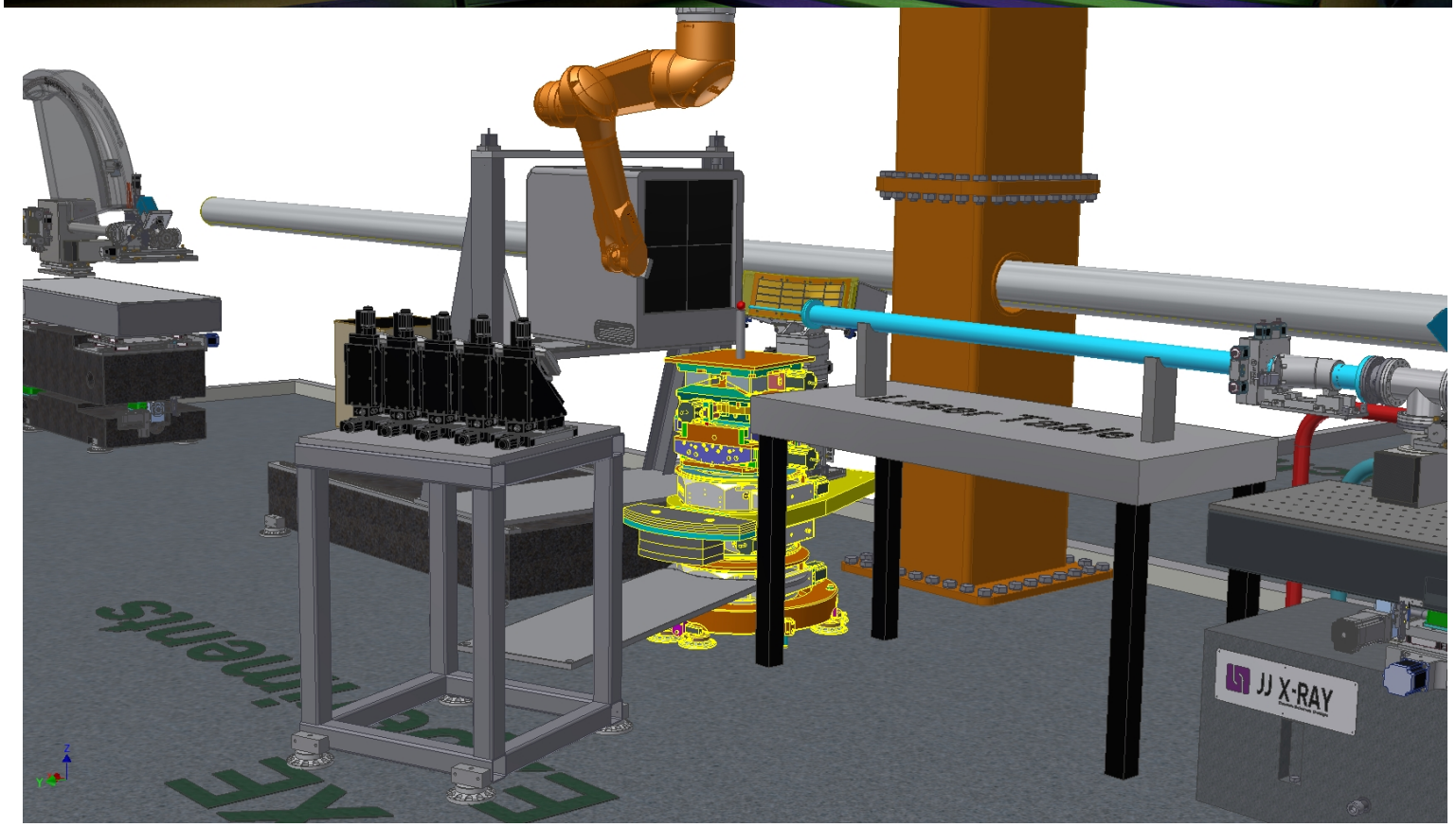
Femtosecond X-Ray Experiments at the European XFEL



Christian Bressler, *Femtosecond X-ray Experiments (FXE) Instrument*
European XFEL

XFEL User Meeting, Hamburg, Jan 29, 2014

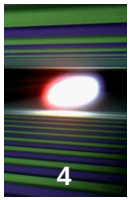
European XFEL

Experiment Hall, June 2013

European XFEL

Experiment Hall Integration

Solvation dynamics using the FXE instrument



Parameter	Monochromatic	Pink beam
Energy range	5-20(25) keV	5-20(25) keV
Beam position	Sample (fixed)	Sample (fixed)
Energy bandwidth	1.4×10^{-4} Si(111) 3×10^{-5} Si(311)	0.3-1 %
Bunch charge	≤ 250 pC	≤ 250 pC
X-ray pulse duration	< 25 fs	< 25 fs
Optical pulse duration	15 fs	15 fs
Sample delivery: Liquid flat-sheet jets	Up to 15 m/s (sapphire nozzles) Up to 100 m/s (colliding µjets)	Up to 15 m/s (sapphire nozzles) Up to 100 m/s (colliding µjets)
X-ray beam spot	1-10 µm in focus Up to 0.1 mm out of focus	1-10 µm in focus Up to 0.1 mm out of focus
Energy resolution	ca. 1 eV (cylindrical) 0.3 - <1eV (spherical)	ca. 1 eV (cylindrical) 0.3 - <1eV(spherical)
Q range (XDS)	0.7 – 13 $Å^{-1}$	0.7 – 13 $Å^{-1}$

FXE Overview Specifications

- FXE will offer world-wide unique and versatile end station for dynamical studies of guest-host interactions
- It will exploit the high repetition rate, x-ray photon flux and ultrashort pulse duration of the European XFEL
- FXE will offer a flexible sample environment optimized for liquid-phase photochemistry using a suite of complementary x-ray spectroscopic and scattering techniques in pump-probe arrangement.
- Simultaneous measurements of several observables deliver a more complete picture of the dynamics both of the solute (guest) and solvent molecules (host).

Coupled electronic, spin and nuclear changes of solute and solvent molecules can be resolved in "real-time"

European XFEL FXE instrument

2007 : Decided to build science instrument dedicated to

Femtosecond Diffraction Experiments –

Time-resolved structural dynamics investigations of solids, liquids, gases using various techniques: diffraction, scattering

2009 : The scientific scope was refined in a science scope Workshop (Budapest, Dec. 2009) for the

Femtosecond X-ray Experiments instrument –

emphasizing the combination of X-ray scattering and X-ray spectroscopy to study liquid & solvation dynamics.

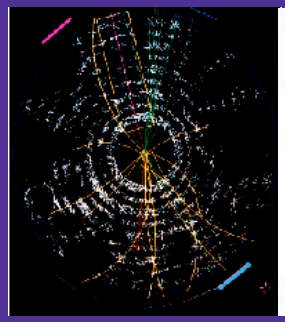
Targets:

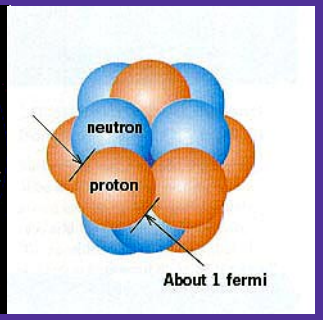
- electronic rearrangements (charge transfer/transport)
- spin state changes
- nuclear rearrangements (including the solvation cage)

…and all this simultaneously (→single shot)

What are the fundamental timescales?

