



Femtosecond X-Ray Experiments

Christian Bressler
FXE

Hamburg, January 25, 2017

- FXE Workshop Dec 2016: Users overall very happy with implemented components

Scientific Instrument FXE

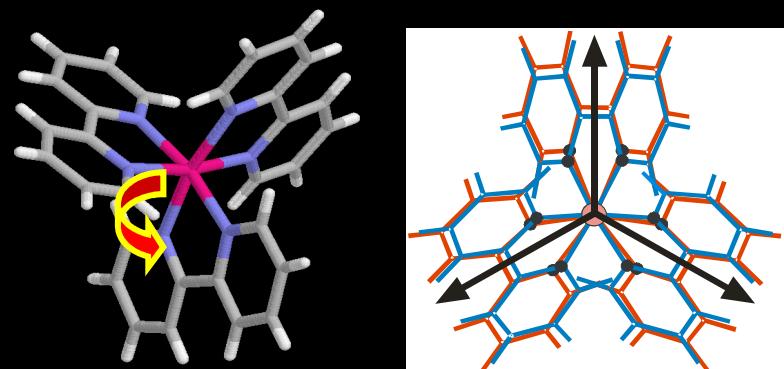
- The FXE scientific instrument will serve a broad scientific community and will embrace several fields of ultrafast X-ray science and their applications. State-of-the-art femtosecond instrumentation and techniques, both for X-rays and optical lasers, will deliver new information about geometric and electronic structures serving applications in many fields, and particular in the areas of
 - Chemical dynamics
 - Photovoltaic applications
 - Photosynthesis
 - Catalytic processes
 - Material physics
 - ...



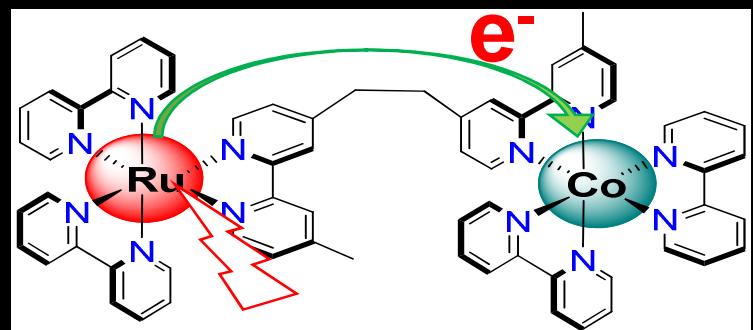
www.xfel.eu/research/instruments/fxe

FXE MISSION: Nuclear, Charge and Spin Dynamics during an ongoing reaction „Elementary Steps in Photochemistry“

