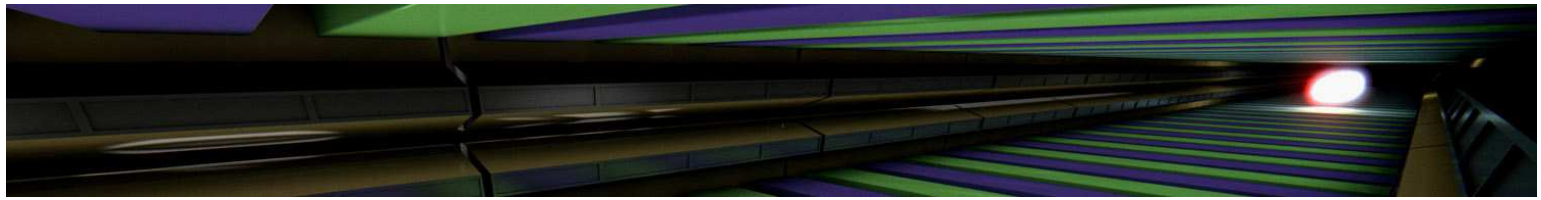


Research Opportunities at European XFEL

Christian Bressler

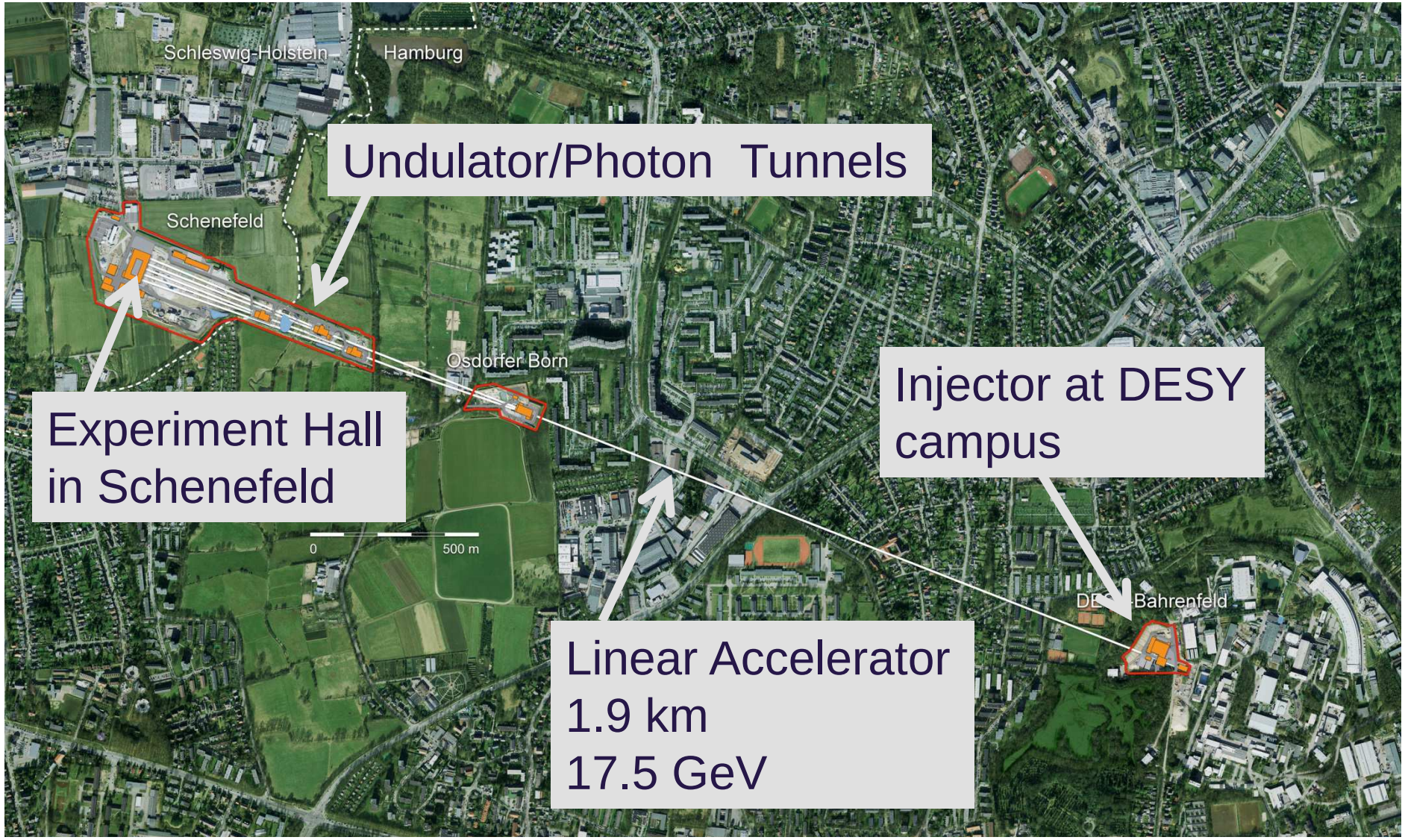
European X-Ray Free-Electron Laser Facility
Hamburg, Germany

christian.bressler@xfel.eu

“Future Research Infrastructures: Challenges and Opportunities", July 09, 2015
Varenna, Lake Como, Italy

European XFEL

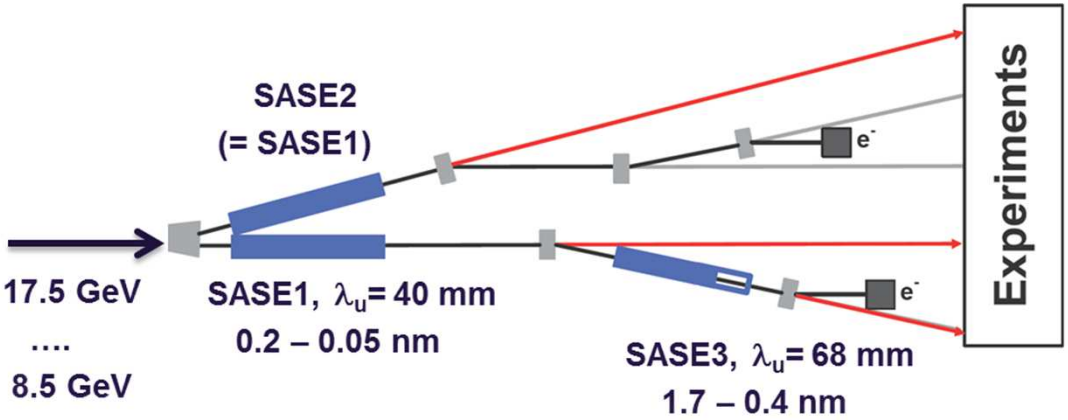
European XFEL layout

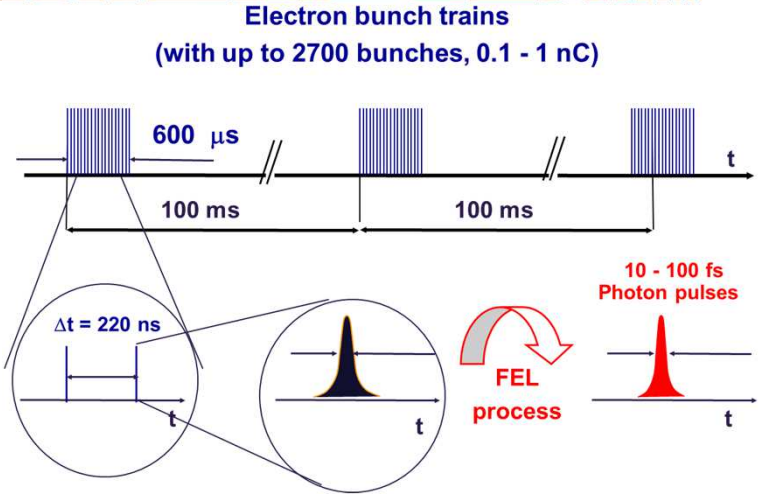


The European XFEL
Project, Challanges, Expected Performance

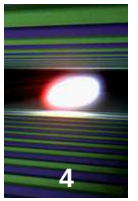
E-beam parameters

Burst repetition rate	10 Hz
Burst length	600µs
#bunches per burst	2700
Bunch length (compressed)	2-180 fs (FWHM)
Bunch charge	0.02-1 nC
Slice emittance	0.4-1.0 mm mrad
Slice energy spread	4-2 MeV





Current timetable…



2016 Initial commissioning of linac, to bring electron beam in first undulator (SASE1). Enable first lasing.

2017 Bring X-ray FEL beam to XHEXP.

Continue commissioning of accelerator.

Initial commissioning of X-ray beam transports and instruments.

Start “early user experiment” programme (peer-reviewed).

2018 Reach full performance of accelerator.

Development of X-ray beam transports and instruments towards full performance.

Continue “early user experiment” programme (peer-reviewed).

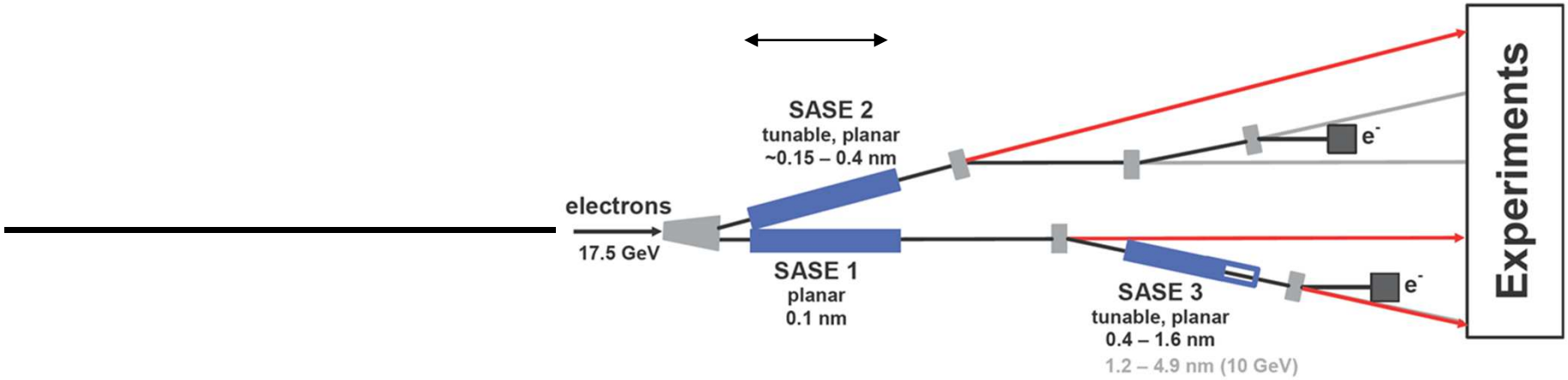
During 2nd half 2018 start full scope user programme (peer-reviewed).

2019 Regular operation (4000 hrs for user programme).

European XFEL (schematic)

- 3.4 km total length

- 200 m undulators



- 2 km linac

- 1 km photon transport

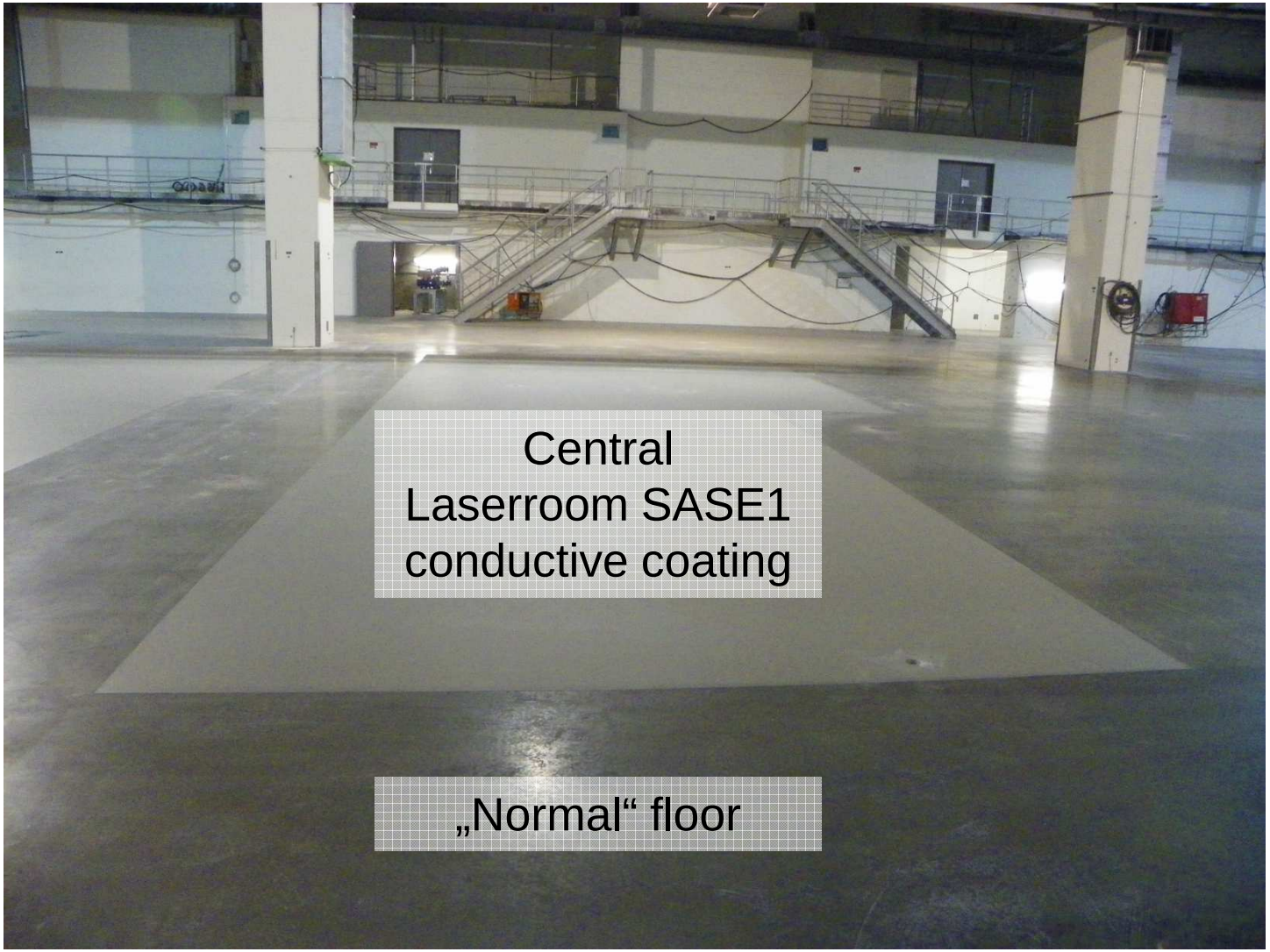
European XFEL: a gigantic construction site (2011)

- XS1 Dec 2010

European XFEL

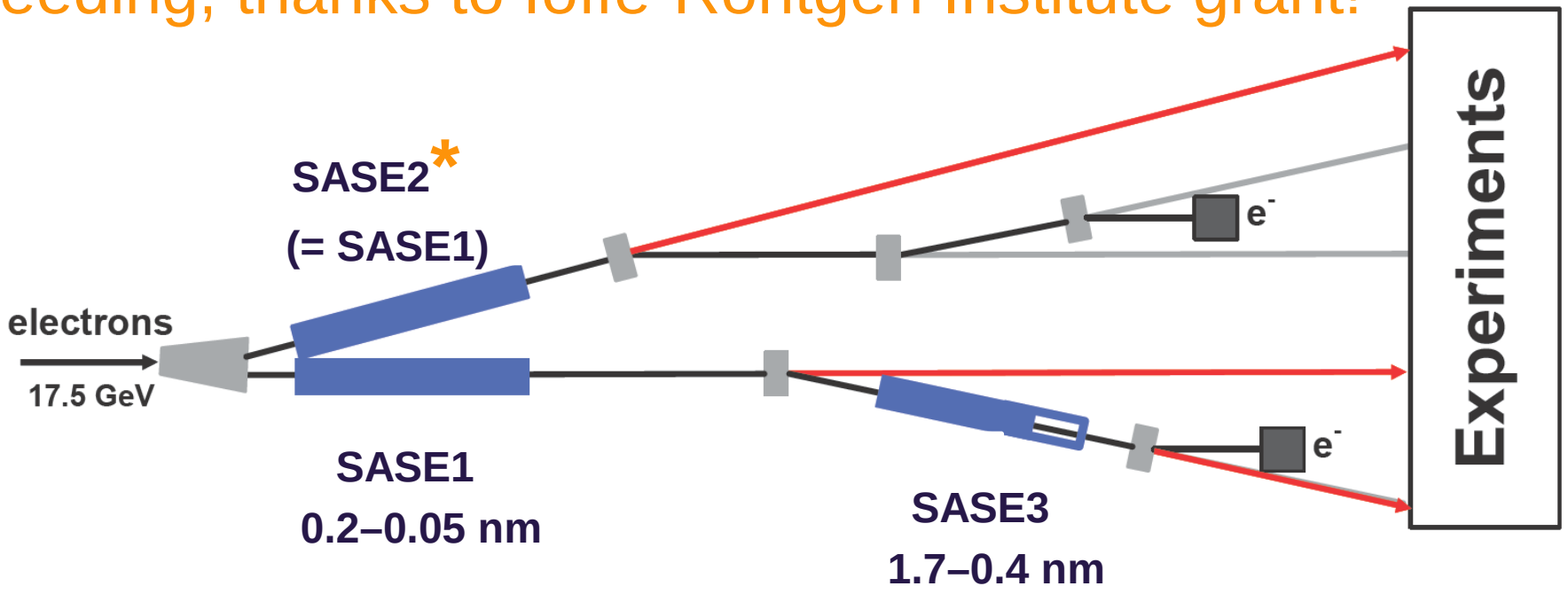
Experiment Hall infrastructure, October 2014

Casting of final floor: Floor was cleaned / polished / coated.