Femtochemistry, Photosynthesis and Catalysis
Solid State Dynamics





Strings, Cosmology

Particle Collisions

Vision

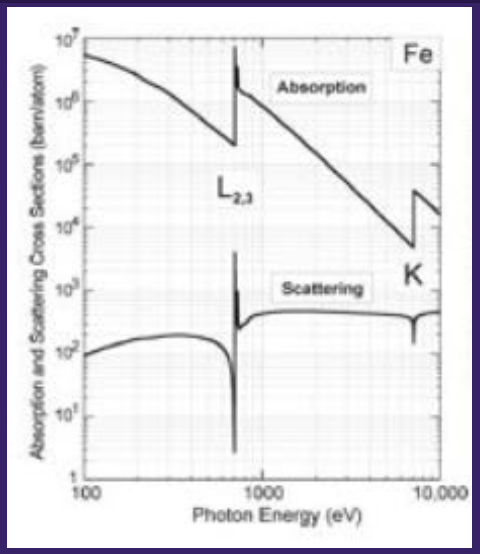
Molecular Vibrations

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

FXE: Make use of all incident x-ray photons

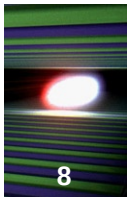


Absorption

Scattering

Combine Femtosecond
-XRD
-XAFS (XANES)
-XES, RIXS, …

Simultaneous Techniques at the FXE instrument

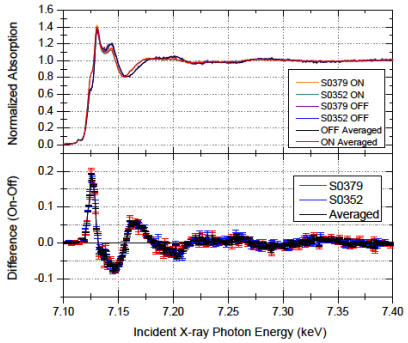


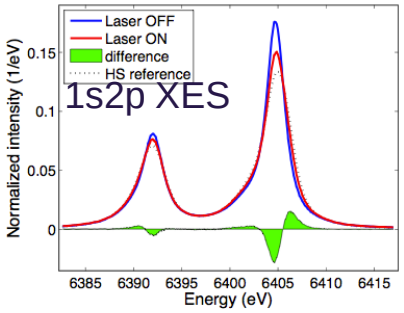
- X-Ray Absorption Spectroscopy
  XANES: oxidation state changes, valence orbitals, DOS…
  EXAFS: coordination shells (geometric)
- X-Ray Emission Spectroscopy
  spin momentum of the absorber, charge state, molecular orbitals,...
- Resonant Inelastic X-Ray Scattering (RIXS)
  Low energy excitations (d-d, charge transfer, even phonons), tunable to different final states, i.e. 3*d* orbitals (dipole-forbidden for 1*s*→n*d* excitation)
- X-Ray Raman Spectroscopy
  Access K-edges of light elements (N, O, C...) constituting solvent molecules
- X-Ray Diffuse Scattering
  Short- and medium-range geometric environment, solute + solvent (cage) contributions to the structural factor

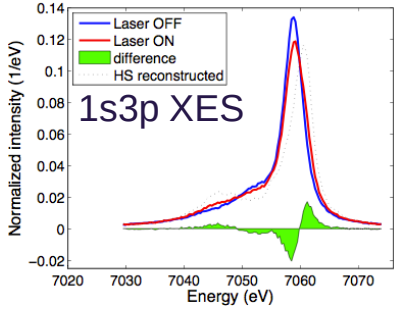
European XFEL

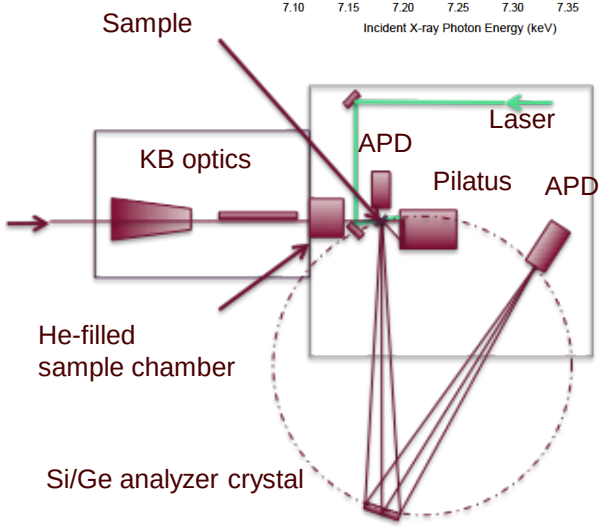
Exploiting complementary techniques

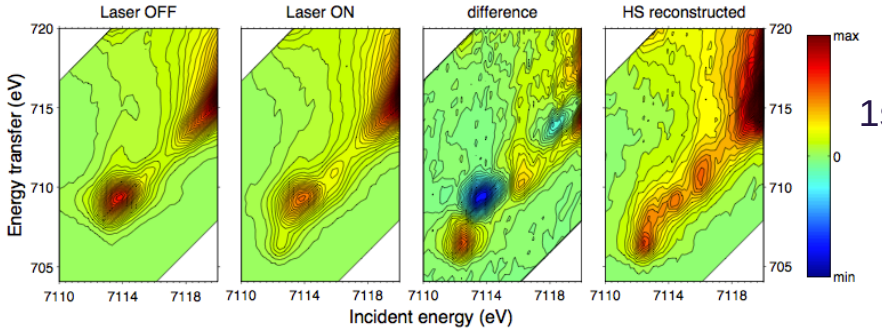
XANES
EXAFS







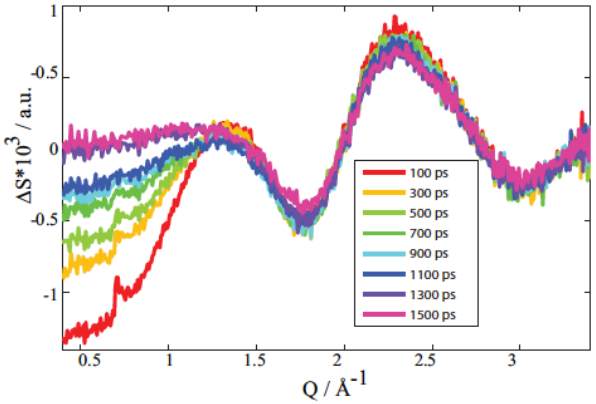




1s2p RXES

UDECS collaboration at work!

Sector 7ID @ APS, Argonne (3.26 MHz)