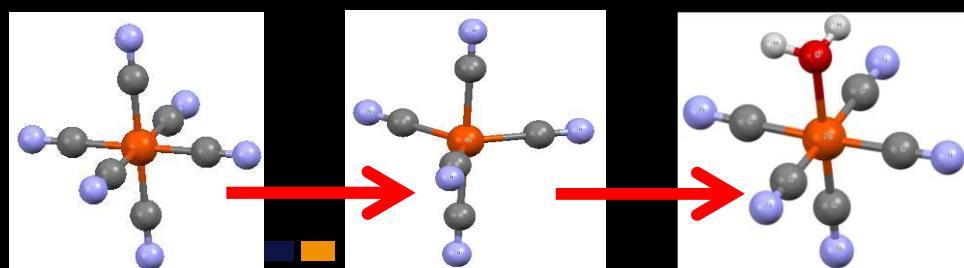
Intramolecular Charge Transfer



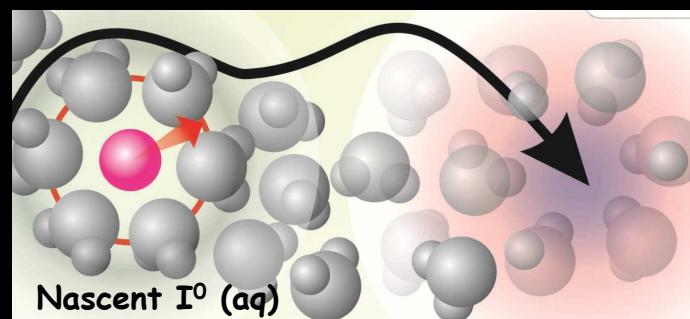
Elementary Steps in Charge Transport



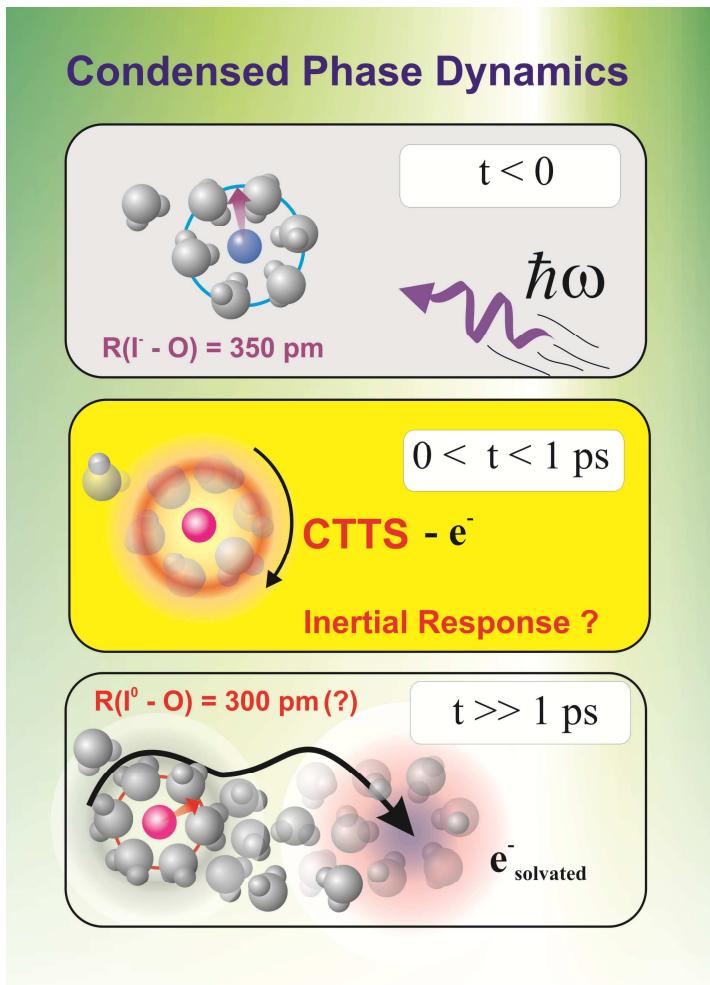
Ligand Detachment/Association



Solvation Dynamics



Imaging Chemical Action



■ X-Ray Spectroscopies

- Intrinsic electronic (XES, XANES) and nuclear dynamics (EXAFS), symmetry changes (XANES, XES)

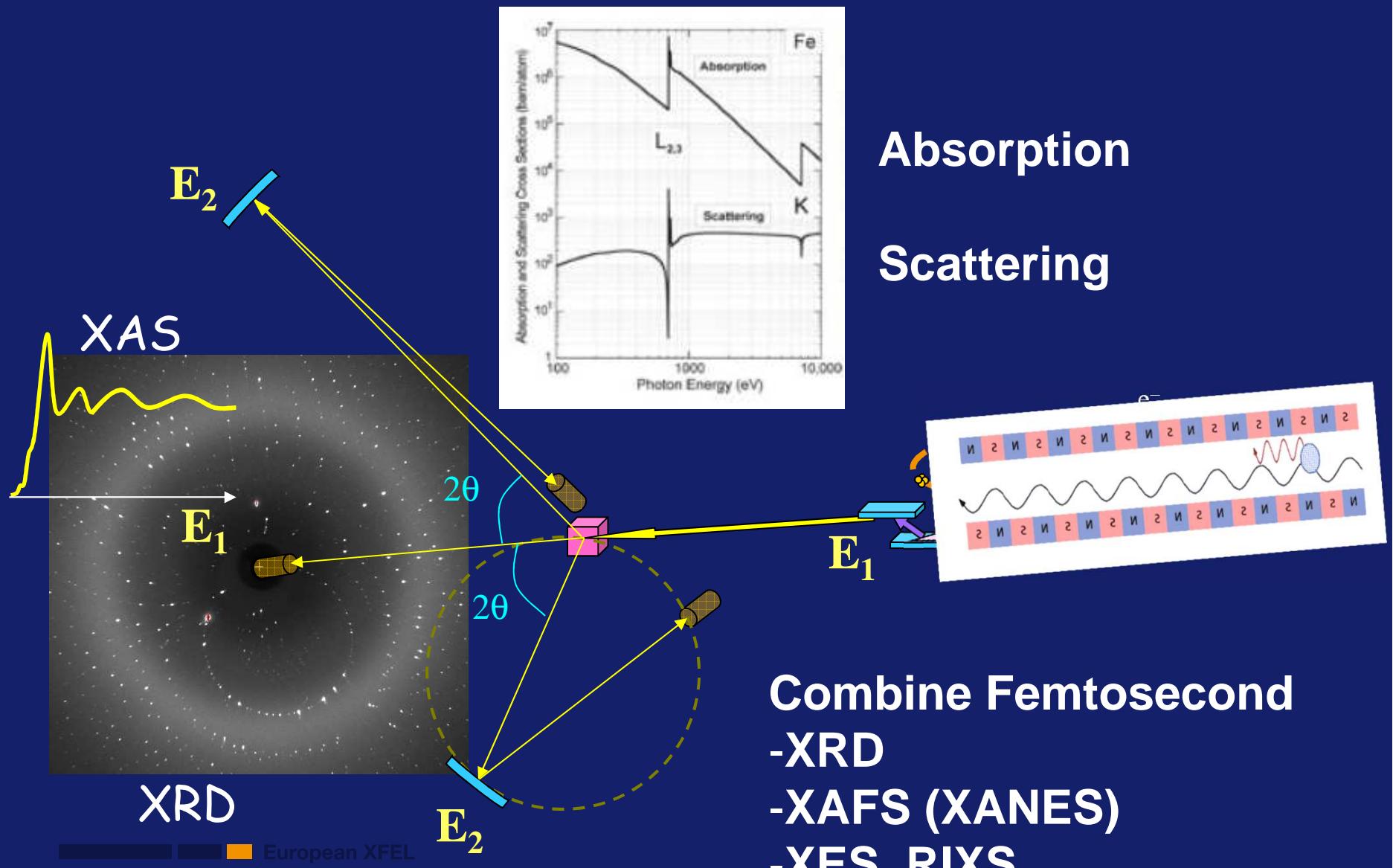
■ X-Ray Scattering

- Guest-Host Interactions, dissociation and association processes

■ Femtosecond shaped pulses

- Excited State Landscape

FXE: Make use of all incident x-ray photons



A Suite of Complementary Structural Tools at FXE

■ 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. 3d orbitals (dipole-forbidden for $1s \rightarrow nd$ excitation)