Undulators and Photon Beamlines

*NEW! : Shall be equipped for hard x-ray self-seeding, thanks to Ioffe-Röntgen Institute grant!

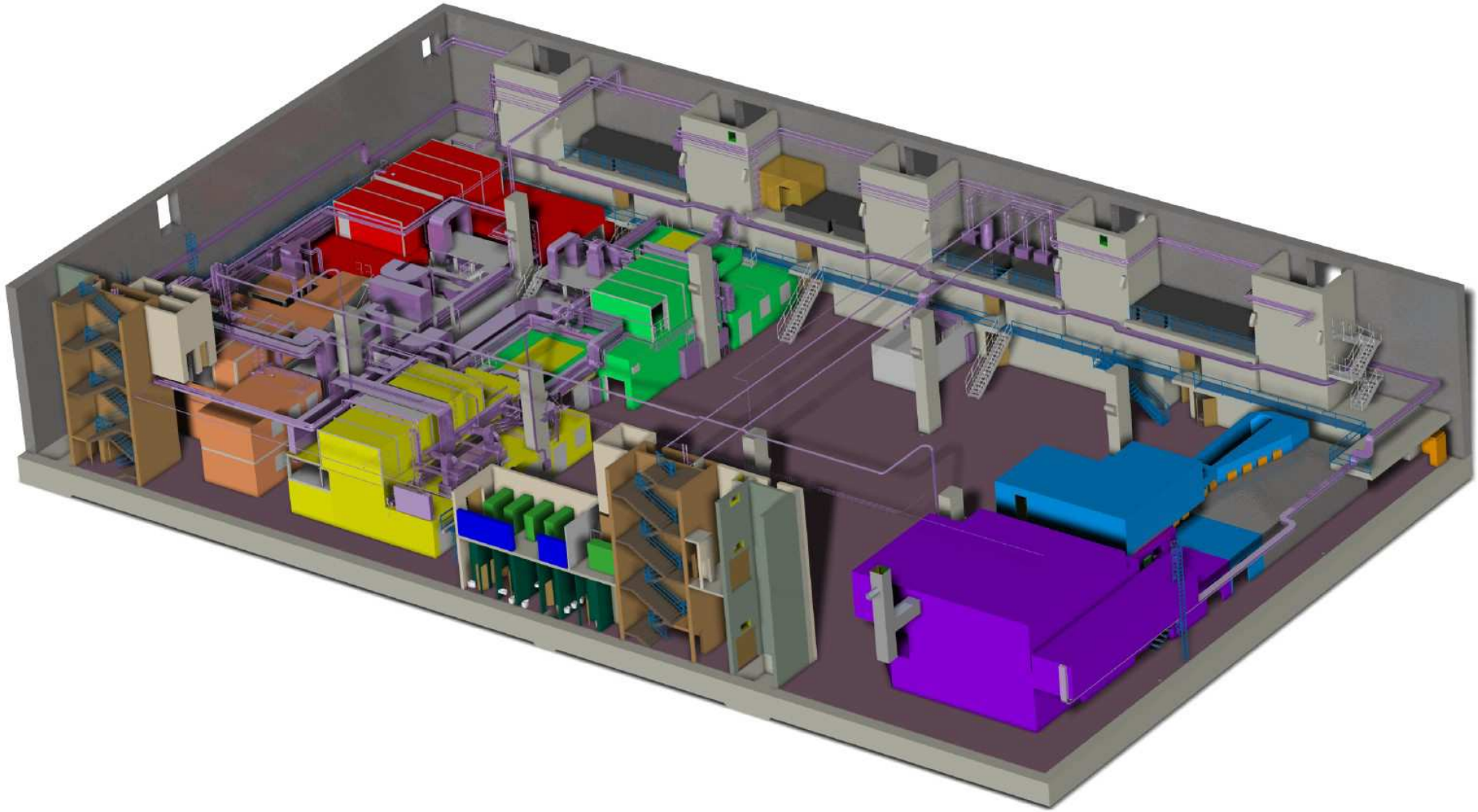


35 X 5m sections,
40 mm period

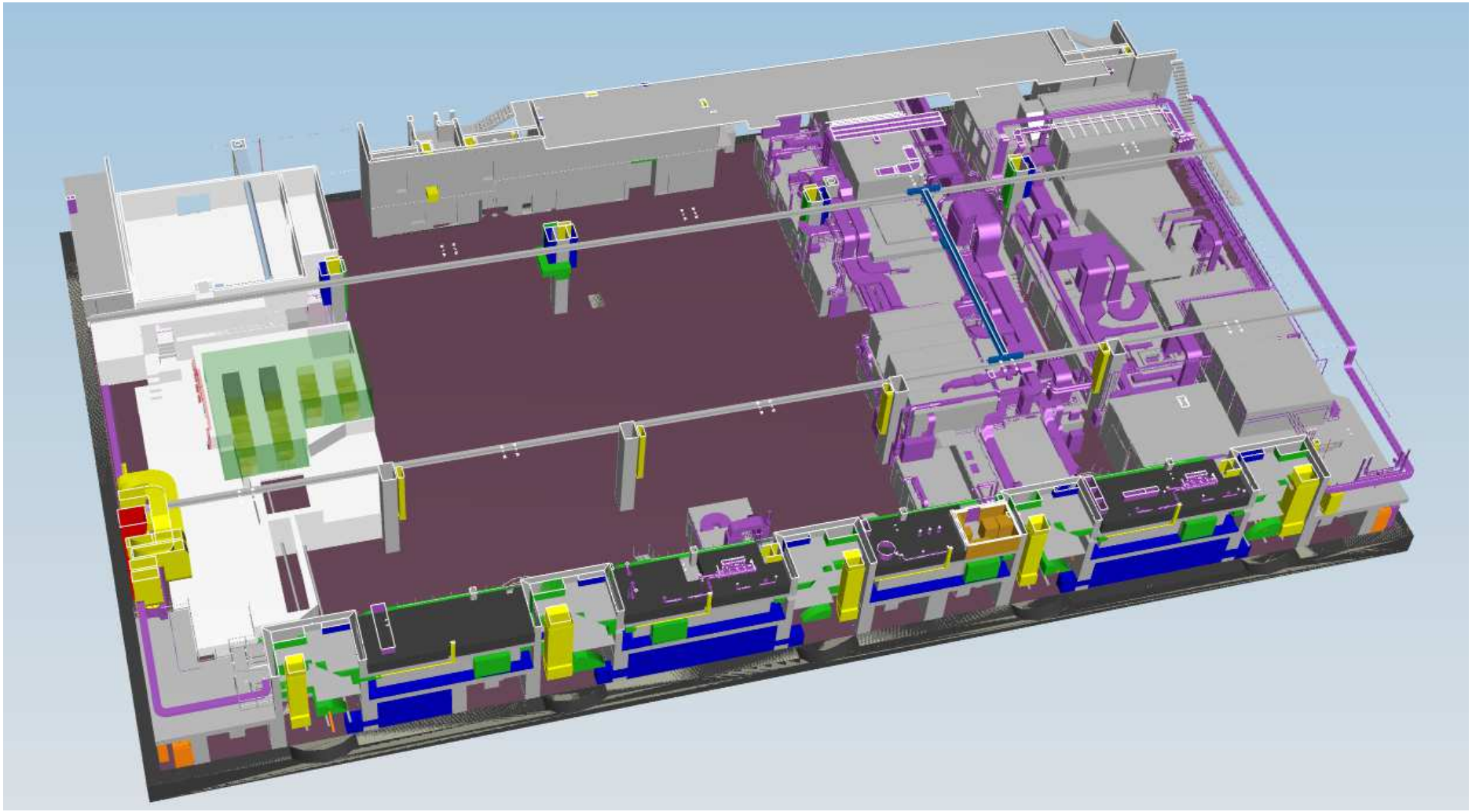
21 X 5m sections,
68 mm period

European XFEL

Experimental Hall Infrastructure

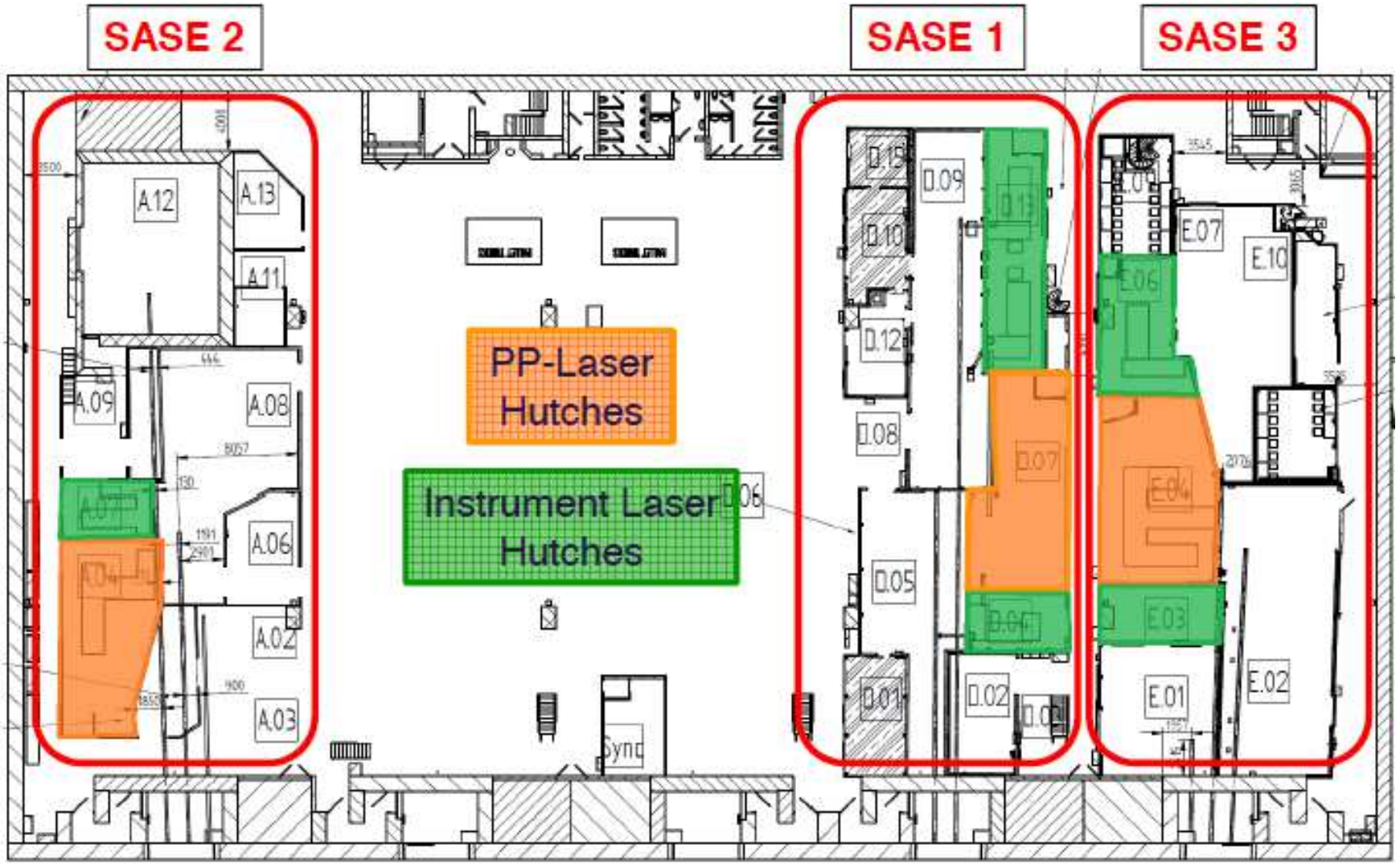


Status of hutch planning + construction: Infrastructure Experimental Hall



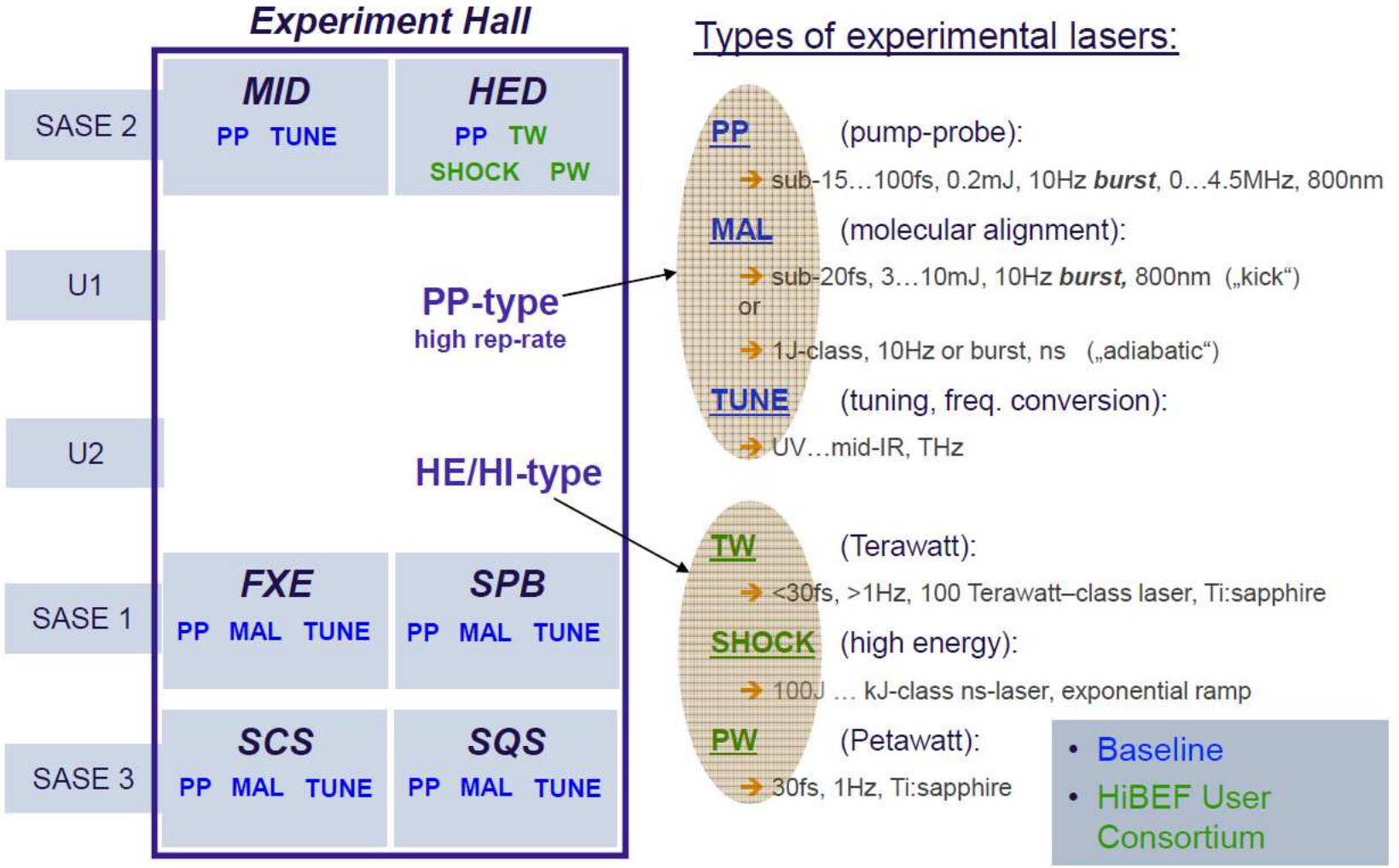
European XFEL

Laser location in the Experiment Hall

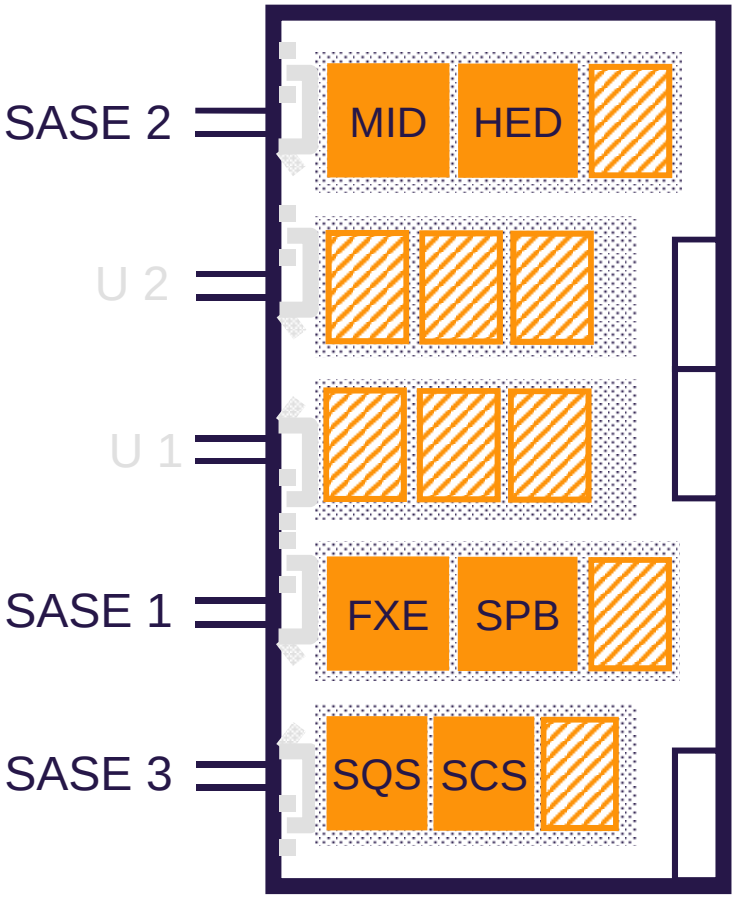


The European XFEL
Many Laser Systems available

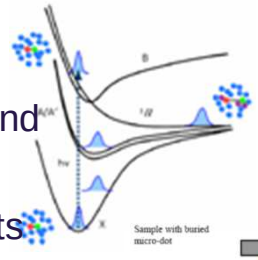
- Optical Lasers WP-78 – Max Lederer & HiBEF UC