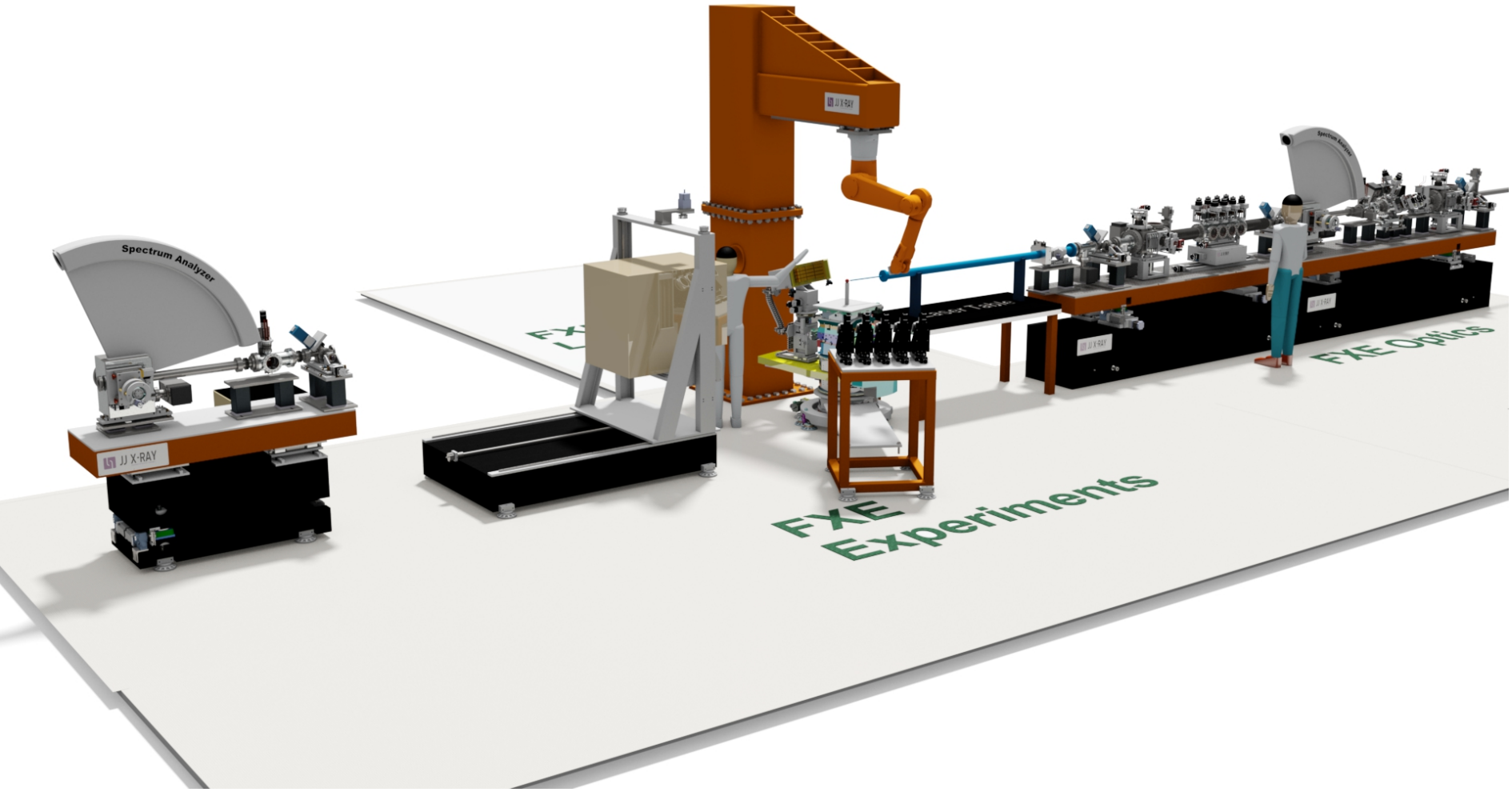


X-ray Diffuse Scattering (XDS)

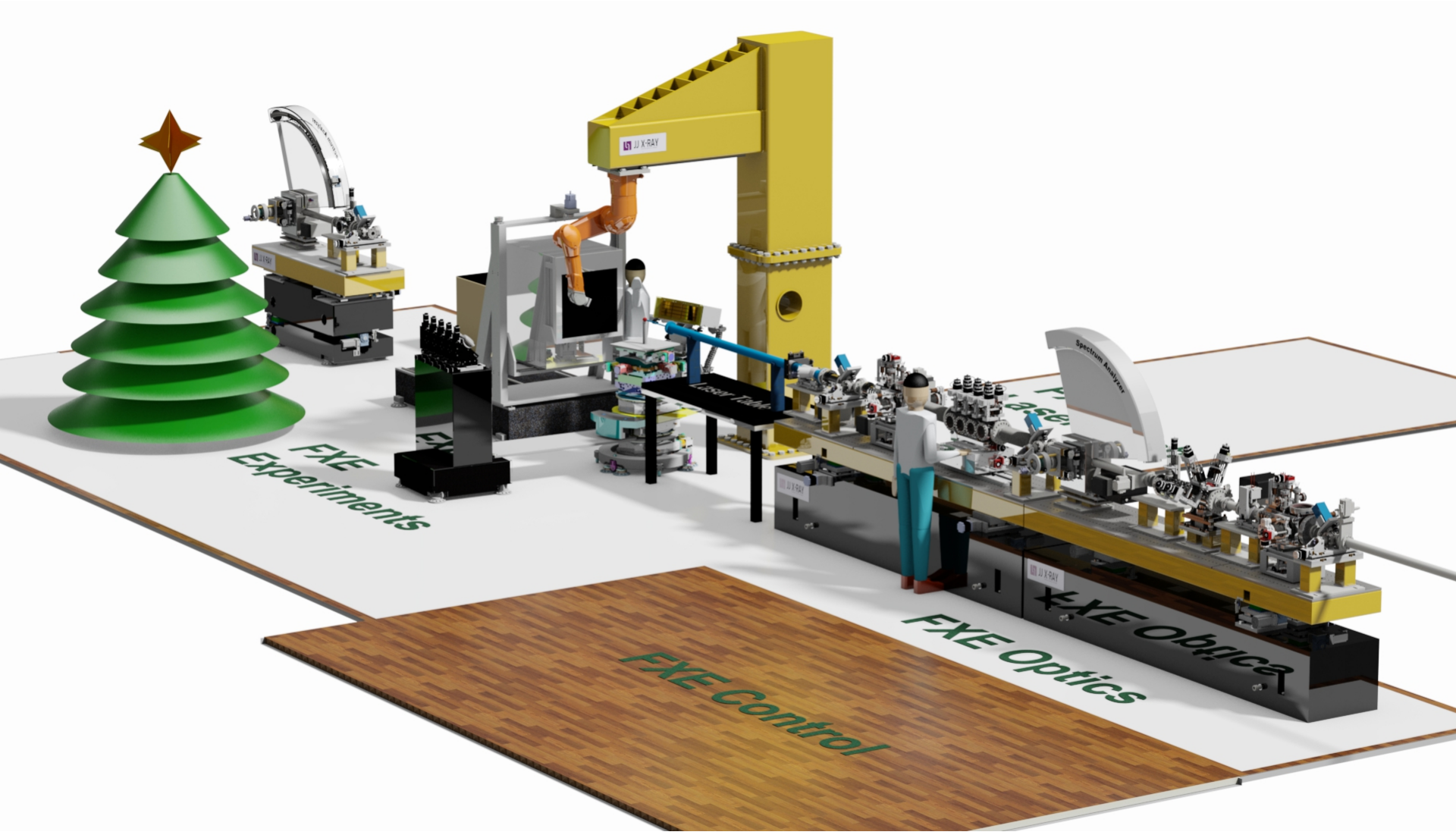
K. Haldrup *et al*, J. Phys. Chem. A **116**, 9878 (2012)

European XFEL

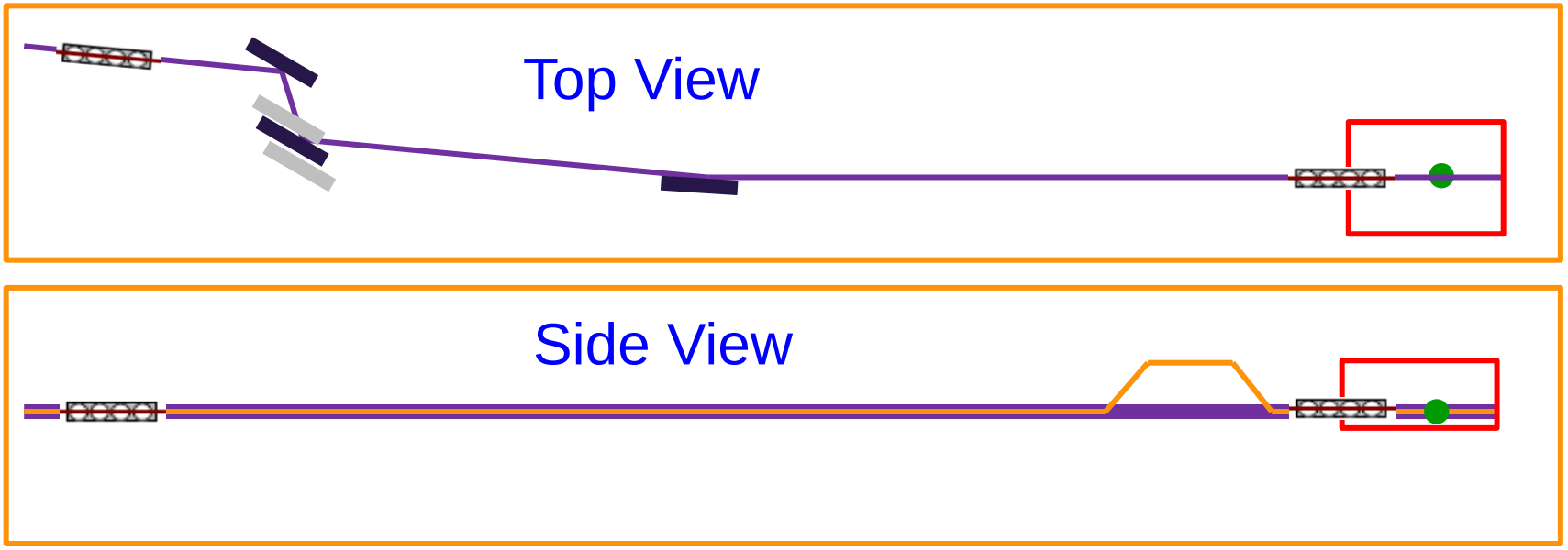
The FXE Instrument (5 – 20 keV)



FXE Instrument (Dec 2013)



On Axis Strategy (pink AND monochromatic)