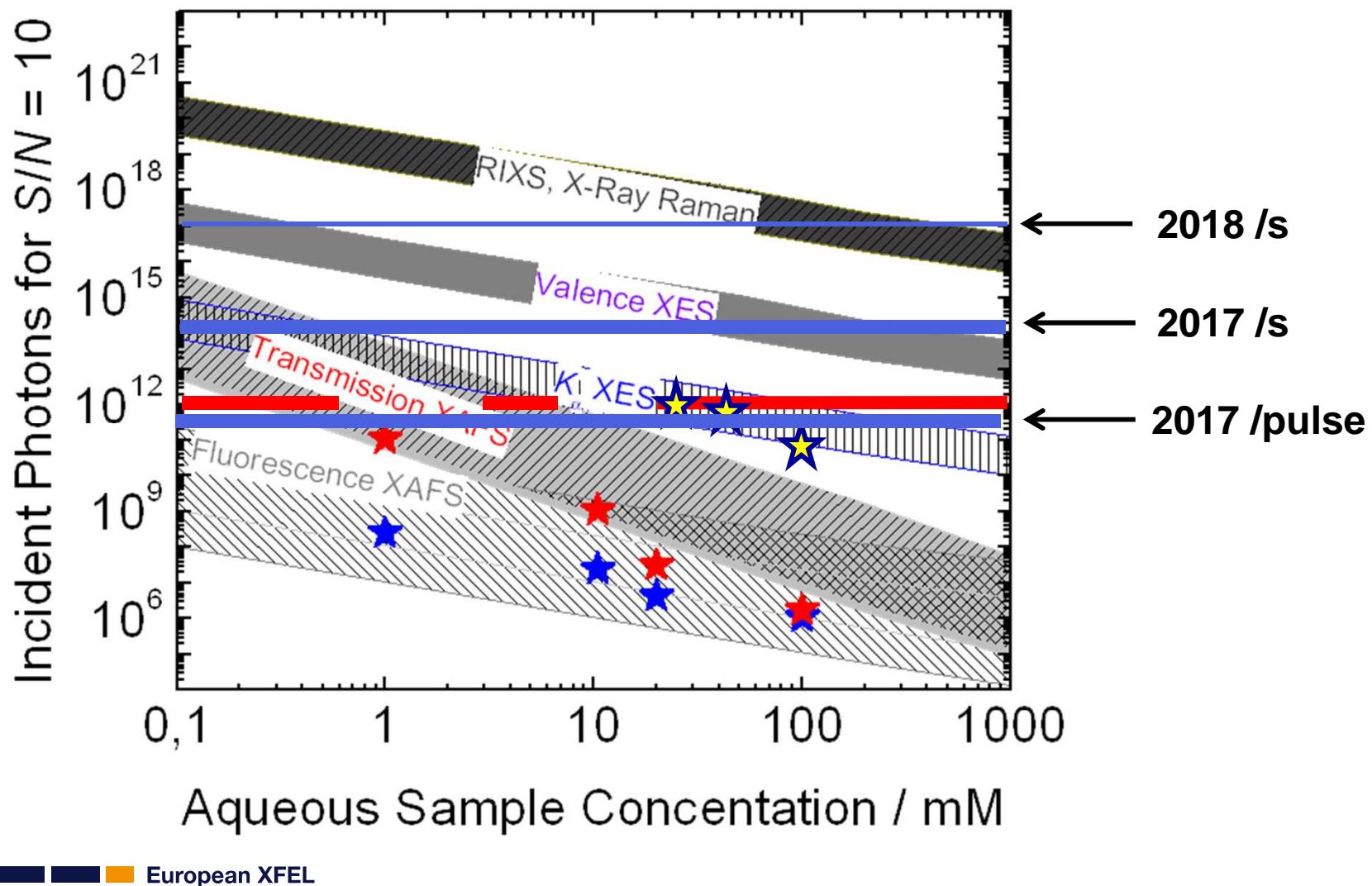
■ X-Ray Raman Spectroscopy

Access K-edges of light elements (N, O, C...) constituting solvent molecules

■ X-Ray Diffuse Scattering

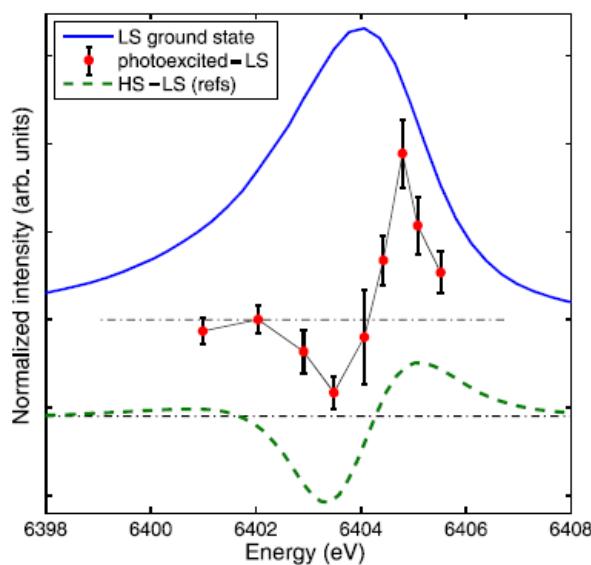
Short- and medium-range geometric environment, solute + solvent (cage) contributions to the structural factor

What you need to get the job done (spectroscopies)