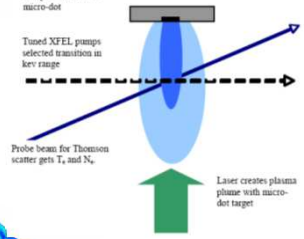
The suite of instruments at European XFEL



- FXE Femtosecond X-ray Experiments

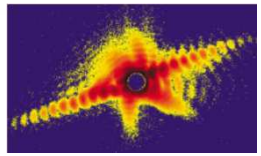


- HED High Energy Density Science

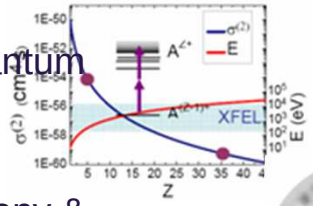


- SPB Single Particle & Biomolecules

- MID Materials Imaging & Dynamics

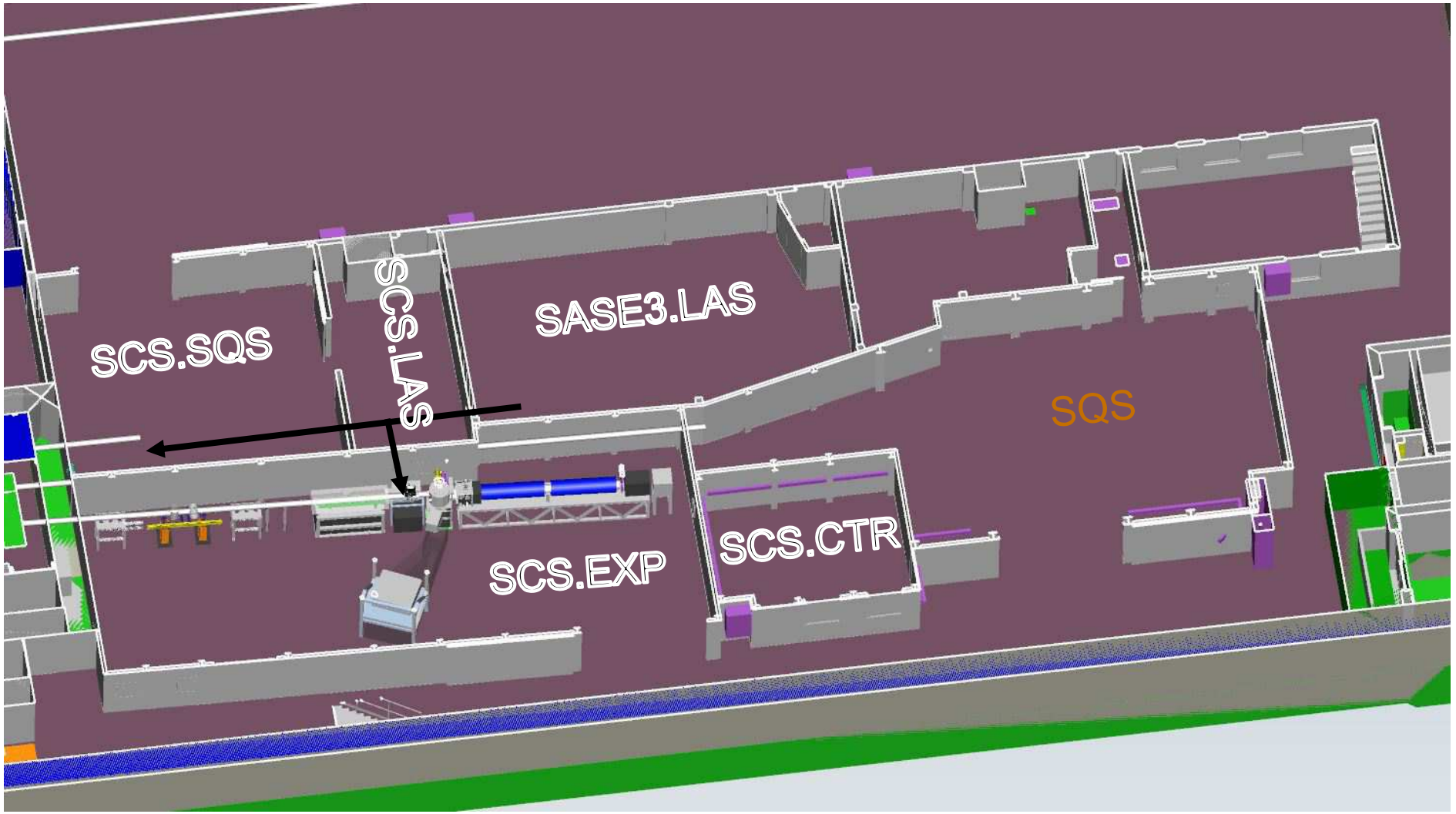


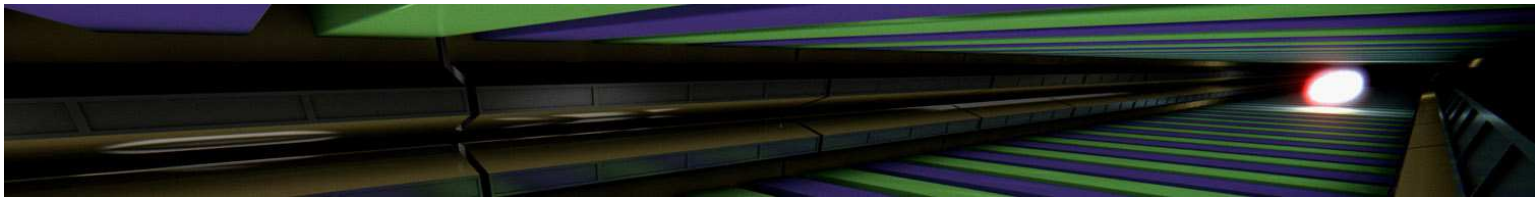
- SQS Small Quantum Systems



- SCS Spectroscopy & Coherent Scattering

Experiment Hall SASE3 Hutches



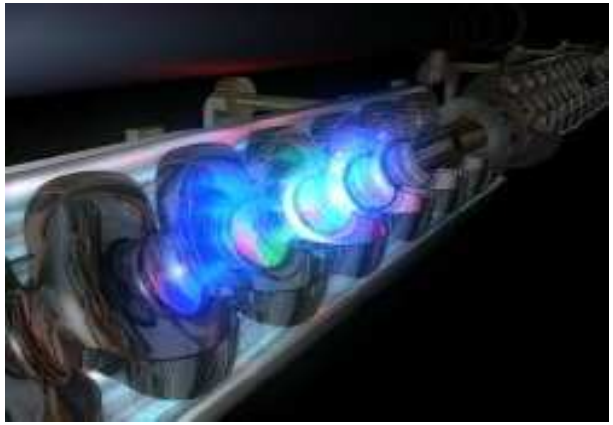


SQS Scientific Instrument

T. Mazza, A. de Fanis, H. Zhang, M. Meyer,
European XFEL GmbH

TDR_2012: http://www.xfel.eu/documents/technical_documents

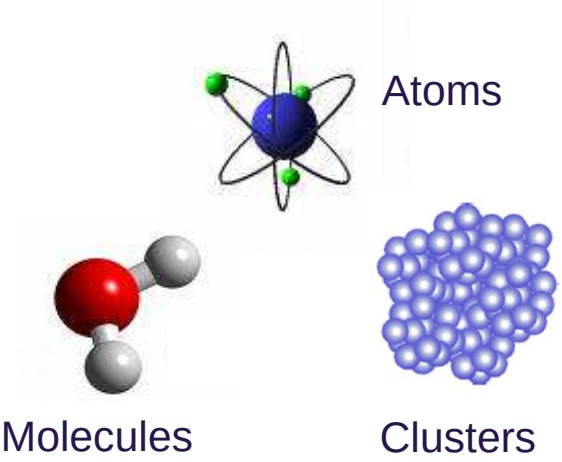
European XFEL



N x hν

2 - 100fs

"Small Quantum Systems"



Scientific Applications at SQS

"Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena"

High intensities: $>10^{15}$ W/cm^2	⇨	**Non-linear phenomena** **Multi-photon processes**
Short pulses: 2 - 100 fs	⇨	**Ultra-fast dynamics** **Pump-probe experiments**
High flux $> 10^{12}$ photons / pulse $> 10^{15}$ photons / sec	⇨	**Extremely dilute targets** **Processes with small cross section**
Spatial coherence	⇨	**Coherent Diffraction Imaging**

European XFEL

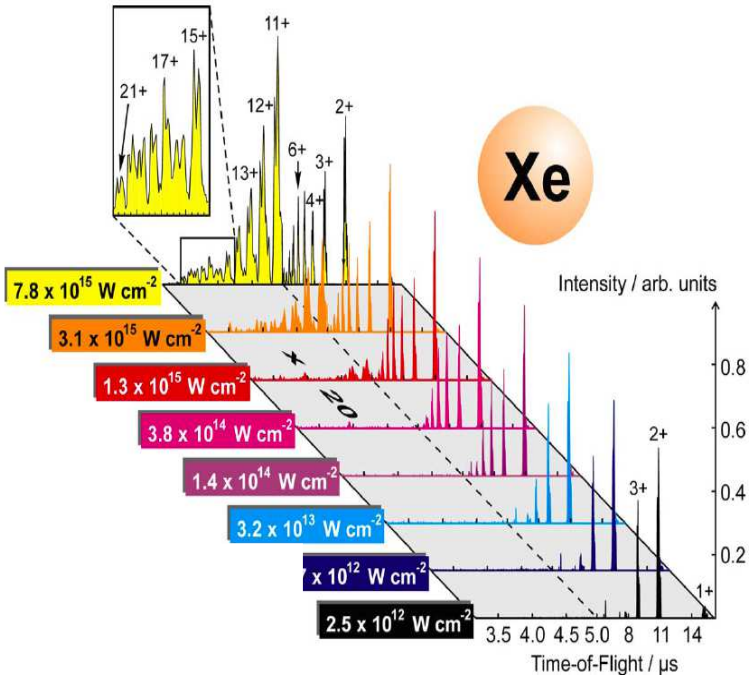
High repetition rate: < 27000 pulses/ sec	➡	**High data collection rate** **Multi-particle coincidences**

1) Multi-photon multiple ionization : Atoms

Multi-electron system: Xe

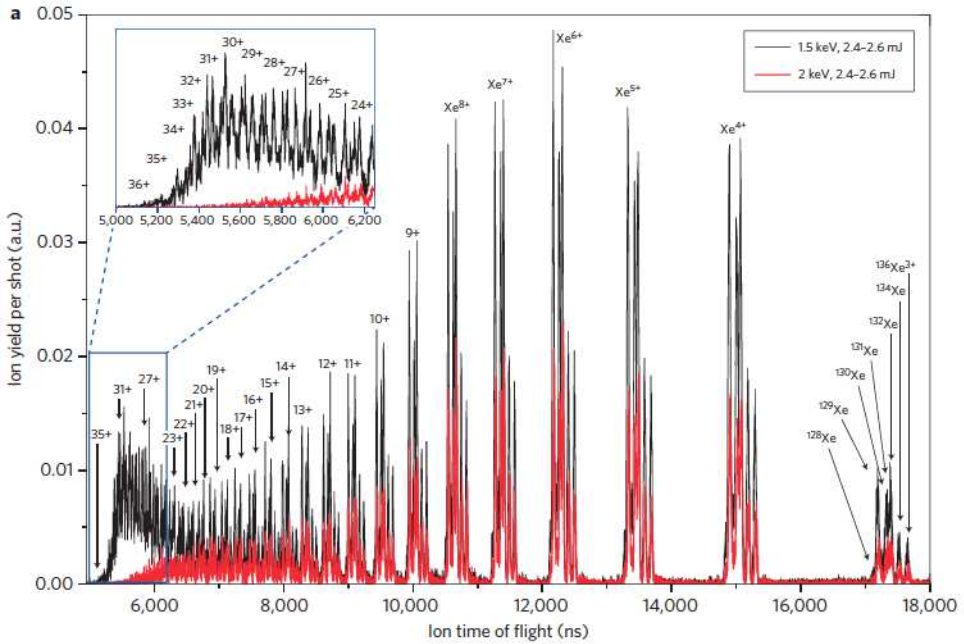
□□(FLASH) = 13.3 nm Sorokin et al., PRL 99, 213002 (2007)

hν = 93 eV



□□(LCLS) = 0.8 nm Rudek et al., Nat.Phot. 6, 858 (2012)

hν = 1.5 keV



IP(Xe 21+) ≈ 5 keV

Xe 35+ (25 keV!!)

1) Multi-photon multiple ionization : Atoms

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□□(FLASH) = 13.3 nm Sorokin et al., PRL 99, 213002 (2007)

hν = 93 eV

□□(LCLS) = 0.8 nm Rudek et al., Nat.Phot. 6, 858 (2012)

????

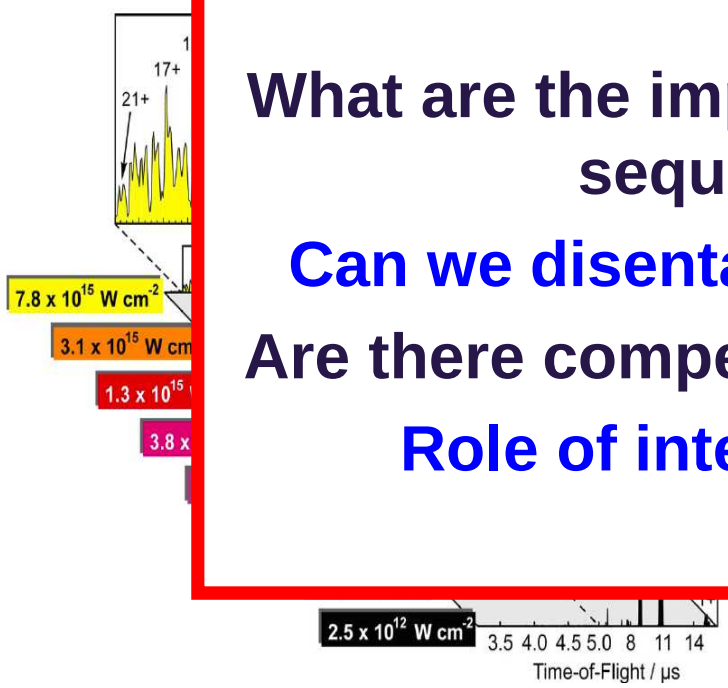
What are the important processes: Direct or sequential ionization?

Can we disentangle the individual steps?

Are there competing / interfering pathways?

Role of intermediate resonances?

????