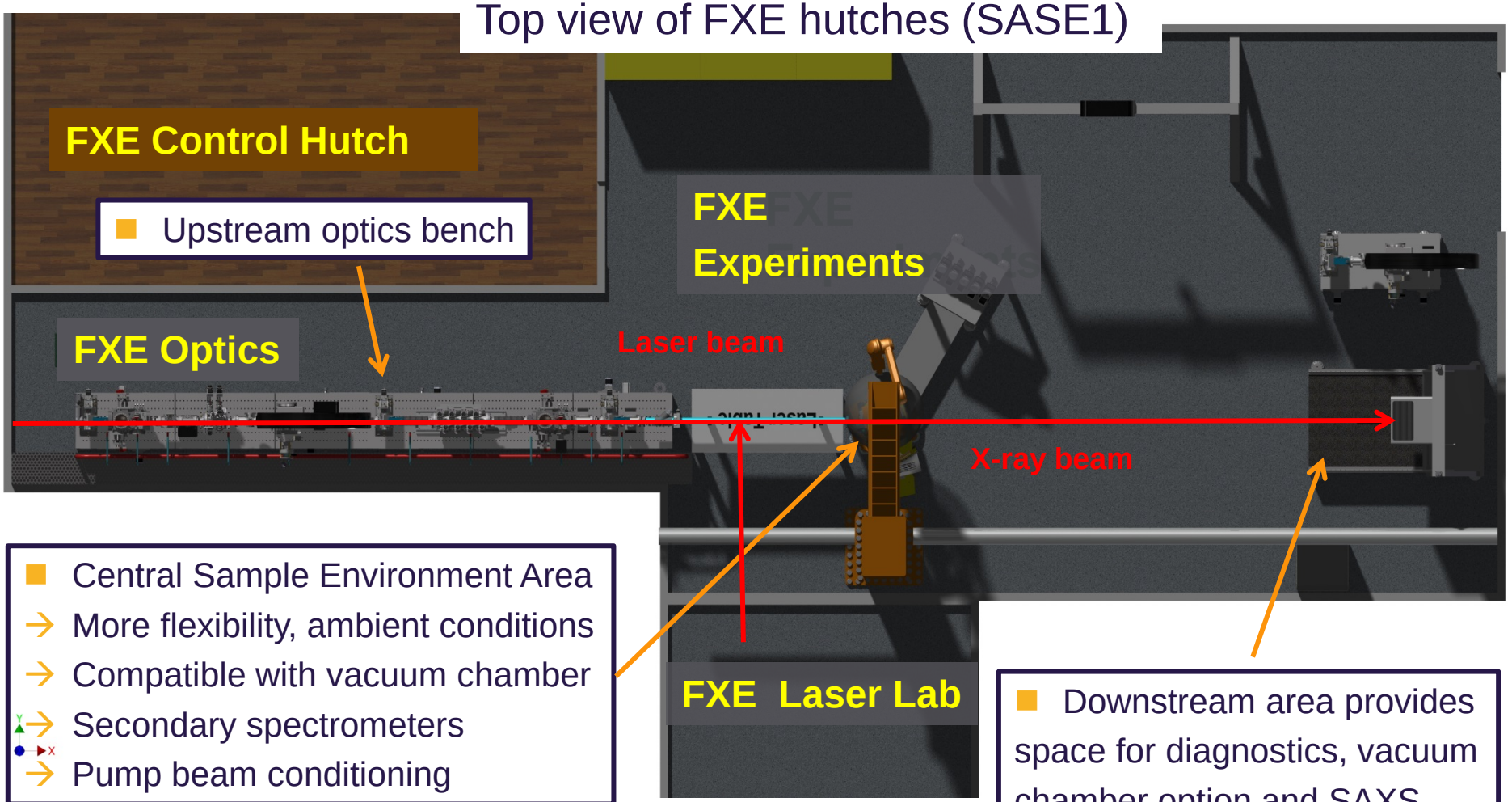


- Find single OM position/angle (5 – 20 keV)
  (maintain flexibility towards changes)
- Use Si(111) 4-bounce for startup

→ Emphasis for „on-axis“ configuration

FXE Instrument: Overall

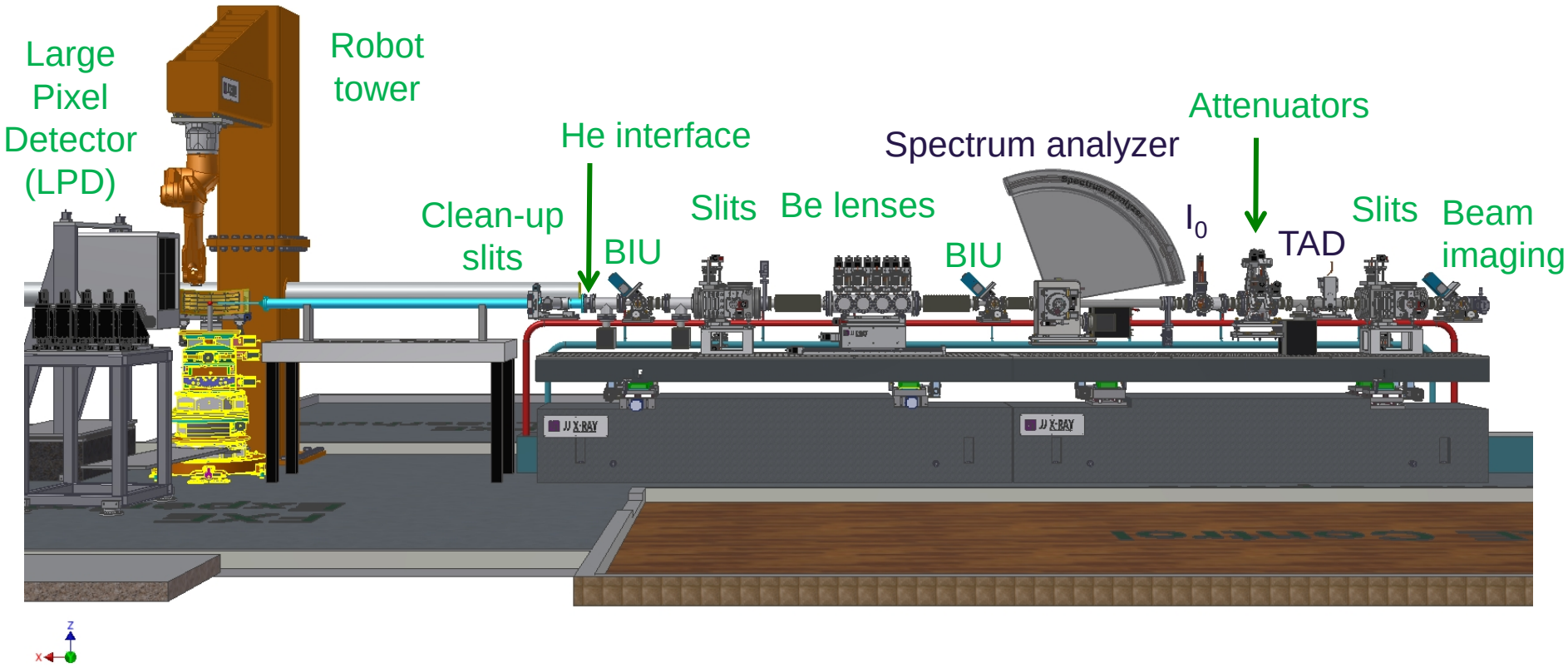
Top view of FXE hutches (SASE1)



- Central Sample Environment Area
  - → More flexibility, ambient conditions
  - → Compatible with vacuum chamber
  - → Secondary spectrometers
  - → Pump beam conditioning

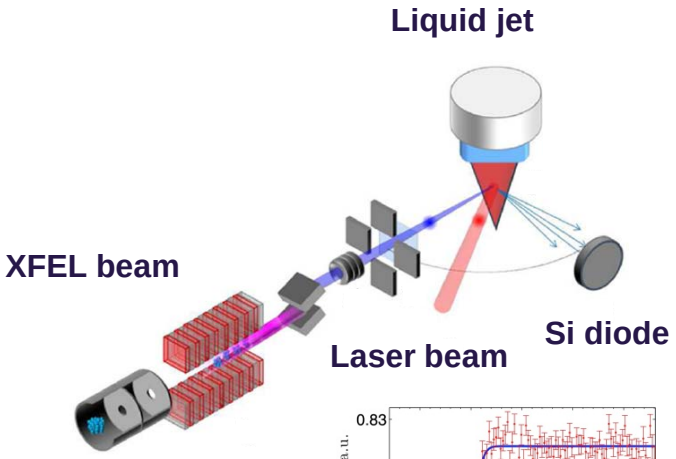
- Downstream area provides space for diagnostics, vacuum chamber option and SAXS.