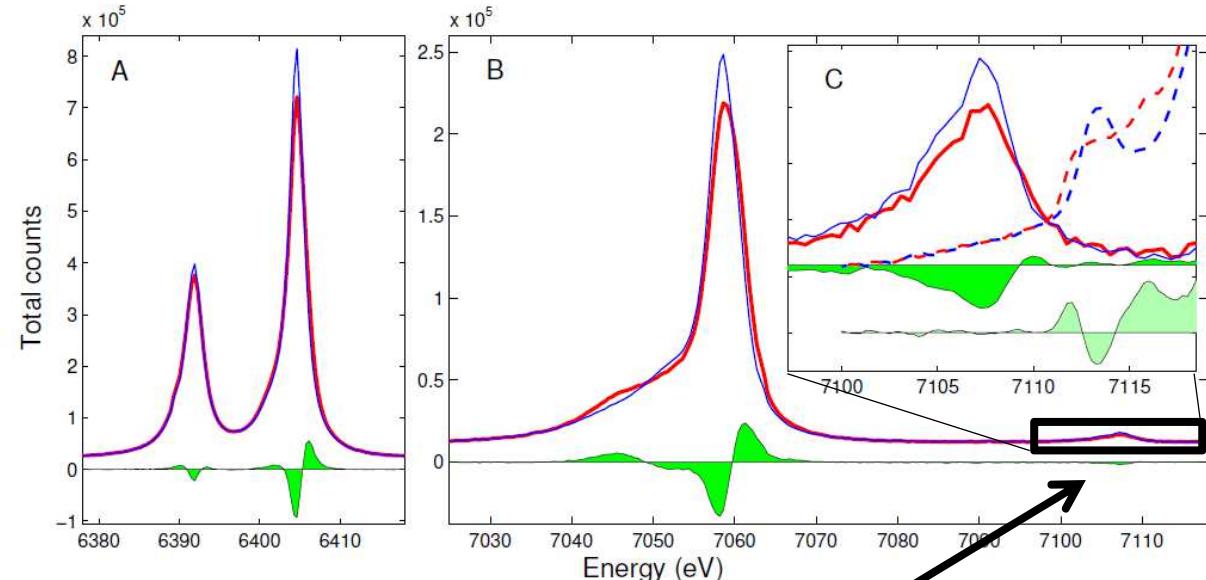


One new key ingredient: TR x-ray emission spectroscopy

2008/9: Vankó, Glatzel, Bressler

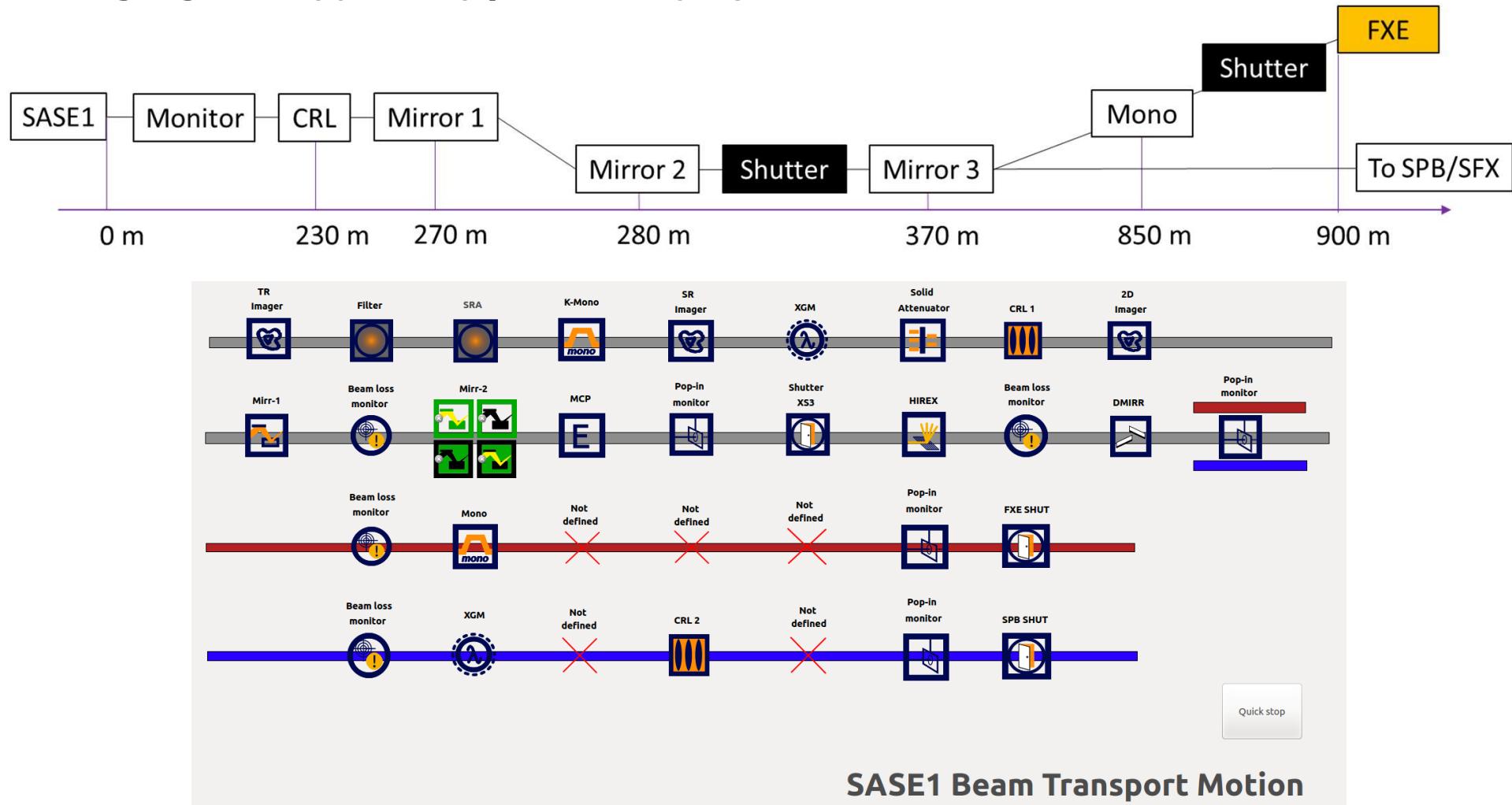


2015/16: Vankó, Gawelda, Bressler



Needs many Photons

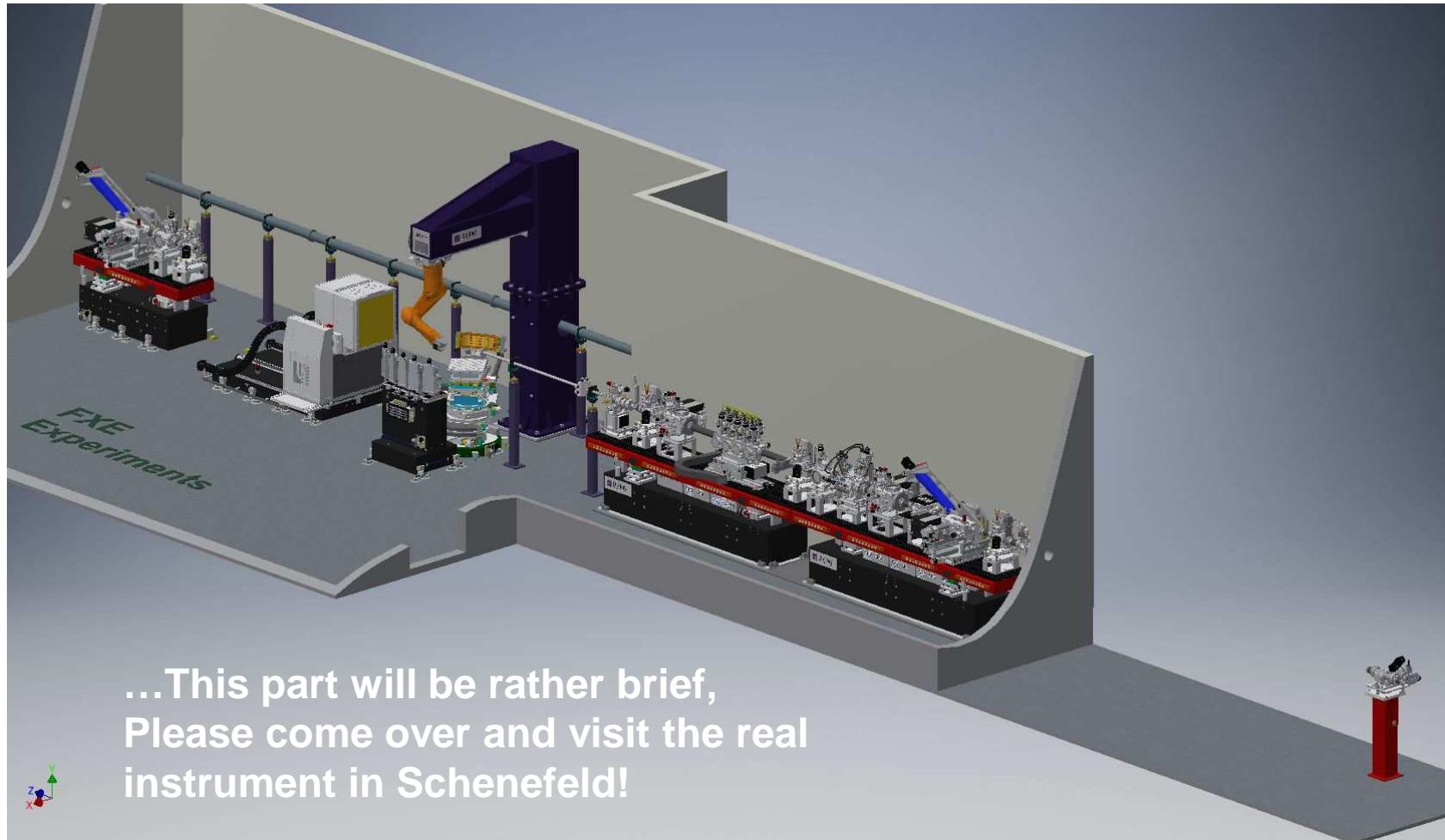
SASE1 Beamline / FXE Branch



SASE1 beam parameters

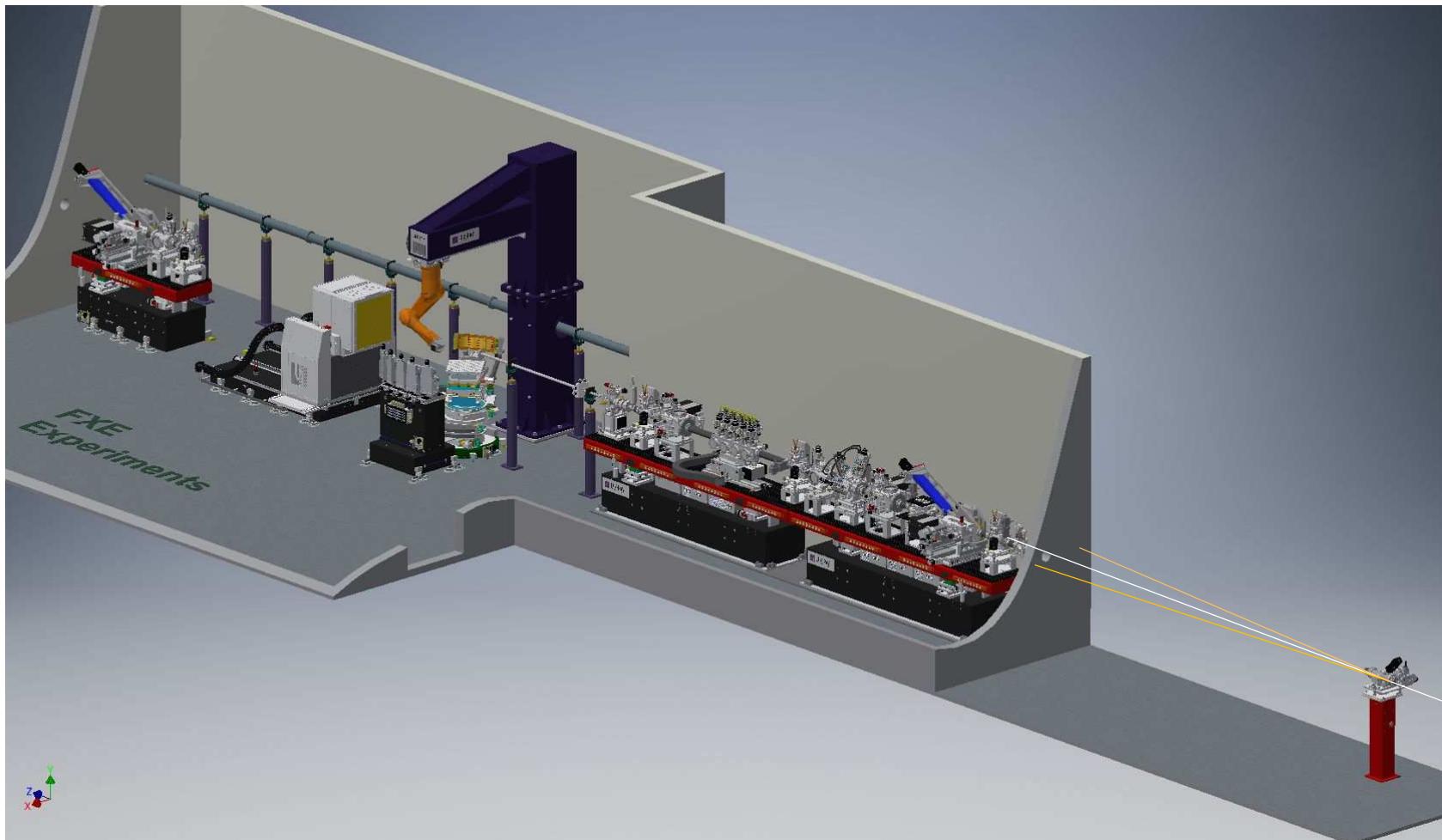