IP(Xe 21+) ≈ 5 keV

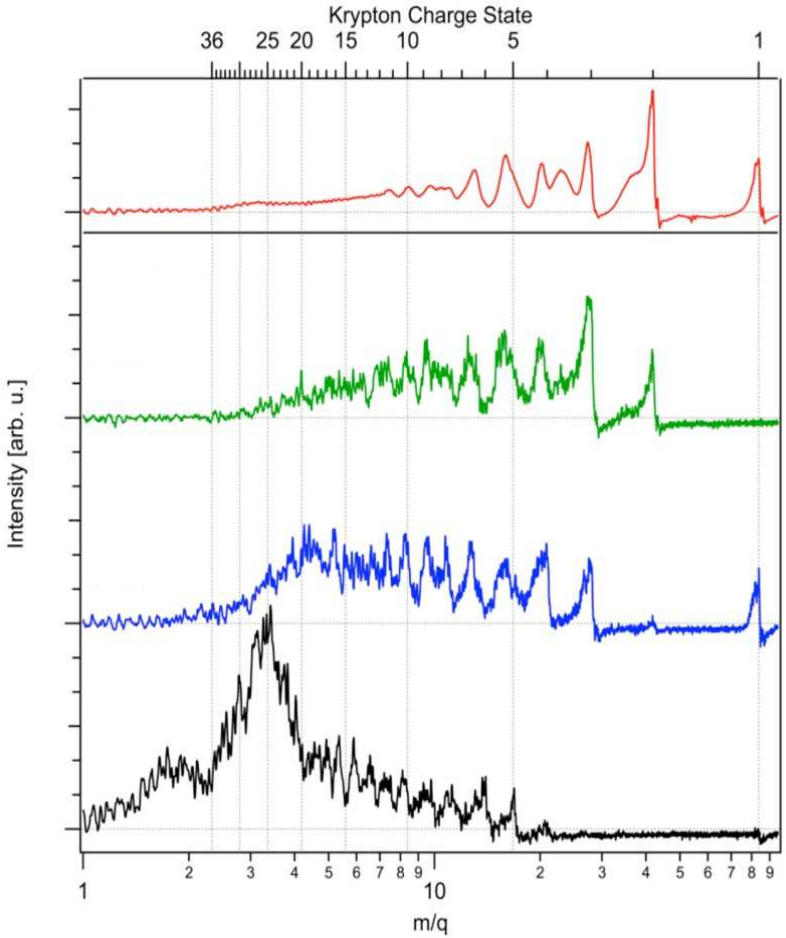
Xe 35+

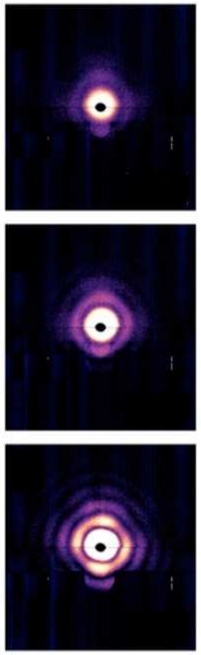
2) Multi-photon multiple ionization : Cluster

Size dependence of multiple ionization in clusters

averaged spectrum (300 Shots)

Single shot, single cluster spectra





LCLS: 1.5 keV, 3 mJ

Kr-cluster

Ion - TOF spectroscopy

Imaging

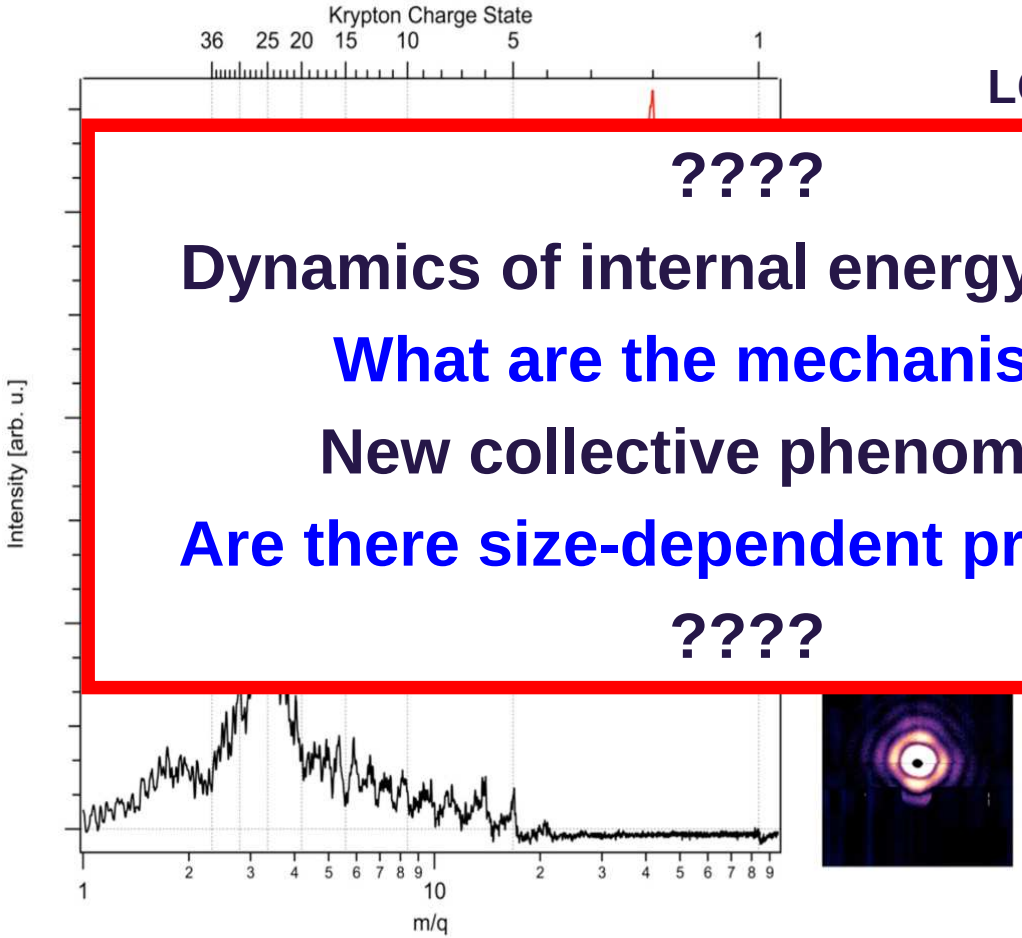
Principal investigator:
Christoph Bostedt (LCLS)

2) Multi-photon multiple ionization : Cluster

Size dependence of multiple ionization in clusters

averaged spectrum (300 Shots)

Single shot, single cluster spectra



LCLS: 1.5 keV, 3 mJ

ter

????

Dynamics of internal energy transfer:

What are the mechanisms?

New collective phenomena?

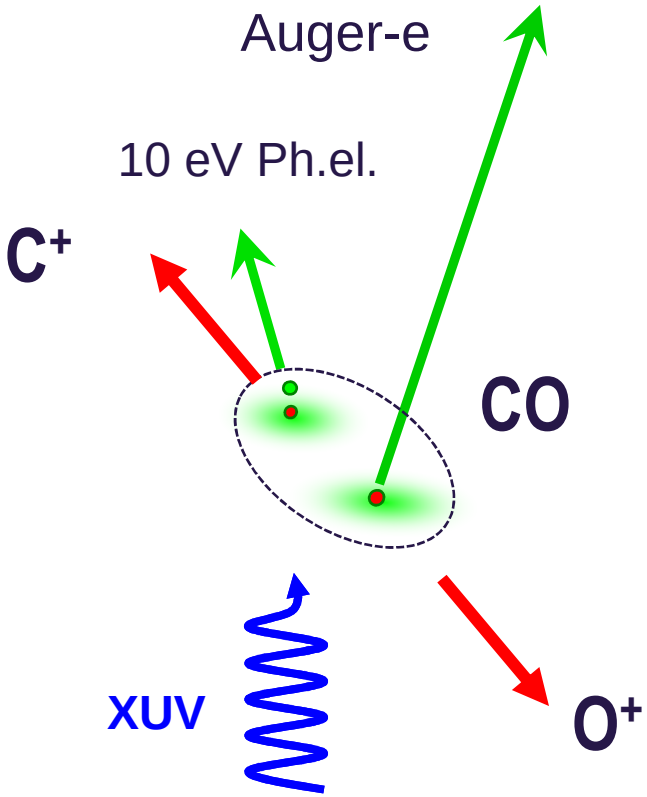
Are there size-dependent processes?

????

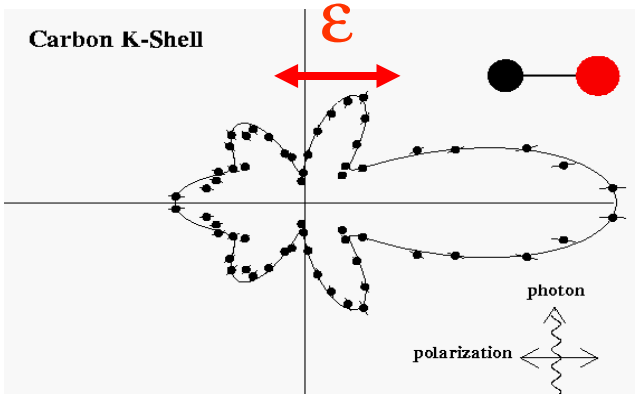
Principal investigator:
Christoph Bostedt
(LCLS)

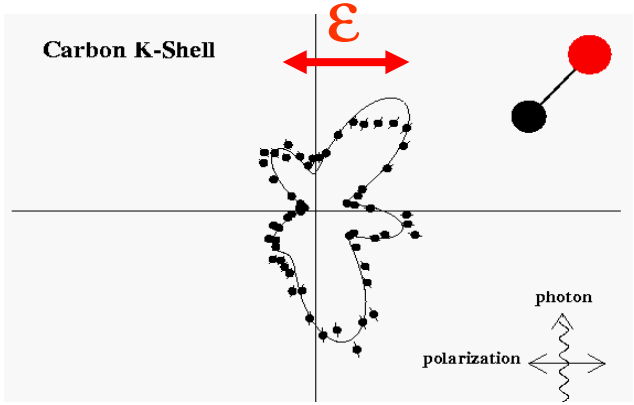
3) Ultra-fast molecular fragmentation

Molecular Dissociation Dynamics



Landers & Dörner
PRL 87 (2001)





Coincidences:
electron – ion –ion
1 pulse = 1 event !!

COLTRIMS:
high collection efficiency

ALS:
MHz rep. rate

~~**fs-dynamics**~~

3) Ultra-fast molecular fragmentation

Molecular Dissociation Dynamics

Landers & Dörner

PRL 87 (2001)

Coincidences:

electron – ion –ion

!!

Auger-e

Carbon K-Shell

ε

????

10 eV

C^+

What is the temporal evolution:

Can we follow the formation of a fragment?

Are there transient states?

Is there site selectivity?

????

XUV

O^+

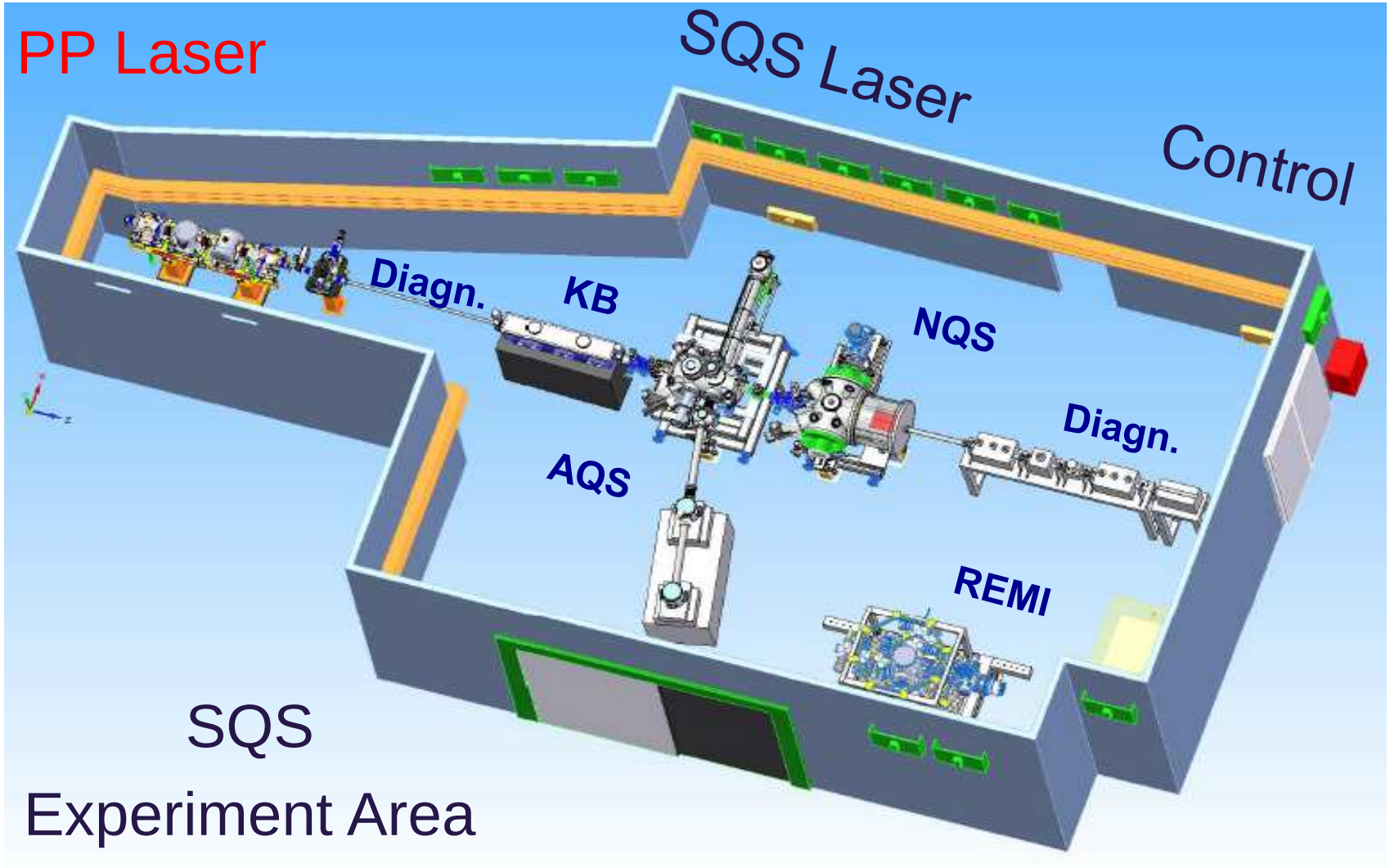
photon

polarization

MHz rep. rate

fs-dynamics

General Layout of SQS Scientific Instrument



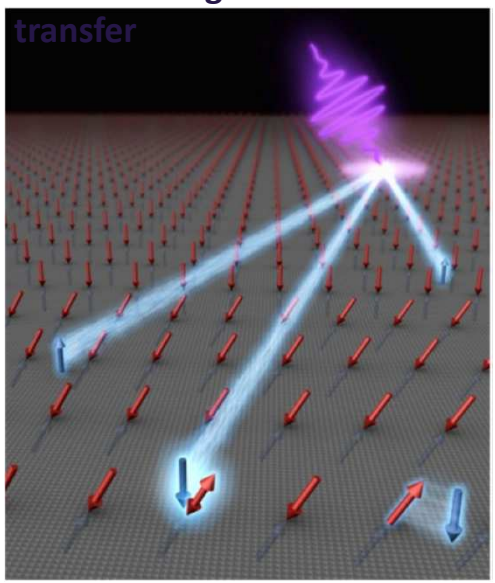
Soft Coherent Scattering (SCS, Andreas Scherz):
Study of solid state lattice, charge, orbital and spin structures

Resonant X-ray Diffraction and Coherent Diffraction [baseline]

Single-shot imaging, time-resolved resonant x-ray diffraction and x-ray photon correlation spectroscopy in forward-and backscattering geometry of charge, orbital and spin structures

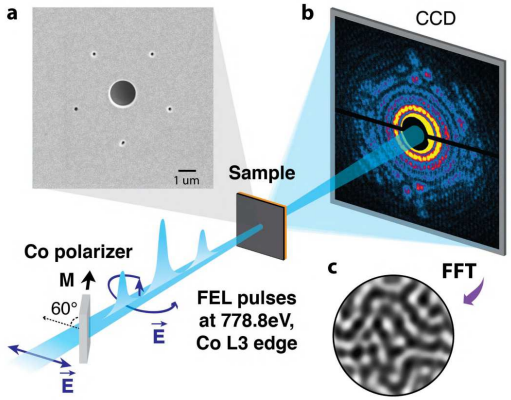
SCS group: A. Scherz, M. Izquierdo, Robert Carley, Jan T. Delitz

Nanoscale spin reversal by non-local angular momentum transfer



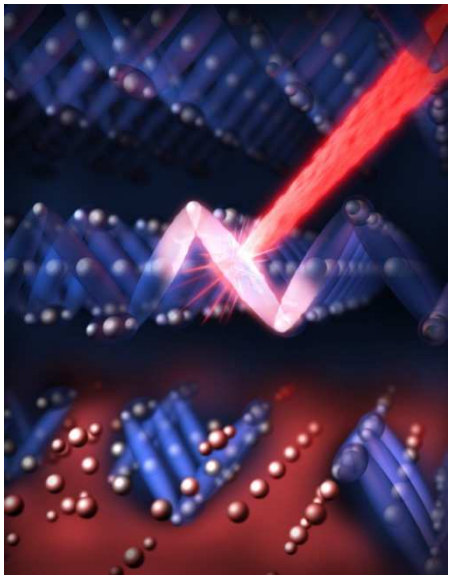
C. Graves *et al*. Nat. materials **12**, 882 (2013)

Single-shot imaging of nanoscale magnetization



Wang, Zhu, Wu *et al*. PRL **108**, 267403 (2012)