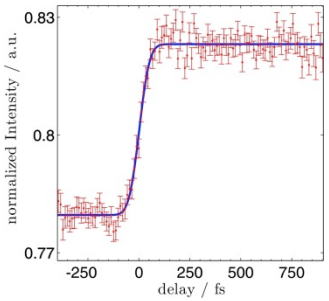
FXE Instrument: Optics Bench + Sample Environment

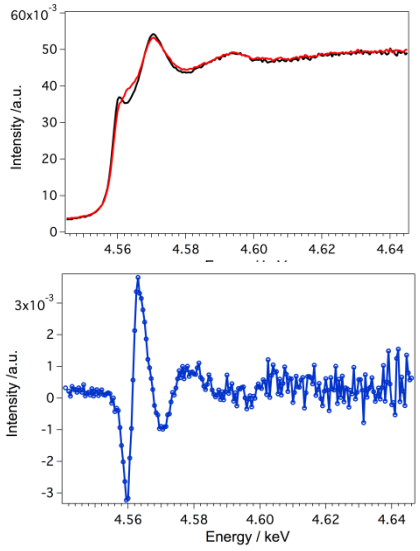


X-ray Absorption studies at FXE

Point-by-point XAS (scanning mode)



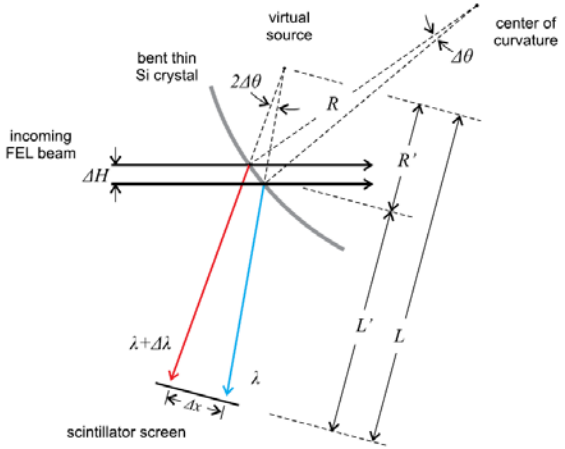


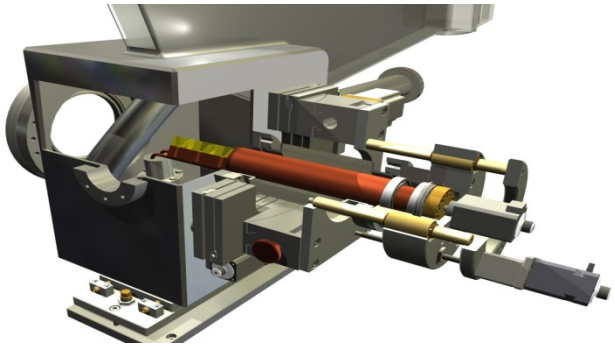


A. Galler *et al.*, **I^-/H_2O @ XPP-LCLS**
(January 2013)

- Scanning mode → 4-bounce monochromator
- Beam focusing chromaticity → transfocator
- Requires reliable intensity normalization!
- (Single energy @ time delay) /shot
- Gated point detector (APD)

Dispersive XAS (single-shot mode)





- Single-shot measurements→ require 2 Spectrum Analyzers (SA)
- Pink beam would provide up to 1% bandwidth
- (Entire XANES spectrum @ time delay) /shot
- Self-normalization!
- Requires a fast readout gated 1D detector (Gotthard)

X-ray Emission Spectroscopy at FXE

Non-resonant XES with moderate energy resolution (0.3 - 2 eV) – Johann geometry

High Energy Resolution Fluorescence Detected (HERFD) - XAS

5 spherical analyzers focus the fluorescence on the same detector (different Si and Ge cr

The aim is cover main 1st row TMs and some 2nd and 3rd row as well

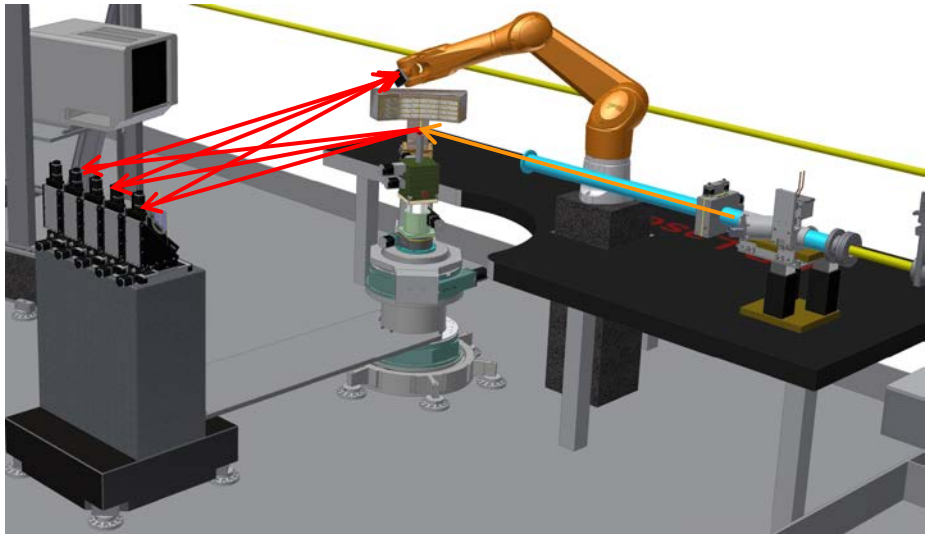
Exact tracking of individual Rowland circles required

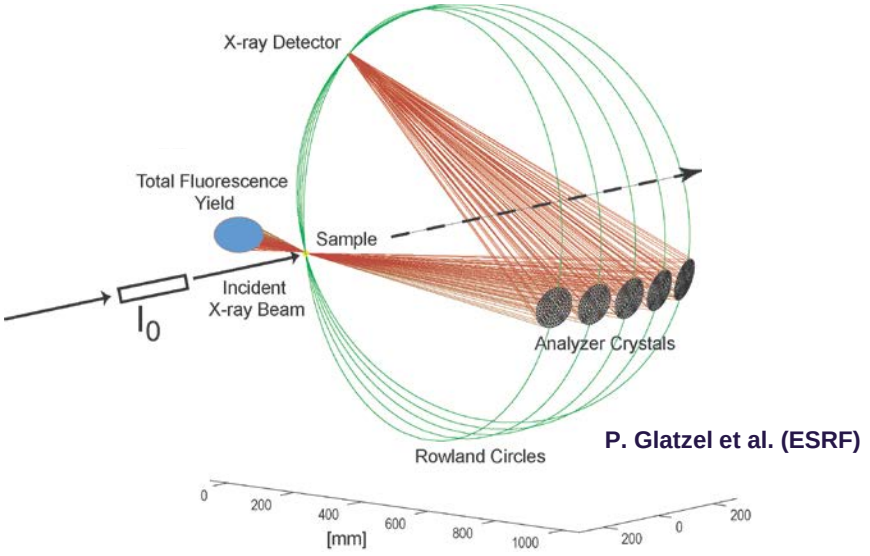
Variable Rowland radii → extension to high energy resolution XES → RXES