photon energy	8.979 keV	potentially variable between 8 keV and 10 keV
pulse energy	0.35 mJ	calculated, at saturation
photons per pulse	2.5×10^{11}	calculated from photon and pulse energy at source
pulse duration	50 fs	calculated from e- beam properties
spot size on sample	~ 2 μm (focus)	calculated, variable up to ~300 μm
photons/μm ² on sample	0.5×10^{11}	derived
train repetition rate	10 Hz	fixed
intra-train repetition rate	1.1 MHz	variable to 4.5 MHz, possibly 100 kHz
no. of bunches per train	60	variable from 1 to 60
$\Delta E/E$	< 0.2%	calculated

Instrument Overview



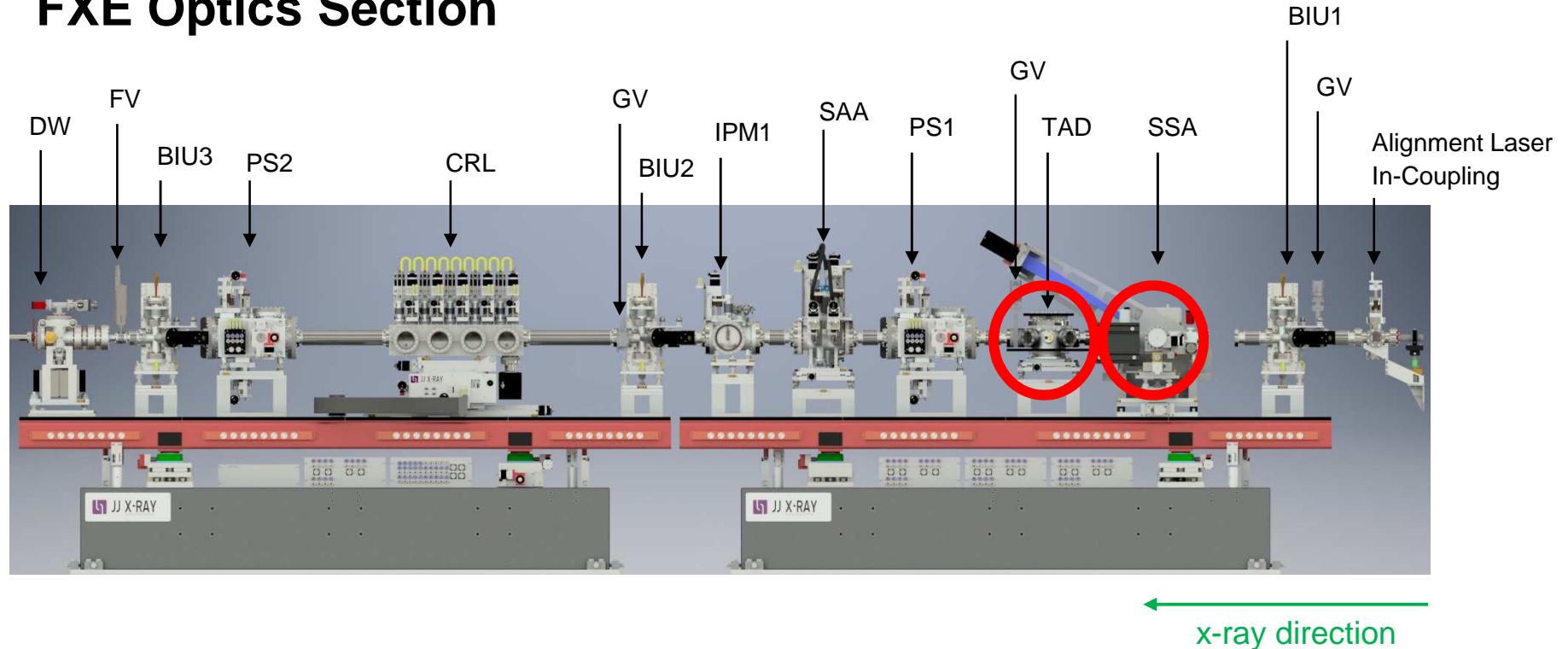
...This part will be rather brief,
Please come over and visit the real
instrument in Schenefeld!