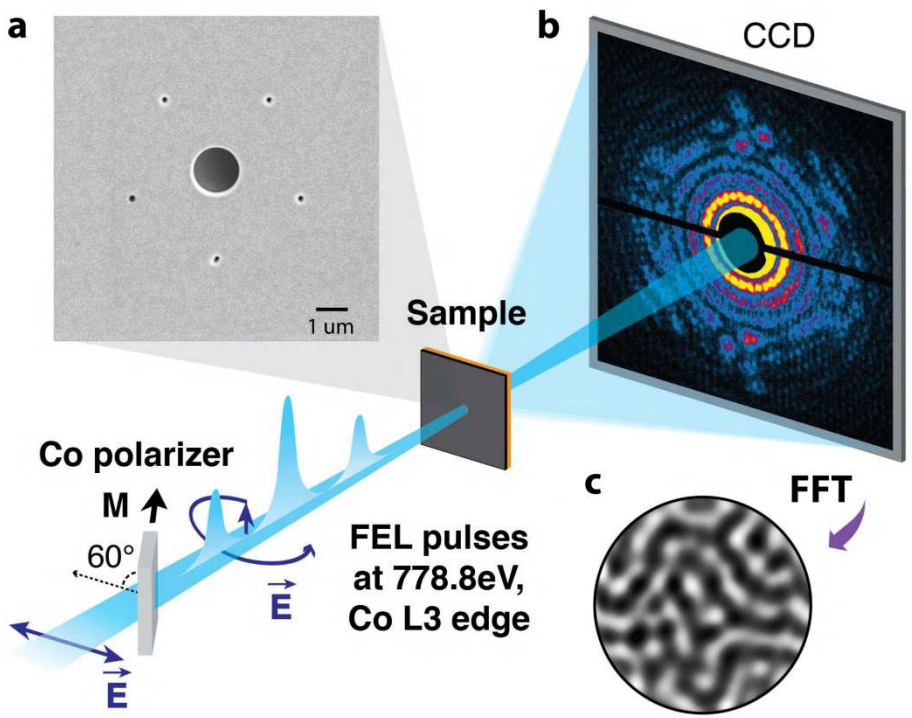
Speed limit of the insulator-metal transition in magnetite



S. de Jong *et al*. Nat. materials **12**, 882 (2013)

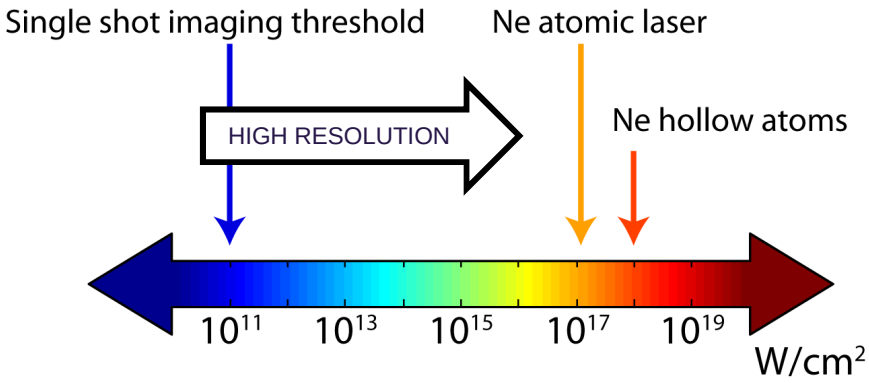
European XFEL

SCS: Single Shot X-ray Holography

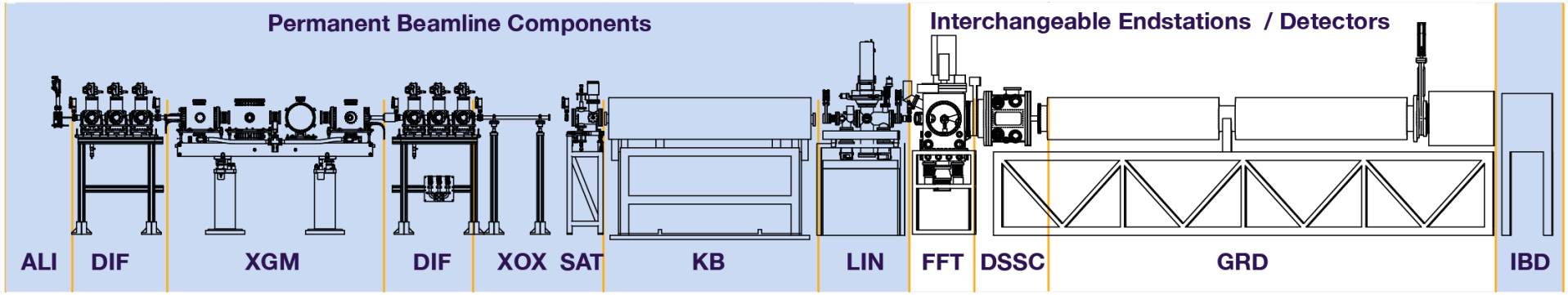


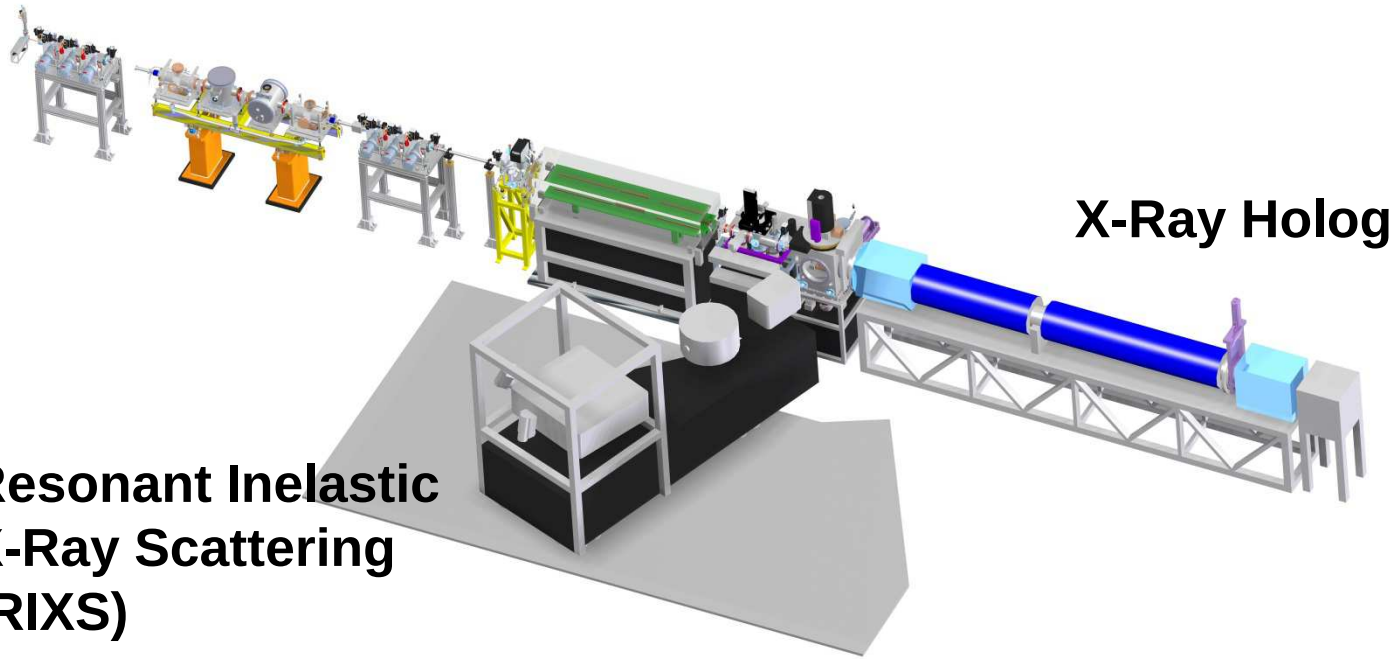
Wang, Zhu, Wu *et al*. PRL **108**, 267403 (2012)

- Using Fourier transform holography, obtain real-space image of magnetic domains.
- Diffraction from a single x-ray pulse (~5 mJ/cm^2).
- We can combine this with pump-probe techniques to make time-resolved movies!



SCS Instrument



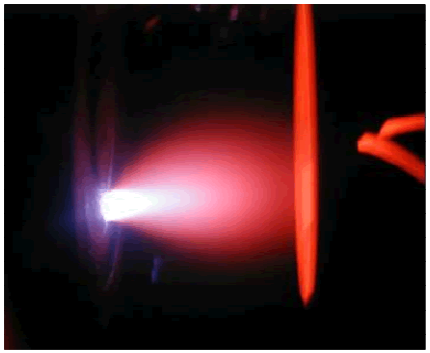


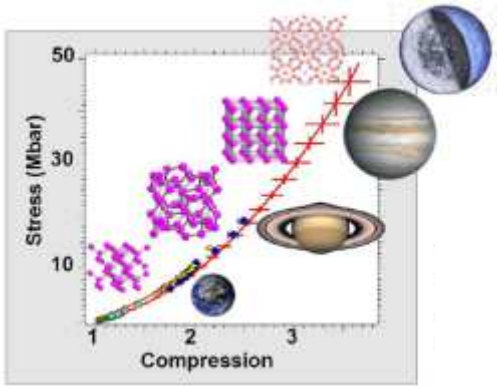
X-Ray Holography

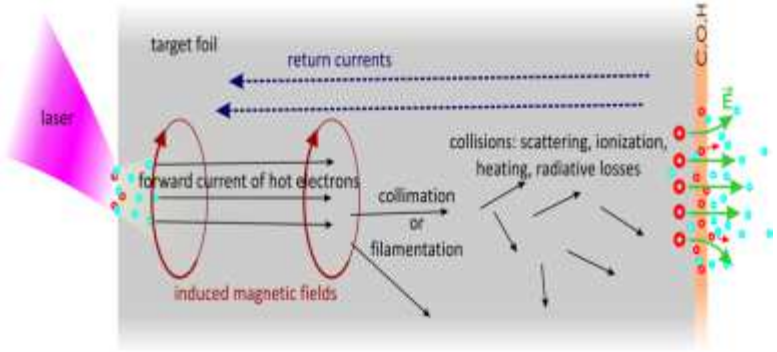
Resonant Inelastic X-Ray Scattering (RIXS)

High-Energy Density instrument (HED)
Ulf Zastrau and Group

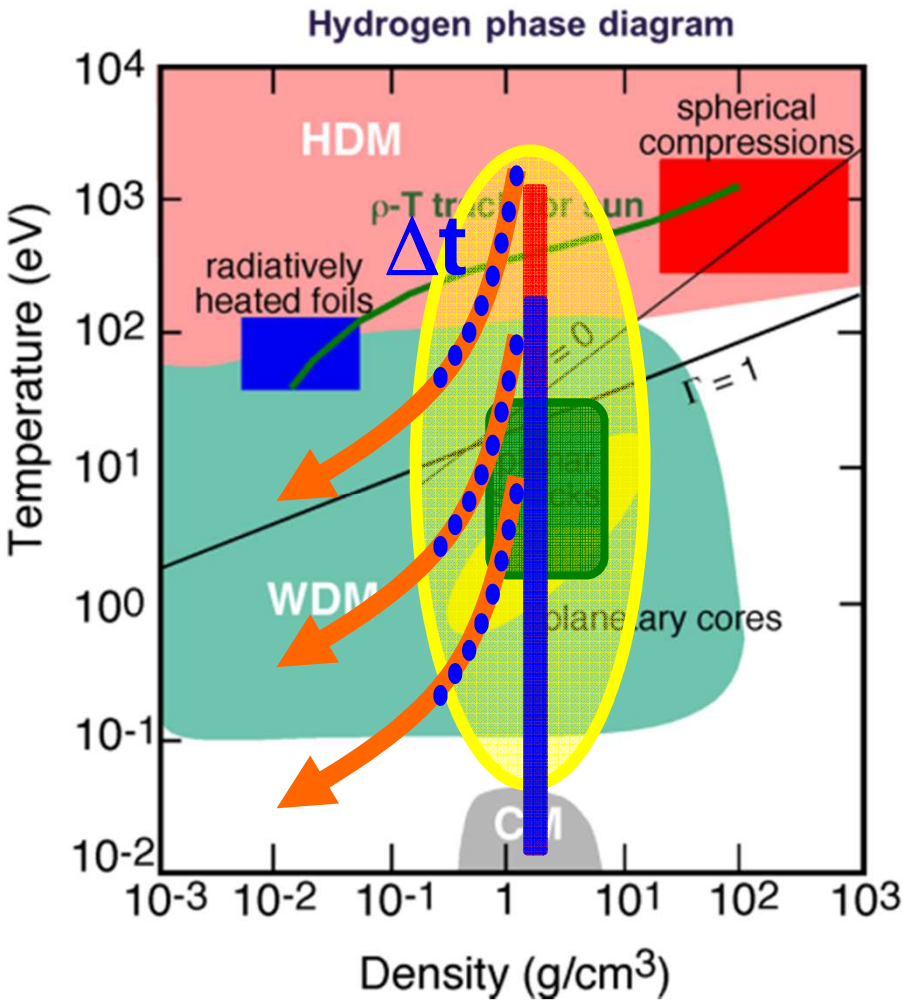
- Ultrafast dynamics and structural properties of matter at extreme states
  - **Highly excited solids**→ laser processing, dynamic compression, high B-field
  - **Near-solid density plasmas**→ WDM, HDM, rel. laser-matter interaction
  - **Quantum states of matter**→ high field QED (future upgrade)







Capabilities at HED – strong drivers available



Three optical lasers

- Pump-Probe (PP) >10^{17} W/cm^2
  - 0.2–3 mJ, 0.2–4.5 MHz, 15 fs
  - 4–100 mJ, 0.2–4.5 MHz, 800 ps
- High-Intensity (HI) >10^{20} W/cm^2
  - 3 J, 30 fs, 10 Hz on sample
- High-Energy (HE)
  - 100 J, 2–15 ns, 10 Hz
  - ~3x compression, ~10 Mbar

DAC set-up (static compression):

- dynamic and double stage DACs

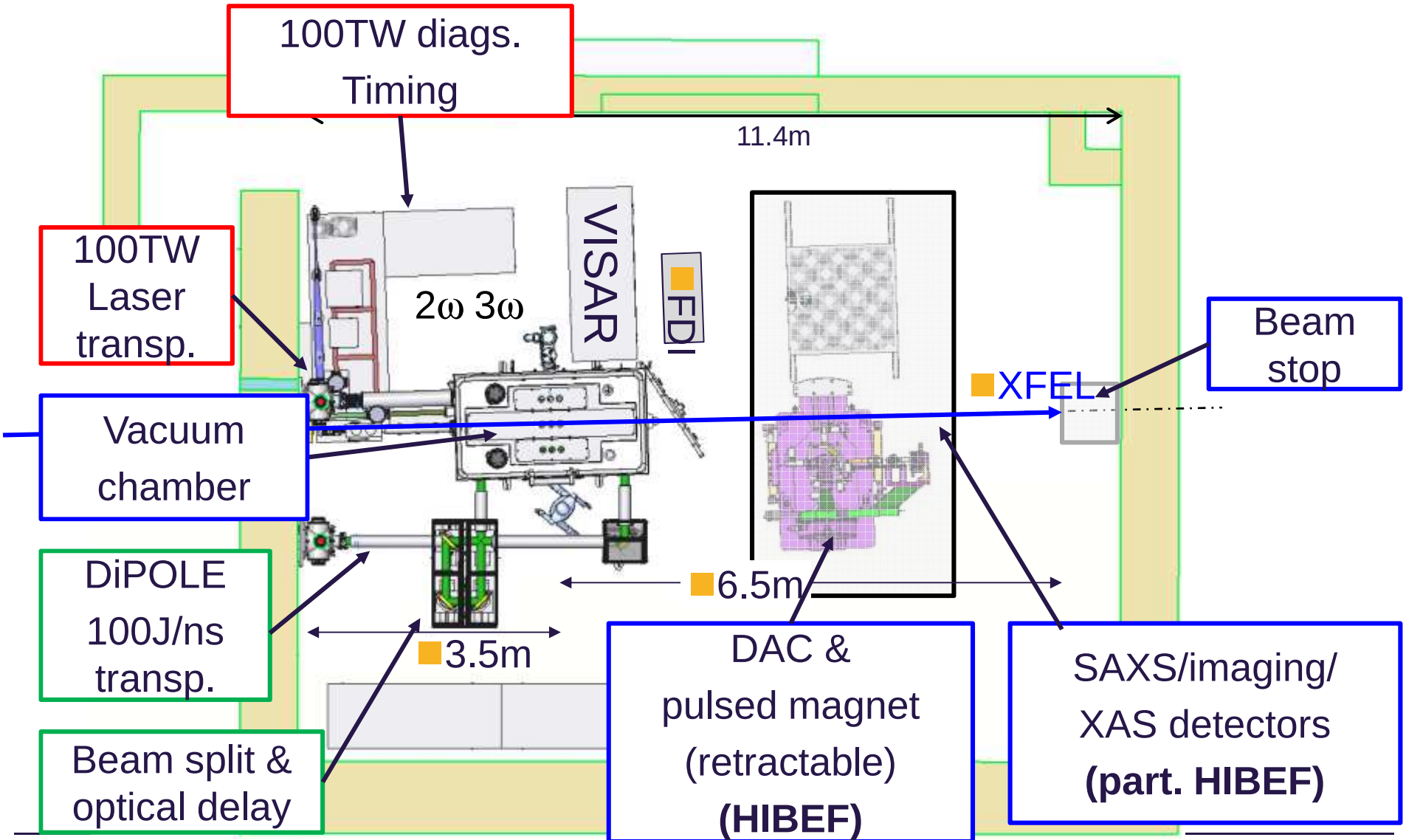
Pulsed magnet

- ~50 Tesla (10 kbar, 1GPa)