Variable scattering angle → opportunity to record RIXS

Both pink and monochromatic beam compatible

Large solid angle coverage/energy interval



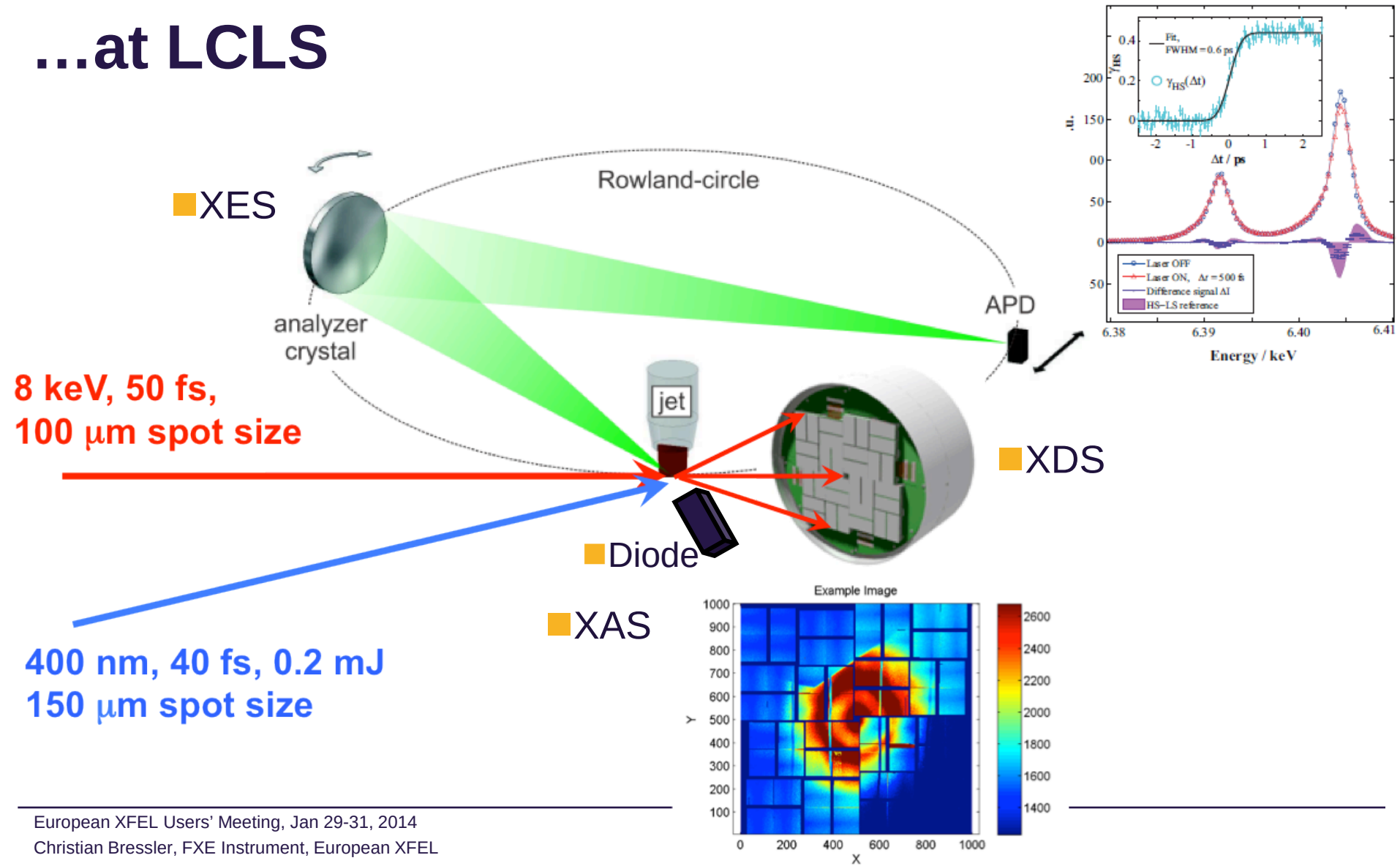


P. Glatzel et al. (ESRF)

European XFEL

Femtosecond XAS/XES/XDS

…at LCLS



X-ray Raman Scattering for solvation studies at FXE

X-ray Raman Scattering (XRS) → study low-Z elements (solvent molecules) with hard x-rays.

Measures inelastic energy loss in the sample → resonant with 1s core-hole excitation of light elements

Requires scanning the incident monochromatic beam energy

Von Hamos (dispersive) geometry allows to measure the entire spectrum in a single shot

Self-normalized → crucial!

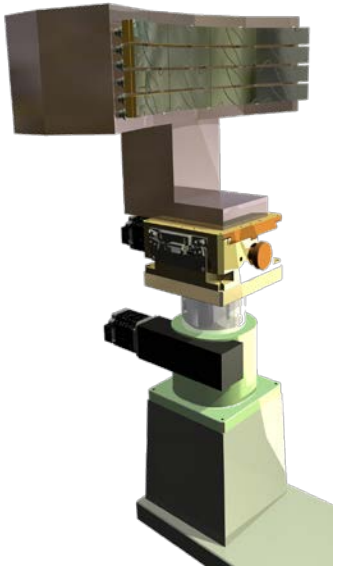
Energy resolution → 1-1.2 eV (segmented analyzers ca. 0.3 eV)

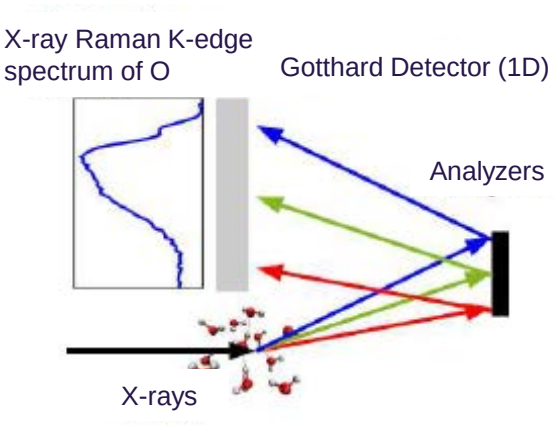
Single-shot NXES and RXES

Does not require scanning the Bragg angle

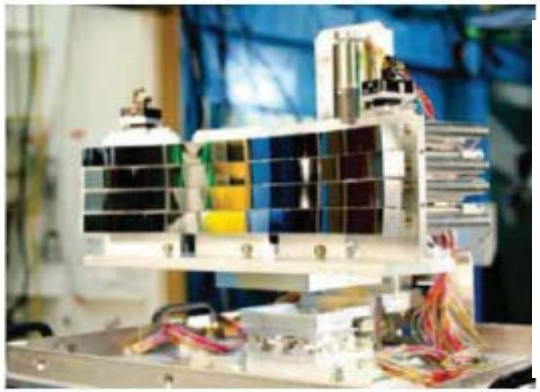
Multiple analyzer crystal can be used to record simultaneously different emission lines