Instrument Overview



■ European XFEL

FXE Optics Section



DW: Diamond Window

FV: Fast Valve

PS: Power Slit

BIU: Beam Imaging Unit

CRL: Beryllium Lenses

GV: Gate Valve

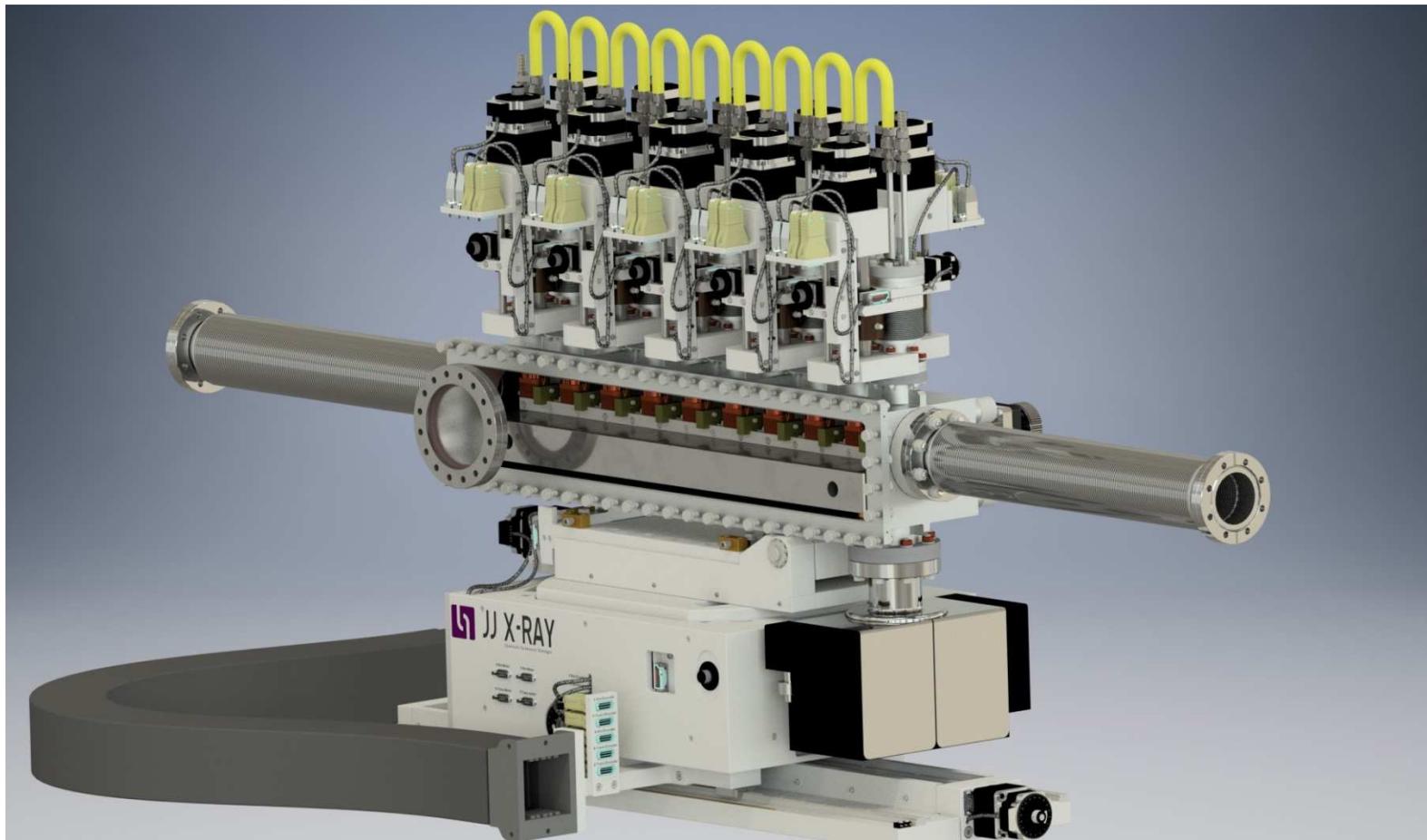
IPM: Intensity Monitor

SAA: Solid Attenuator Assembly

TAD: Time Arrival Detector

SSA: Single-shot Spectrum Analyzer

Beryllium Lens Assembly

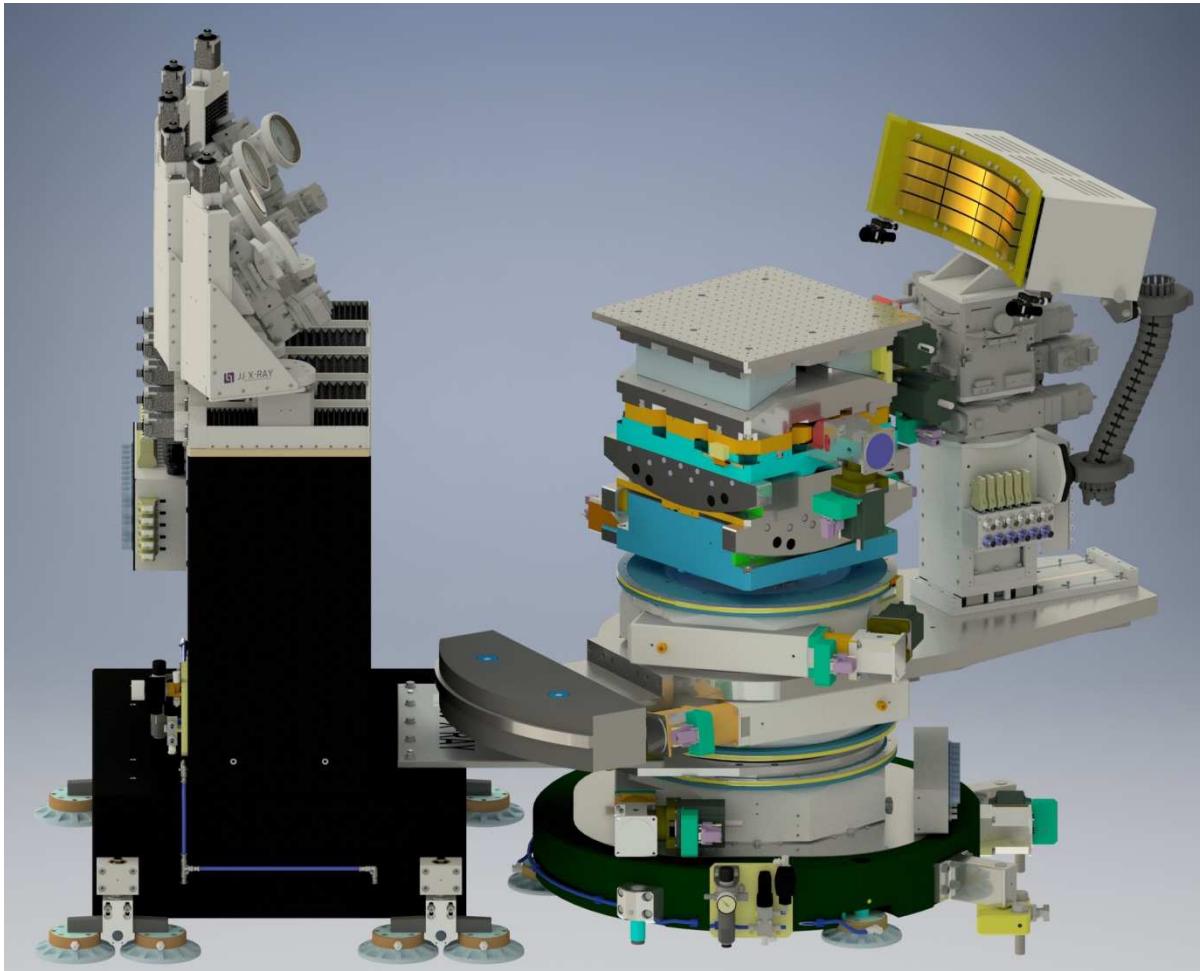


Diamond Window / Fast Shutter



a set of vacuum apertures following a redundant pressure gauge protects the beamline vacuum by means of a fast shutter in case the diamond fails

Sample Environment



ambient condition

offering 10 degrees of freedom, including 2 independent rotations for Johann and von Hamos spectrometers:

x – translation perpendicular to x-ray beam

Lower 2-theta rotation (Johann)
Upper 2-theta rotation (von Hamos)