Isochoric XFEL heating

- >10^{11} phot, <µm, > 10^{19} W/cm^2

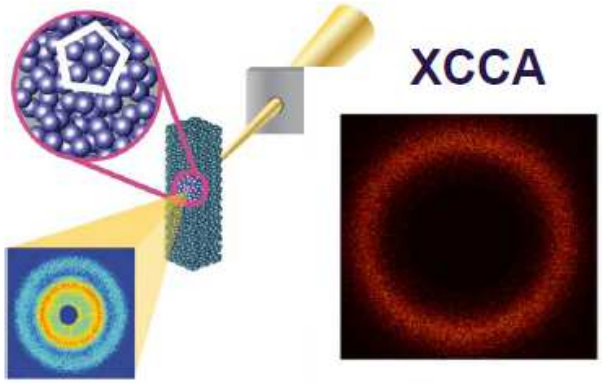
HED Experiment (EXP)



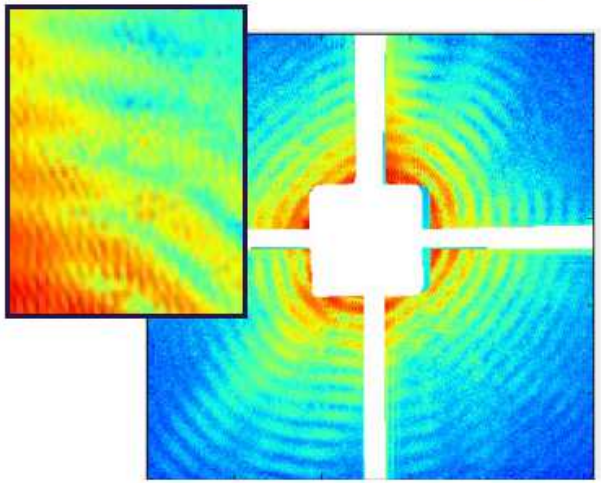
MID Mission (Anders Madsen Group)

The Materials Imaging and Dynamics (MID) instrument aims at the investigation of nanosized **structure** and nanoscale **dynamics** using **coherent radiation**. Applications to a **wide range of materials** from hard to soft condensed matter and biological structures are envisaged

(1st MID workshop, Oct 2009 @ ESRF, Grenoble)

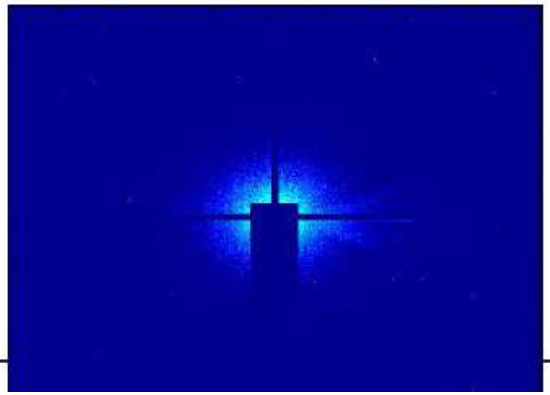


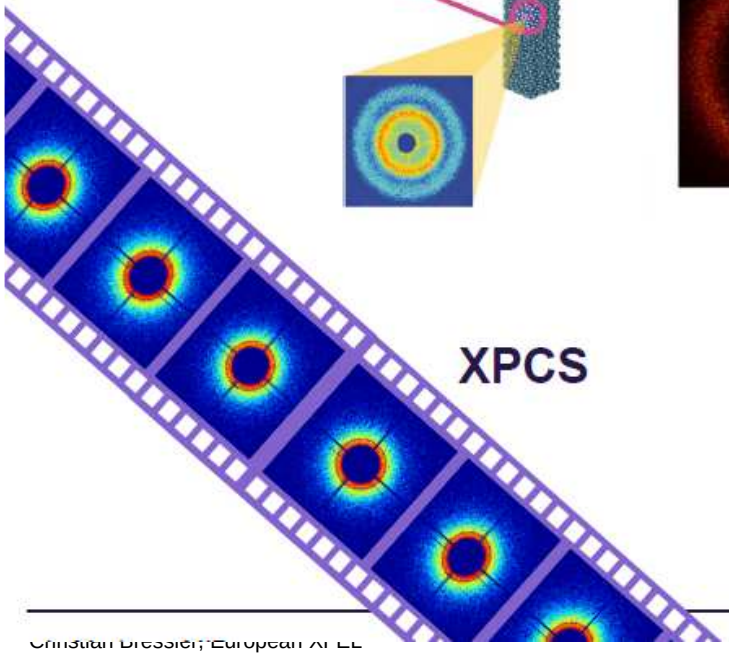
XCCA



X-Ray holography

CDI





XPCS

Hi-res techniques
Self-seeding…

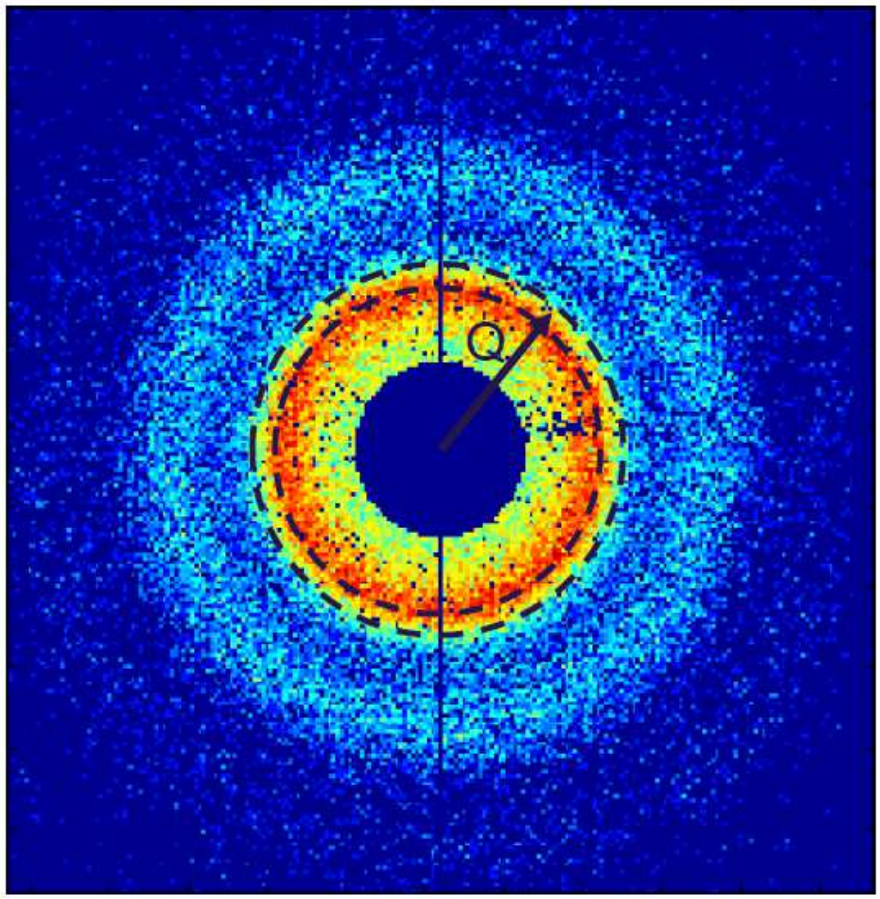
European XFEL

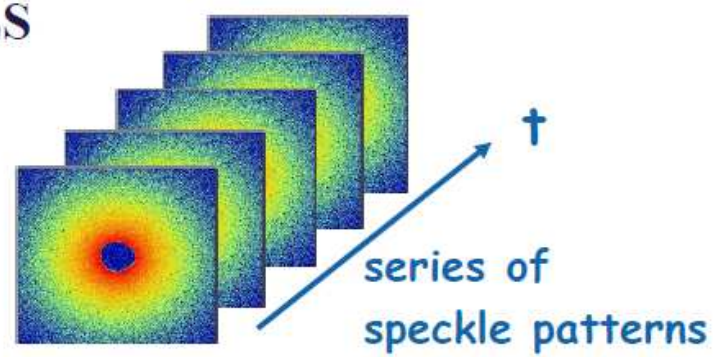
X-Ray Photon Correlation Spectroscopy (XPCS)

ESRF

X-ray version of DLS

Multi-speckle approach





$$g^{(2)}(t_1,t_2)=\frac{\langle I(t_1)I(t_2)\rangle}{\langle I(t_1)\rangle\langle I(t_2)\rangle}$$

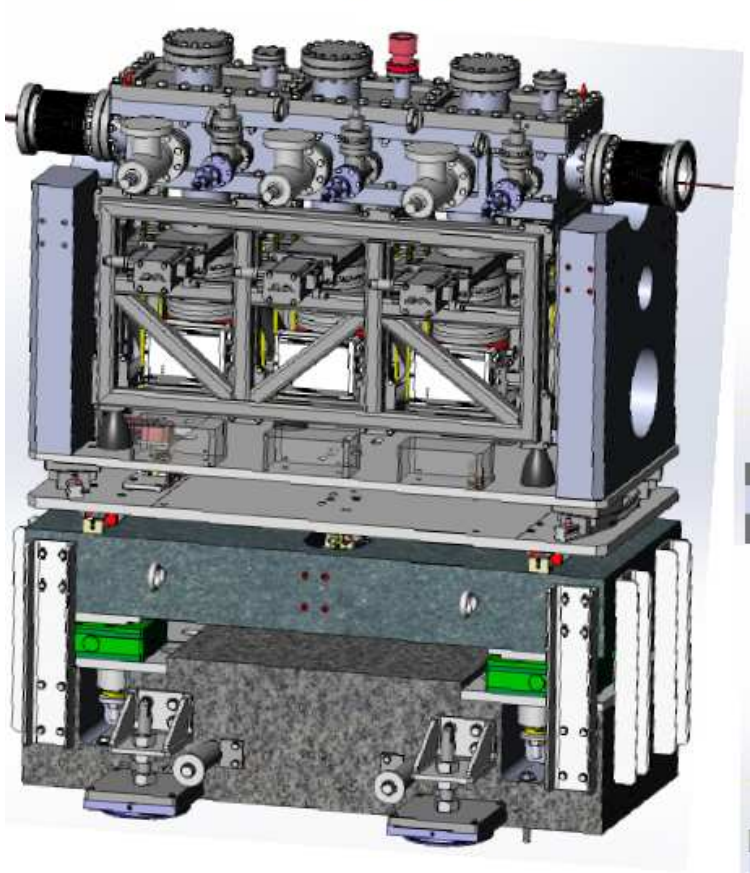
Average over ensemble of pixels (e.g. constant Q region) and/or time

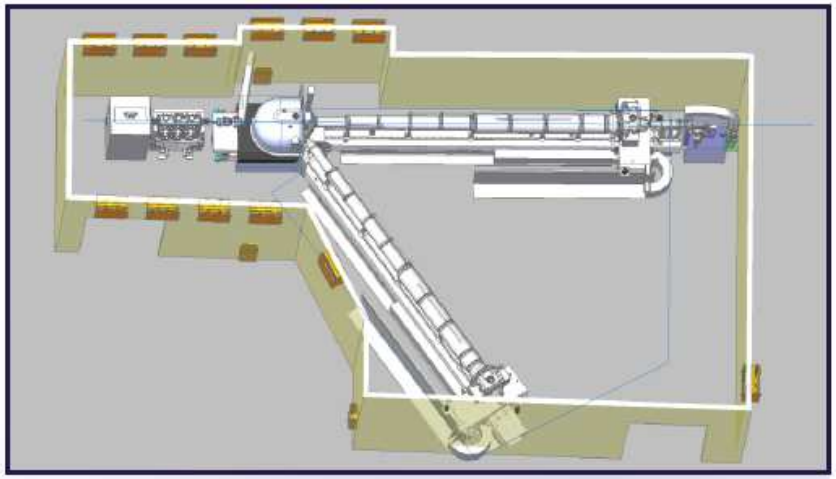
Applications:
Study of structural dynamics
in soft- and hard condensed matter

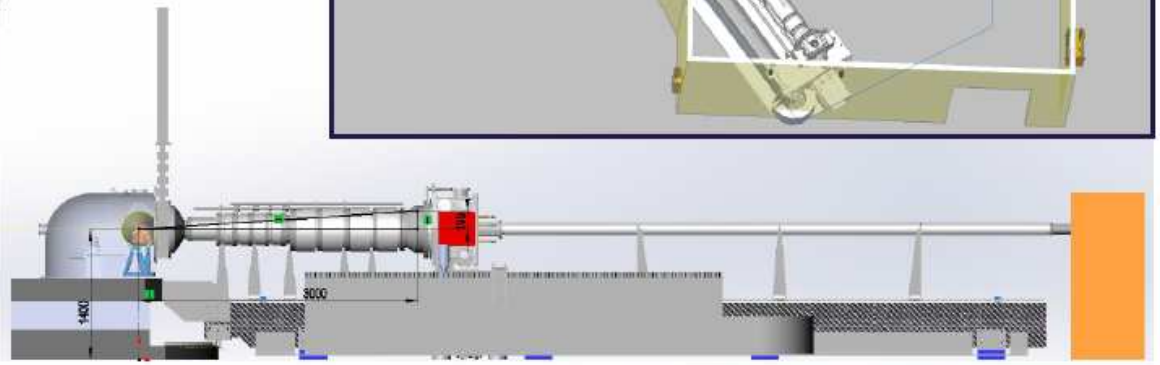
A. Madsen *et al.*,
New Journal of Physics **12**, 055001 (2010)

Design of MID Components

Differential pumping section







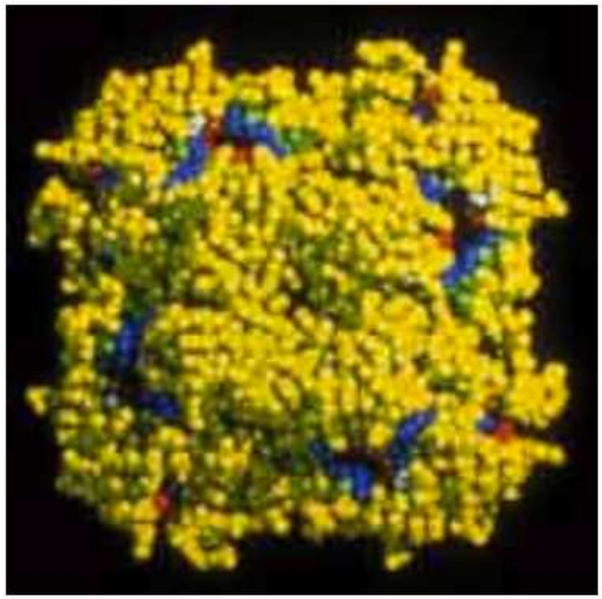
Side-view, exp. chamber and long arm

Diff. pump section out for tender

Finalize 3D models of chamber/arm/detector stand by summer 2015

SPB Mission: Image *single* biomolecules (Adrian Mancuso group)

- Structure of a molecule -> function
- Structure allows, eg, Rational Drug Design, Understanding of human biochemistry.
- Photons (X-rays) allow depth information from intact systems.
- Single Particle Imaging seeks to image molecules and structures that are *unable to be imaged by other means*. These are structures < microns in size and include membrane proteins.