Extension to RXES → scanning the incident x-ray photon energy

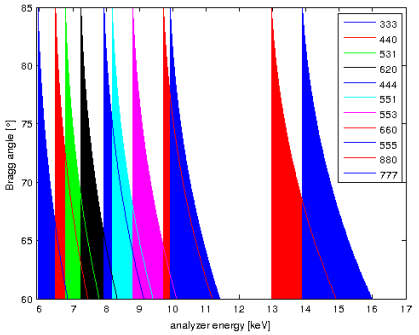




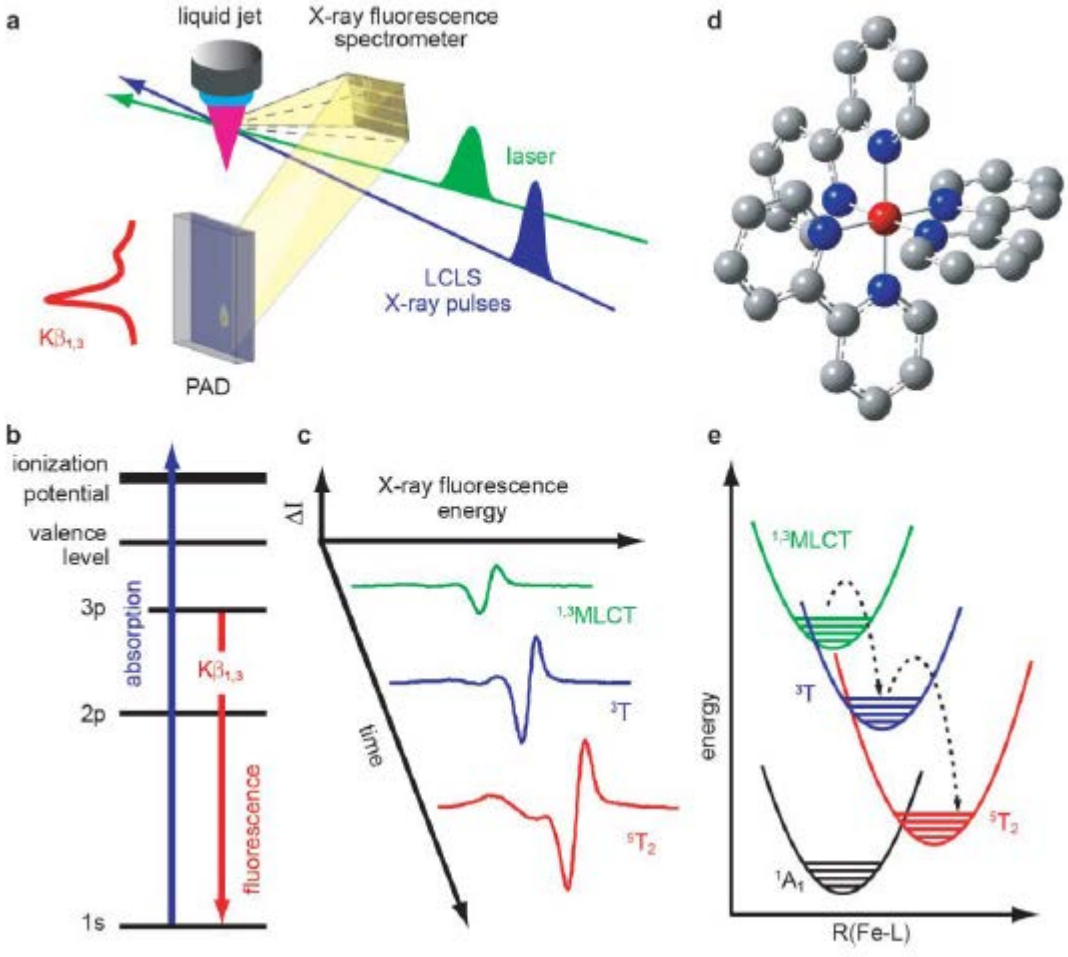
C. Sternemann *et al.(TU Dortmund)*

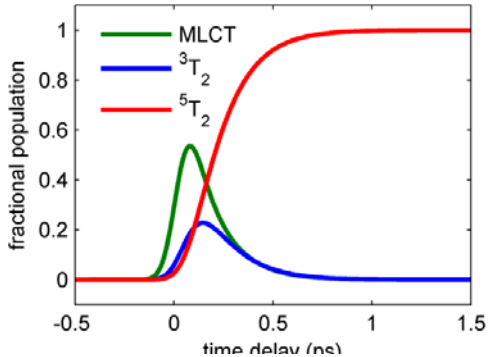


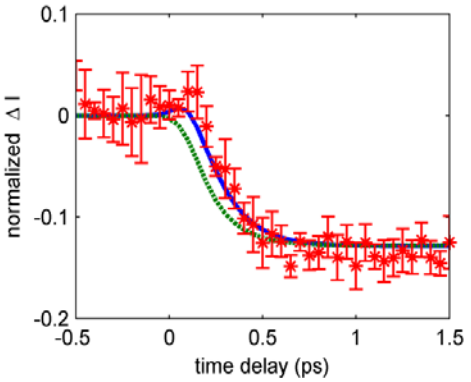
R. Alonso Mori, U. Bergmann *et al. (SLAC)*

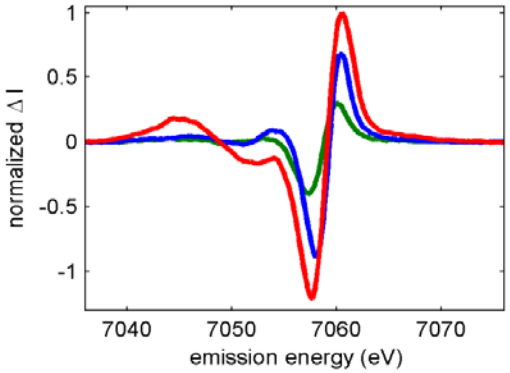


Femtosecond Kβ XES during Spin Transition: First Observation of Intermediate States





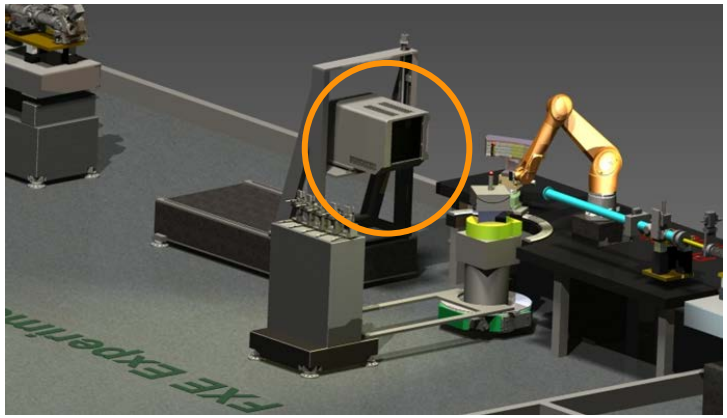


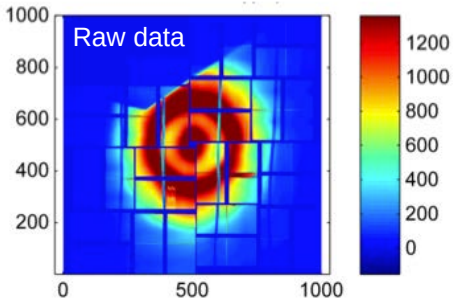


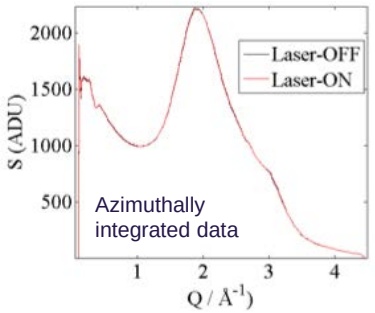
W. Zhang and K. Gaffney *et al.*, accepted in Nature (2014)

X-ray Diffuse Scattering: towards probing the solvation dynamics

Wide-angle X-ray scattering delivers global geometric structural dynamics of the solute and the surrounding solvent



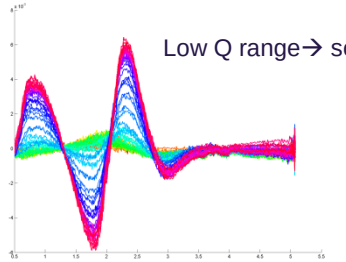




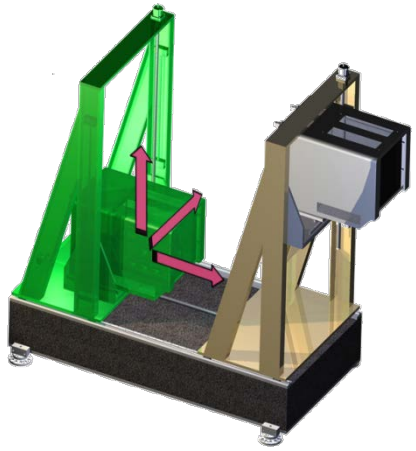
Diffuse scattering rings reflect the disordered nature of the liquid

Radially integrated scattering factor → mainly due to the solvent

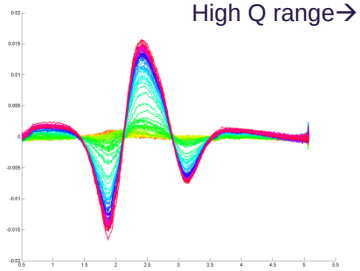
Difference scattering factor ΔS → solute and solvent changes