Lower vertical (y) translation

Theta rotation

Phi and Chi rotations

x, z crossed translations

Upper vertical (y) translation

LPD mount



motorized mount for LPD

3 degrees of freedom, i.e.

z – translation

y – translation

x – translation

Post Experiment Diagnostics

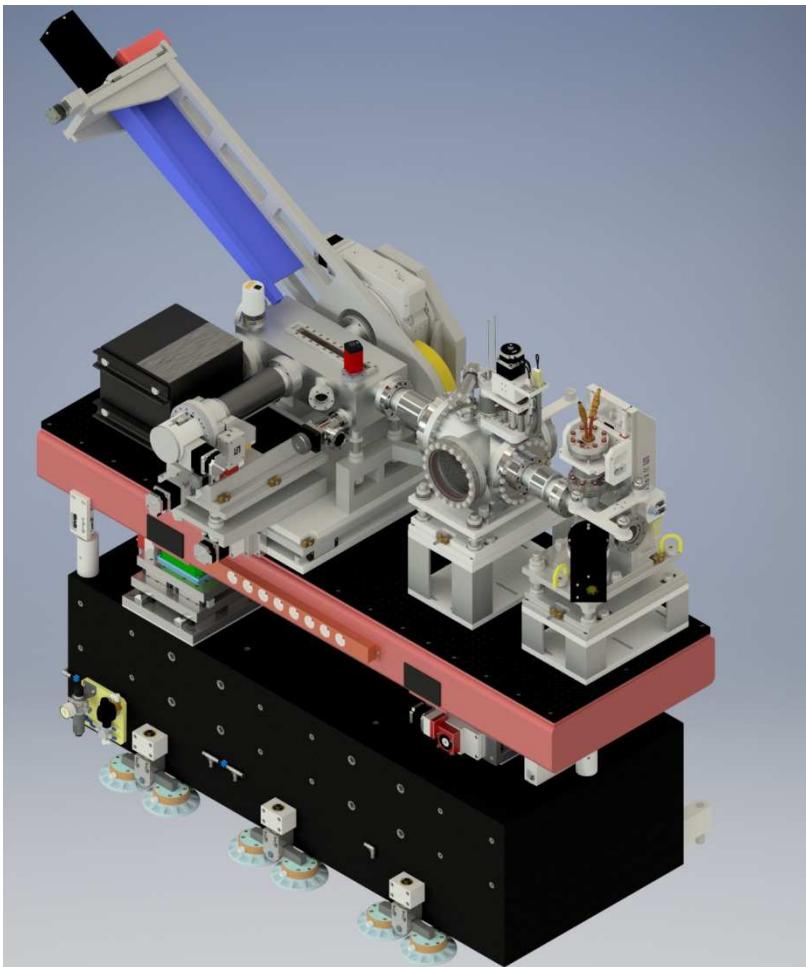


table components:

beam imaging unit for x-ray beam alignment

intensity monitor for I1 (post experiment) measurements

single-shot spectrum analyzer allowing for single shot transient XANES if used in conjunction with upstream Single-Shot Spectrum Analyzer

Acknowledgements

FXE

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C. Mammen and Team



Congratulations to the first two PhD graduates from European XFEL !!!

European XFEL

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