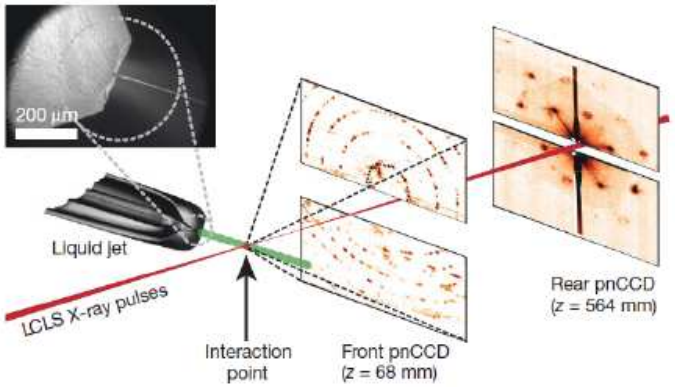
Influenza virus structure - A protein from the influenza virus

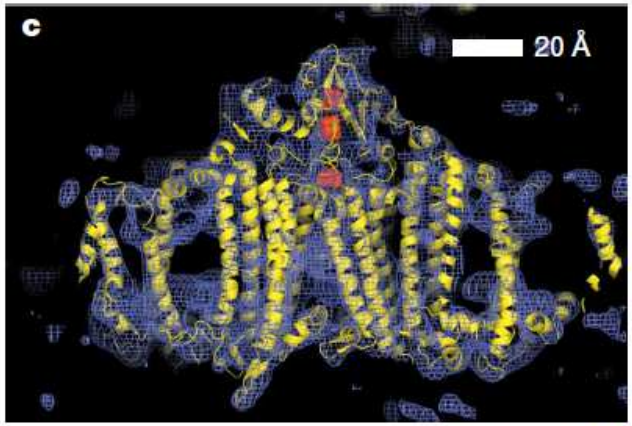
Image: J. Varghese et al, CSIRO Health Sciences & Nutrition

Review: A. P. Mancuso, *et al*, J. Biotechnol. **149** (2010) 229–237

Nanocrystallography: between single molecules (SPB) and everyday crystallography (→ SFX)

- Extends the scope of XFEL imaging (i.e. class of possible samples broader than macromolecular crystallography)
- Has first been demonstrated at LCLS, USA (Chapman, et al., Nature, 2011)
- The measurement shown required > 3 million LCLS pulses (~1 day)
- The European XFEL will produce that many pulses in about 2 min





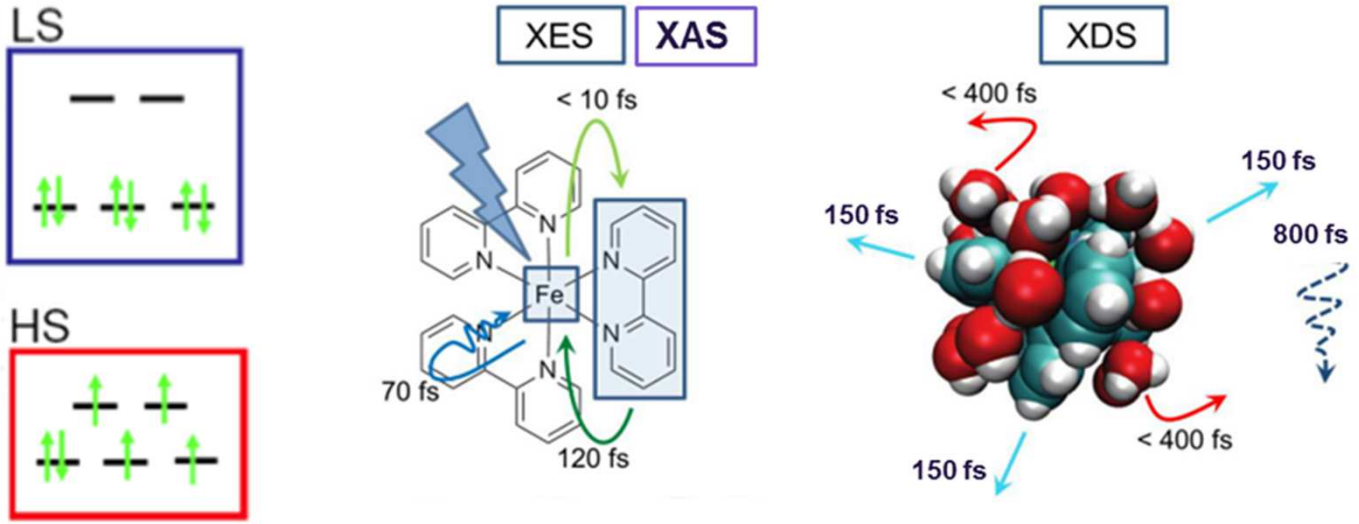
Chapman et al., Nature, 2011

- FEL Nanocrystallography perhaps opens crystallography to a broader range of samples that form small, but not larger, crystals

FXE: Towards a High Speed Molecular Camera
Christian Bressler and FXE Group

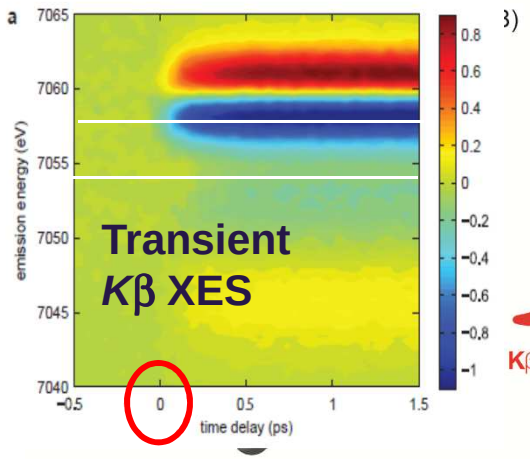
GOAL:

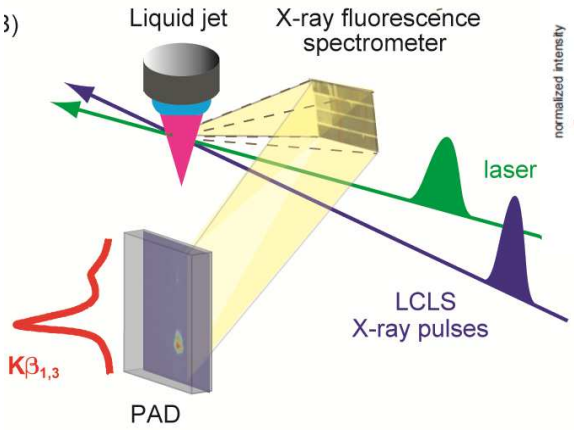
Record a Movie with a Suite of *Simultaneous* Smart Cameras:

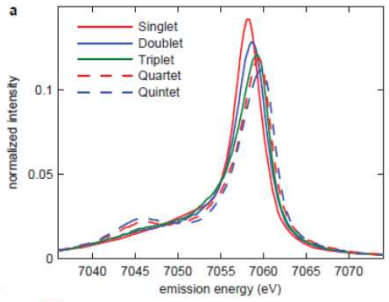


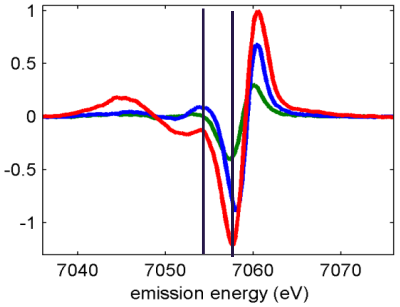
- Camera for electronic orbital changes
- Camera for spin state changes
- Camera for internal structural changes
- Camera for involved external molecular interactions

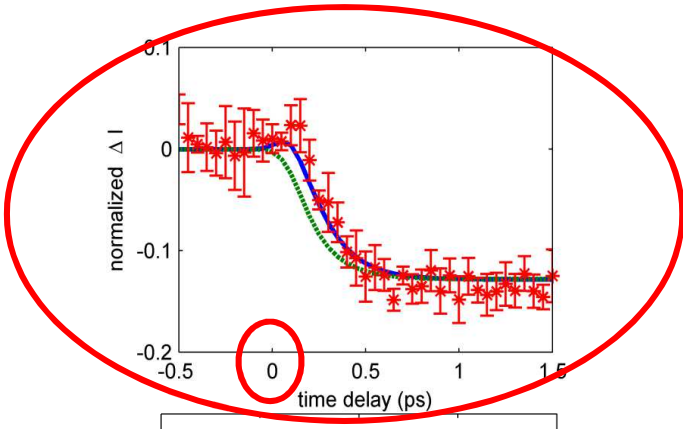
Femtosecond Kβ XES on $[Fe(bpy)_3]^{2+}$: First Observation of Intermediate State

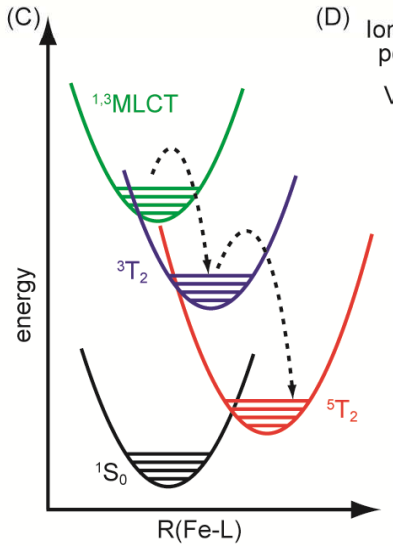


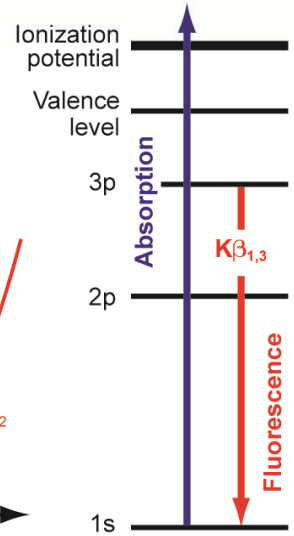


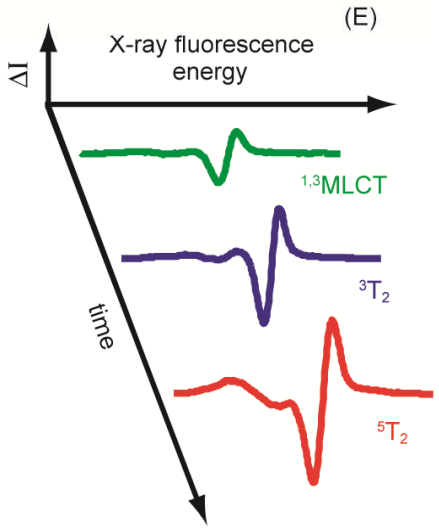


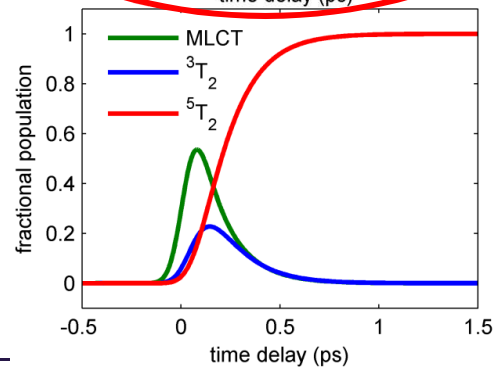








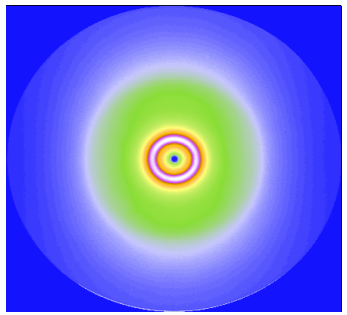




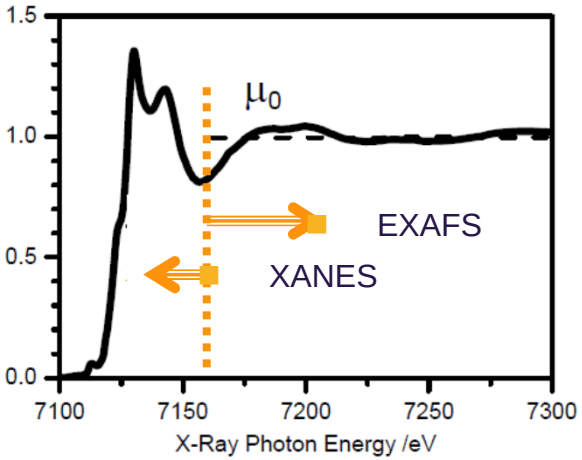
W. Zhang *et al.*, Nature 509, 345 (2014)

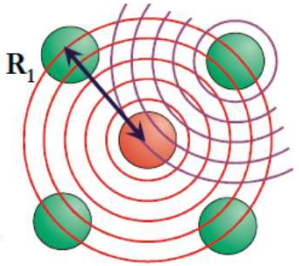
Combination of x-ray techniques: added value!

- X-ray diffraction (XRD)
  - atomic positions
  - lattice vibrations (acc- & opt. phonons)
  - long/short-range order

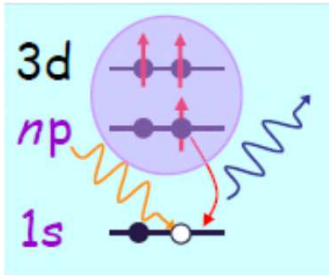


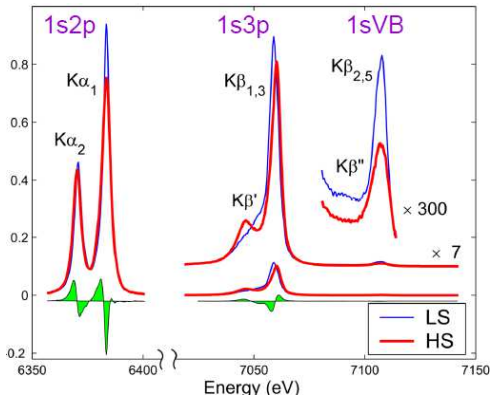
- **X-ray absorption (XAS)**
  - empty states (DOS)
  - local symmetry
  - bond length /neighbours
  - short-range order





- **X-ray emission (XES)**
  - sensitivity to fine structure of excited electronic states
  - e.g. spin states

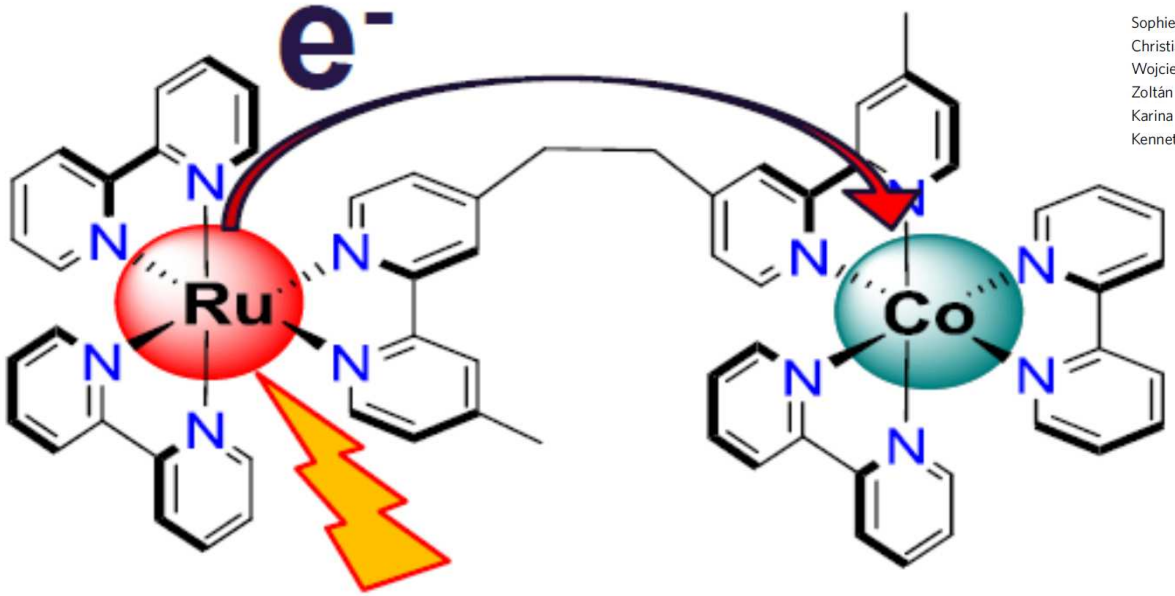




European XFEL

A model complex: observe the invisible

- Photo-excited electron transfer in metallo-complexes
  - Ru(II) → Ru (III) XAS, XES, optical
  - Co(III) → Co (II) XAS, XES, optical
  - IVR & e^- transport XRD, optical
  - Co (II) HS → LS XAS, XES