Low Q range→ solute + cage

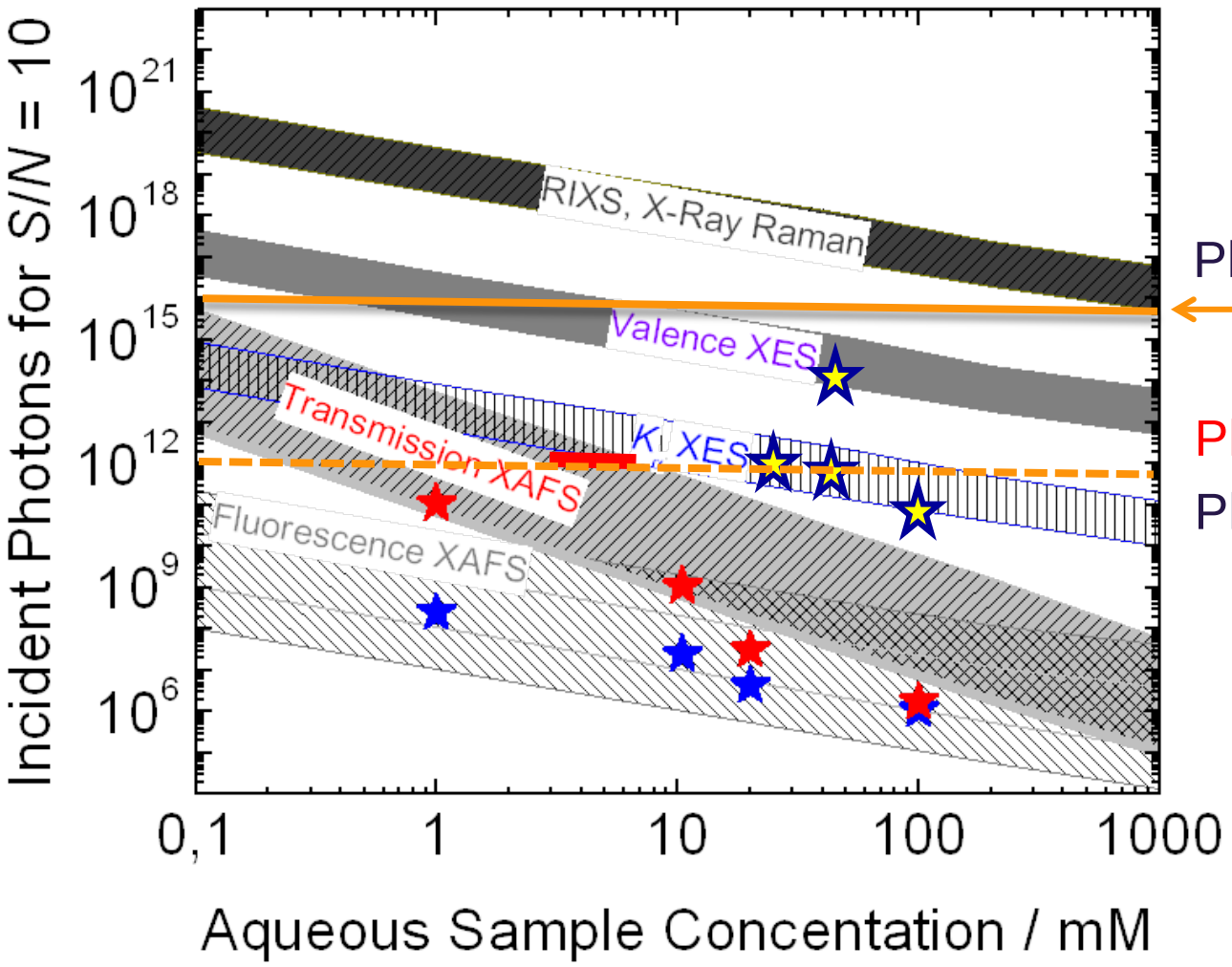


- Requires large area detector → 1 Mpix LPD detector
- LPD → 4.5 MHz output, 5120 images/sec
- No monochromatization needed → pink beam compatible
- Moderate focusing requirements → < pixel size (0.5 mm)
- High repetition rate desired!
- Variable sample-detector distance desired → WAXS/SAXS
- He environment compatible
- High dynamics range (single photon→10^5 photons/pixel)



High Q range→ solvent

Feasibility: solvated molecules (here: H2O)

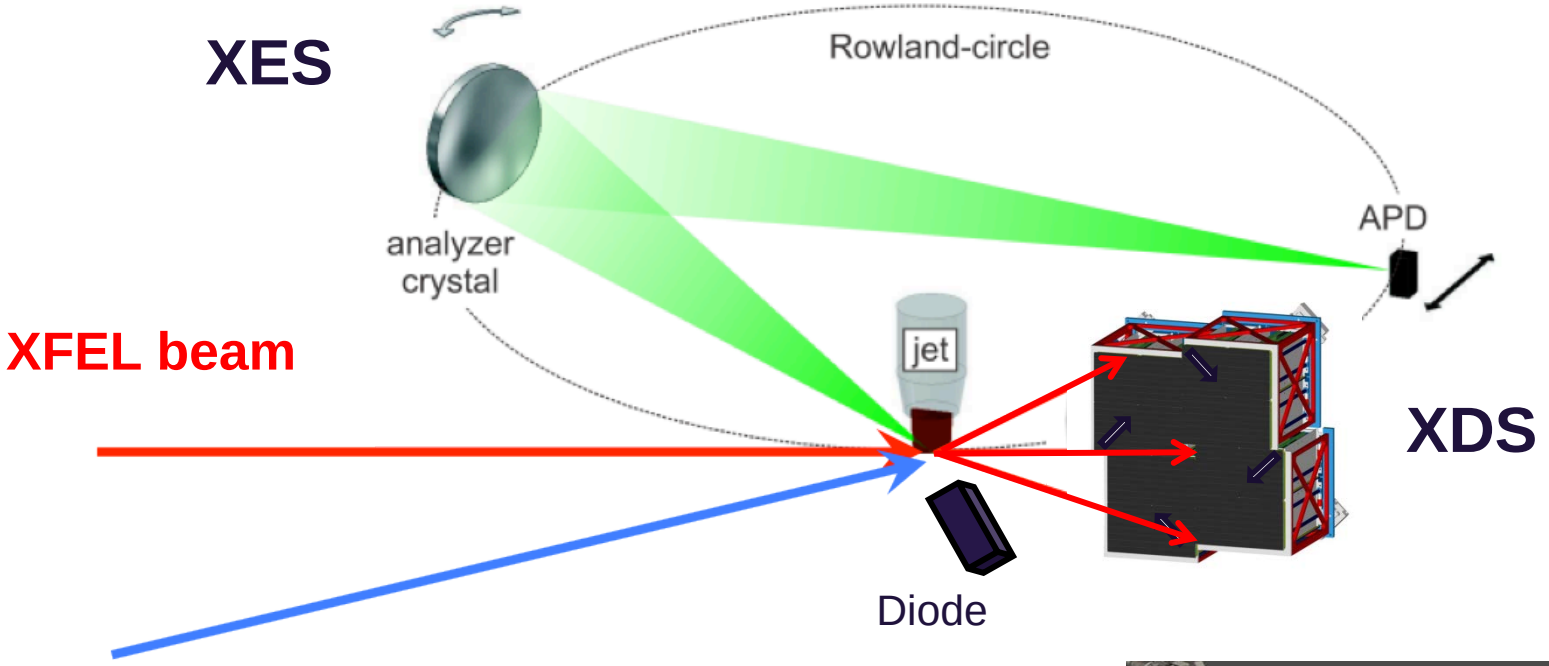


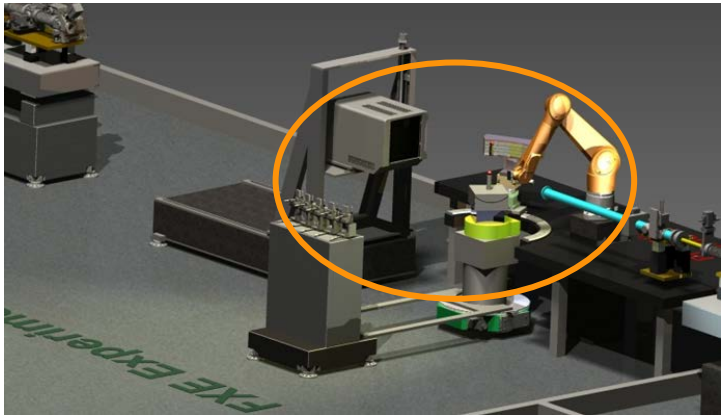
Photons/s

Photons/s (SR)

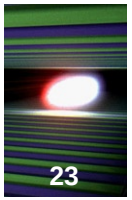
Photons (XFEL)

Summary: simultaneous ultrafast X-ray tools at FXE





Acknowledgments



- Wojciech Gawelda (FXE)
- Andreas Galler (FXE)
- Tadesse Assefa (FXE)
- Alexander Britz (FXE)
- Thomas Tschentscher (European XFEL)
- Martin M Nielsen (DTU)
- Christian Mammen et al. (JJ X-Ray)