 mm ok
  (5 keV)

# Baseline Detectors



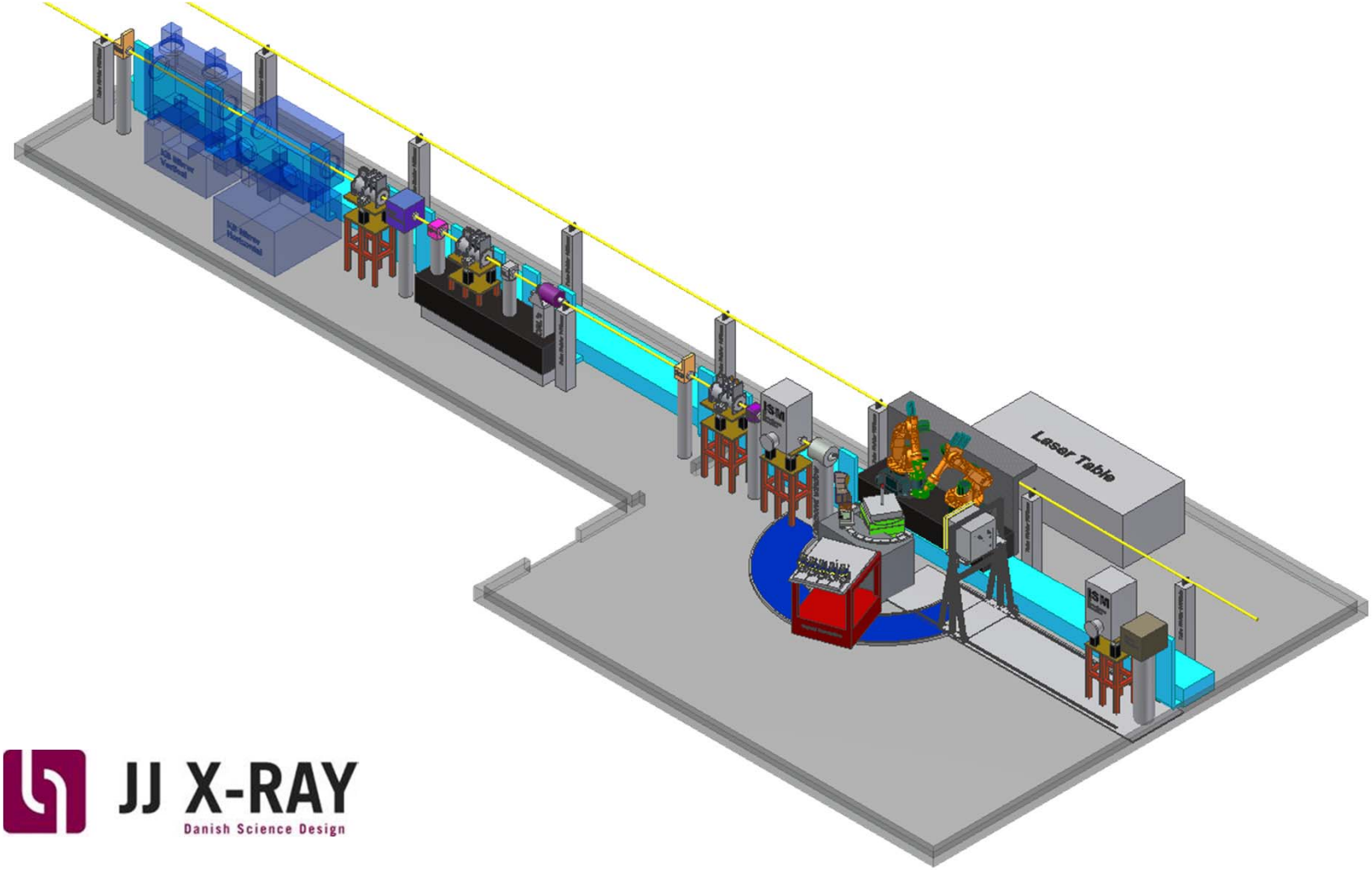
| | Diffuse Scattering | XES Analyzer | Versatile | Time Domain Monitor |
|---|---|---|---|---|
| Detector Type | 2D Pixel | 1D Strip/2D | 2D | 2D |
| Energy Range | 3-20 keV | 3-20 keV | 3-20 keV | UV-vis |
| Energy Resolution | No | No (or < 200 eV@7 keV) | No | No |
| Frame Rate | 4.5 MHz | 4.5 MHz | 4.5 MHz | 4.5 MHz |
| Pixel/Strip Size | < 500 x 500 $\mu m^2$ | 100 x 100 $\mu m^2$ | 100 x 100 $\mu m^2$ | < 100 x 100 $\mu m^2$ |
| Sensitive Area | 22 x 22 $cm^2$ | 2 x 6 $cm^2$ | up to 10 x 10 $cm^2$ (2 x 6) | ca. 1 x 1 $cm^2$ |
| # Pixels | 1M | 200 x 600 | ≥200 x 600 | 100 x 100 |
| Sensor Material | Si | Si | Si | Si |
| Sensor Thickness | 500 µm | 500 µm | 500 µm | - |

# Basic layout (work in progress)



# FXE Layout concept



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# Summary



**FXE Instrument**

- Dynamics of Solids and Liquids (nuclear-lattice, electronic, spin,..)
- Focus on ultrafast time resolution (< 25 fs c.c.)
- Suitable laser conditions (pulse energy, wavelength, pulse width)
- flexible spot size (refresh, damage,…)
- versatile secondary spectrometer instrumentation
- ambient-He environment, + vacuum add-on
- 1M (< 0.5 mm), 100k (0.1 mm), possibly strip (0.05 mm), 0D, …

# Time Line



- April 2011: CDR out
- 2012: TDR
- 2013+: commence ordering of components
- 2014+: Installation in exp. Hall
- Late 2014/2015: ready for beam

# Awcknowledgments




- FXE Team
- Andreas Galler
- Wojciech Gawelda
- European XFEL Team Members

- FXE Instrument Advisory Review Team
- Martin Meedom Nielsen (chair)
- Rafael Abela (SAC representative)
- Pieter Glatzel (ESRF)
- Alke Meents (DESY)
- Simone Techert (MPI)
- Steven Johnson (ETHZ)
- David Fritz (SLAC)
- Aymeric Robert (SLAC)