ARTICLE
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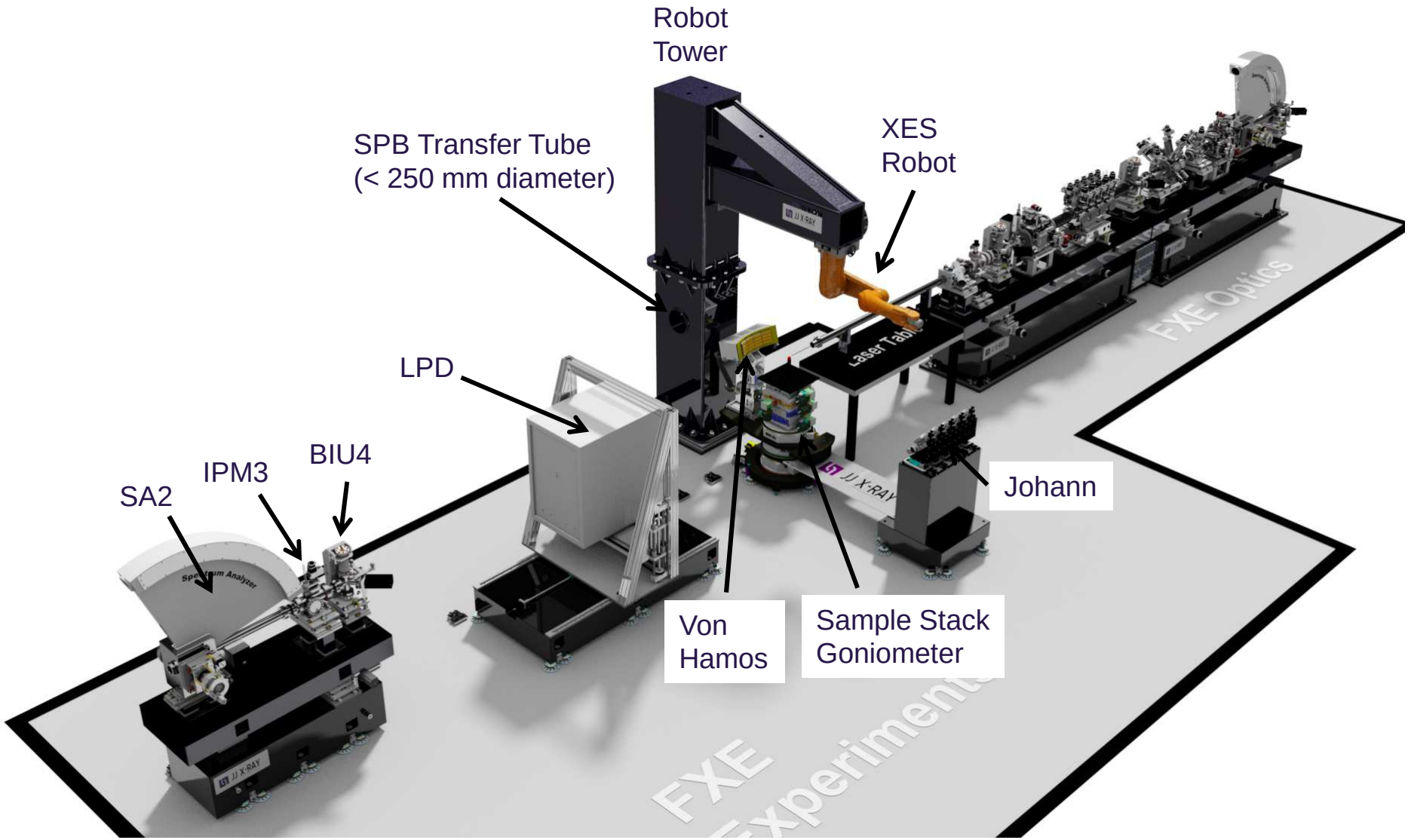
DOI: 10.1038/ncomms7359 OPEN

Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses

Sophie E. Canton[1,*], Kasper S. Kjær[2,3,*], György Vankó[4], Tim B. van Driel[3], Shin-ichi Adachi[5], Amélie Bordage[4,†], Christian Bressler[6], Pavel Chabera[7], Morten Christensen[3], Asmus O. Dohn[8], Andreas Galler[6], Wojciech Gawelda[6], David Gosztola[9], Kristoffer Haldrup[3], Tobias Harlang[7], Yizhu Liu[10], Klaus B. Møller[8], Zoltán Németh[4], Shunsuke Nozawa[5], Mátyás Pápai[4], Tokushi Sato[5,†], Takahiro Sato[11,†], Karina Suarez-Alcantara[1,†], Tadashi Togashi[12], Kensuke Tono[12], Jens Uhlig[7], Dimali A. Vithanage[7], Kenneth Wärnmark[10], Makina Yabashi[11], Jianxin Zhang[10,†], Villy Sundström[7] & Martin M. Nielsen[3]

FXE Instrument: A Suite of Molecular High-Speed Cameras



The European XFEL
Covering several contemporary research fields

Hard X-rays

SPB/SFX: Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules

Structure determination of single particles: atomic clusters, bio-molecules, virus particles, cells.

MID: Materials Imaging & Dynamics

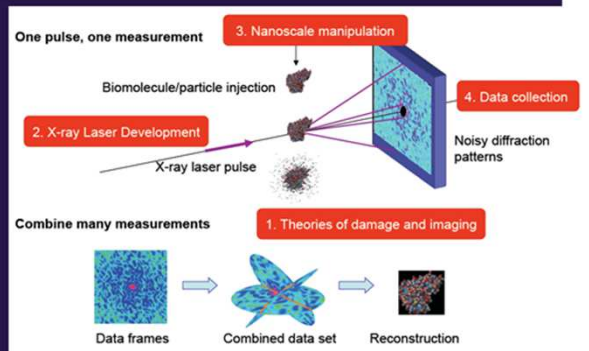
Structure determination of nano-devices and dynamics at the nanoscale.

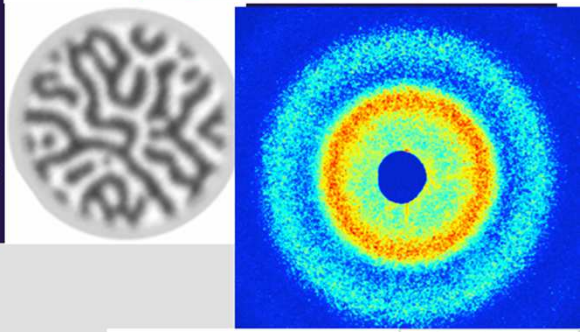
FXE: Femtosecond X-ray Experiments

Time-resolved investigations of the dynamics of solids, liquids, gases

HED: High Energy Density Matter

Investigation of matter under extreme conditions using hard X-ray FEL radiation, e.g. probing dense plasmas





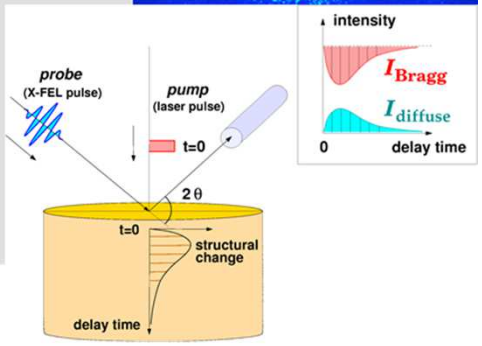
Soft x-rays

SQS: Small Quantum Systems

Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena

SCS: Soft x-ray Coherent Scattering/Spectroscopy

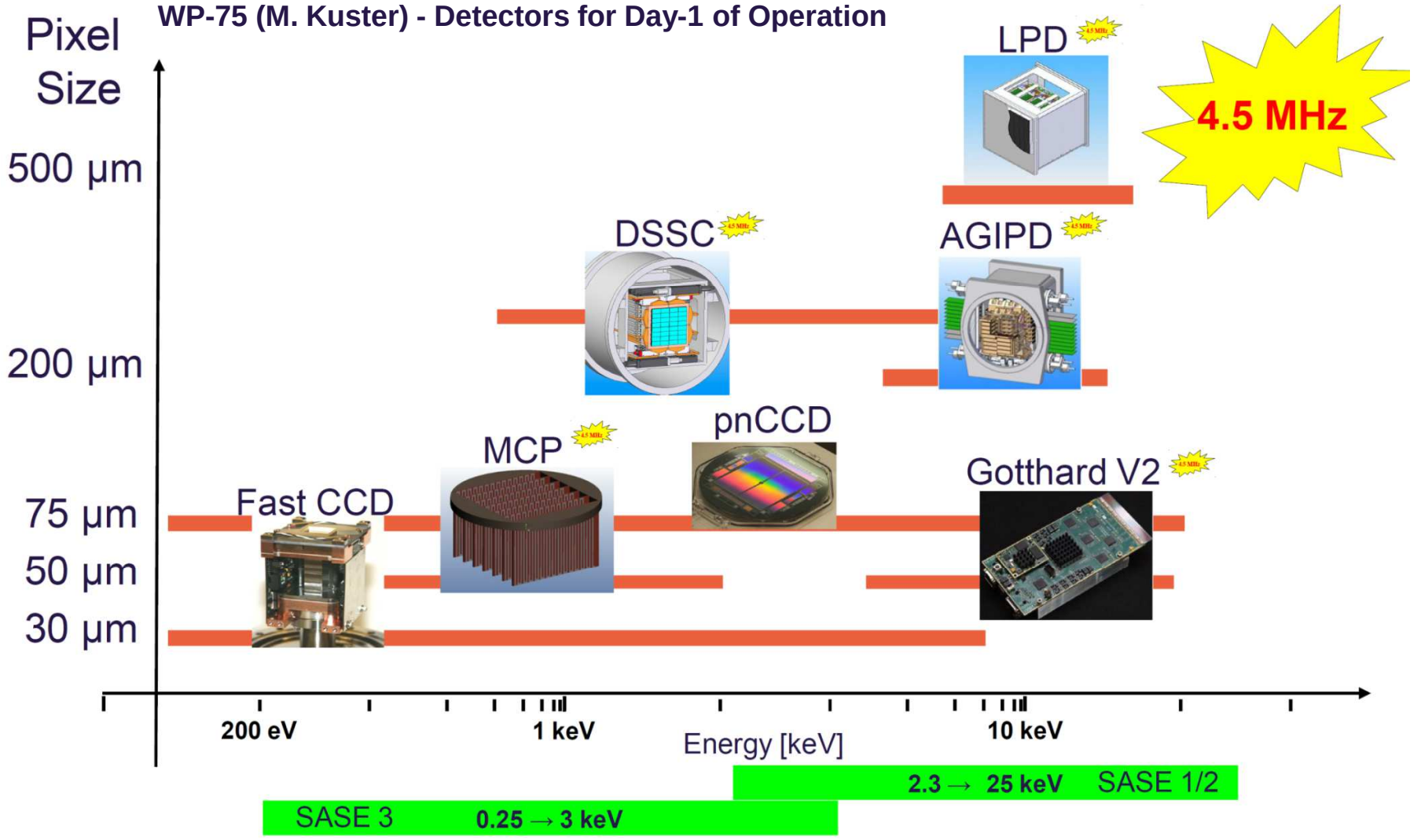
Electronic and real structure, dynamics of nano-systems and of non-reproducible biological objects



Six “day-one” scientific instruments

(SPB/SFX: Mancuso, MID: Madsen, FXE: Bressler, HED: Zastrau, SQS: Meyer, SCS: Scherz)

The European XFEL
Several Detector Projects Well Underway



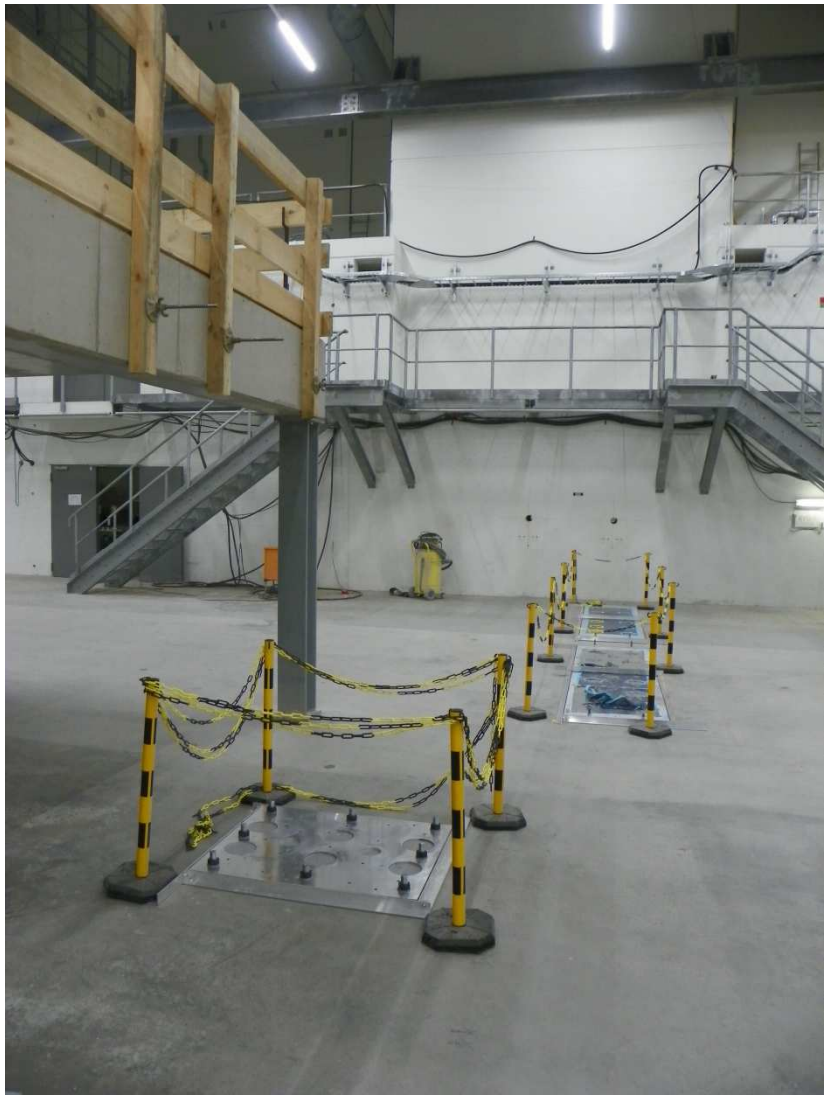
European XFEL

FXE Heavy Equipment (Aug. 5 installation)

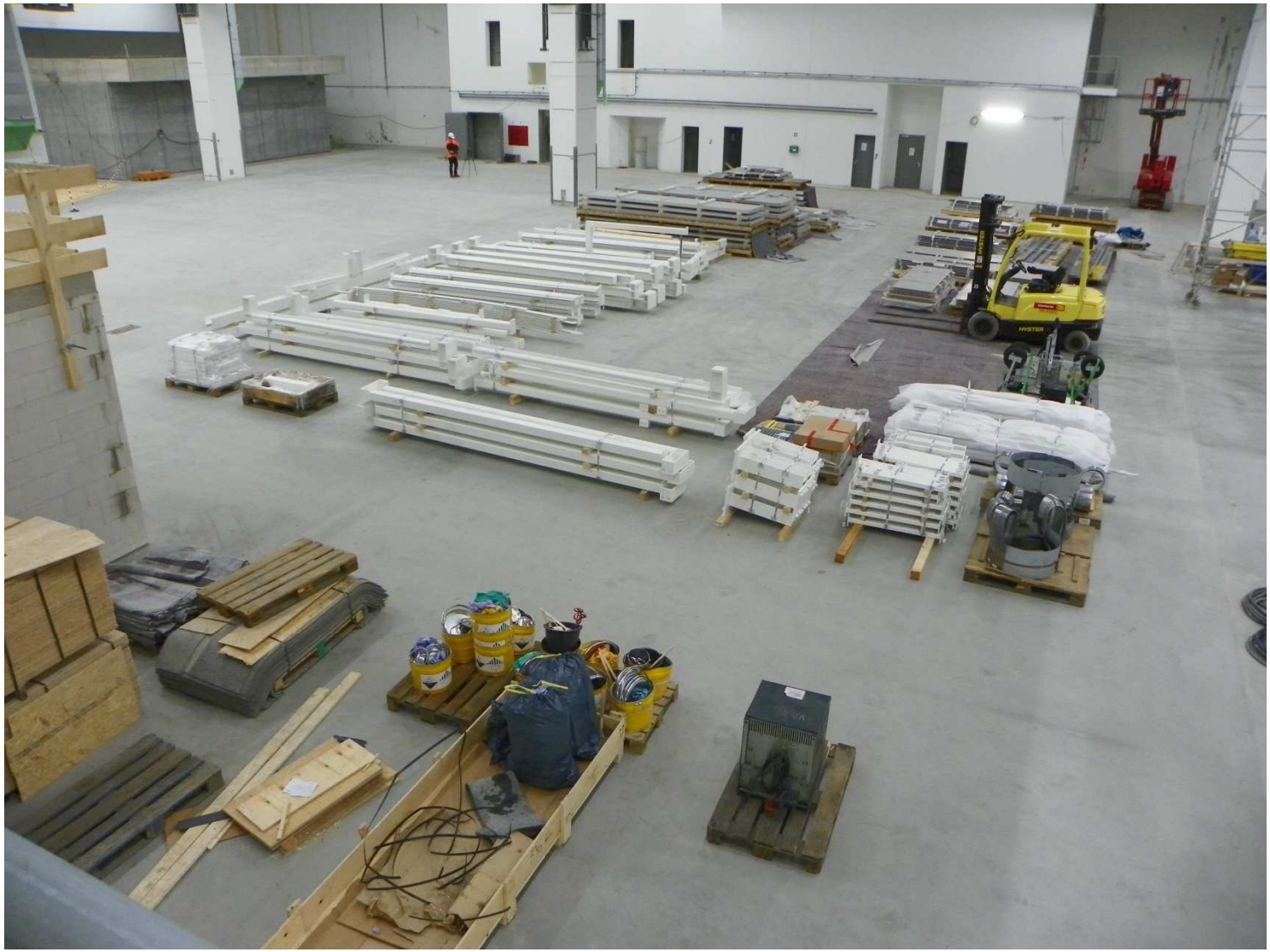
European XFEL

9.6.2015: Laser hutches mostly done

24.6.: FXE-supports of robot tower + granite tables grouted.



29.6.: Pontax + Berdel got parts for SPB-experimental hutch delivered.

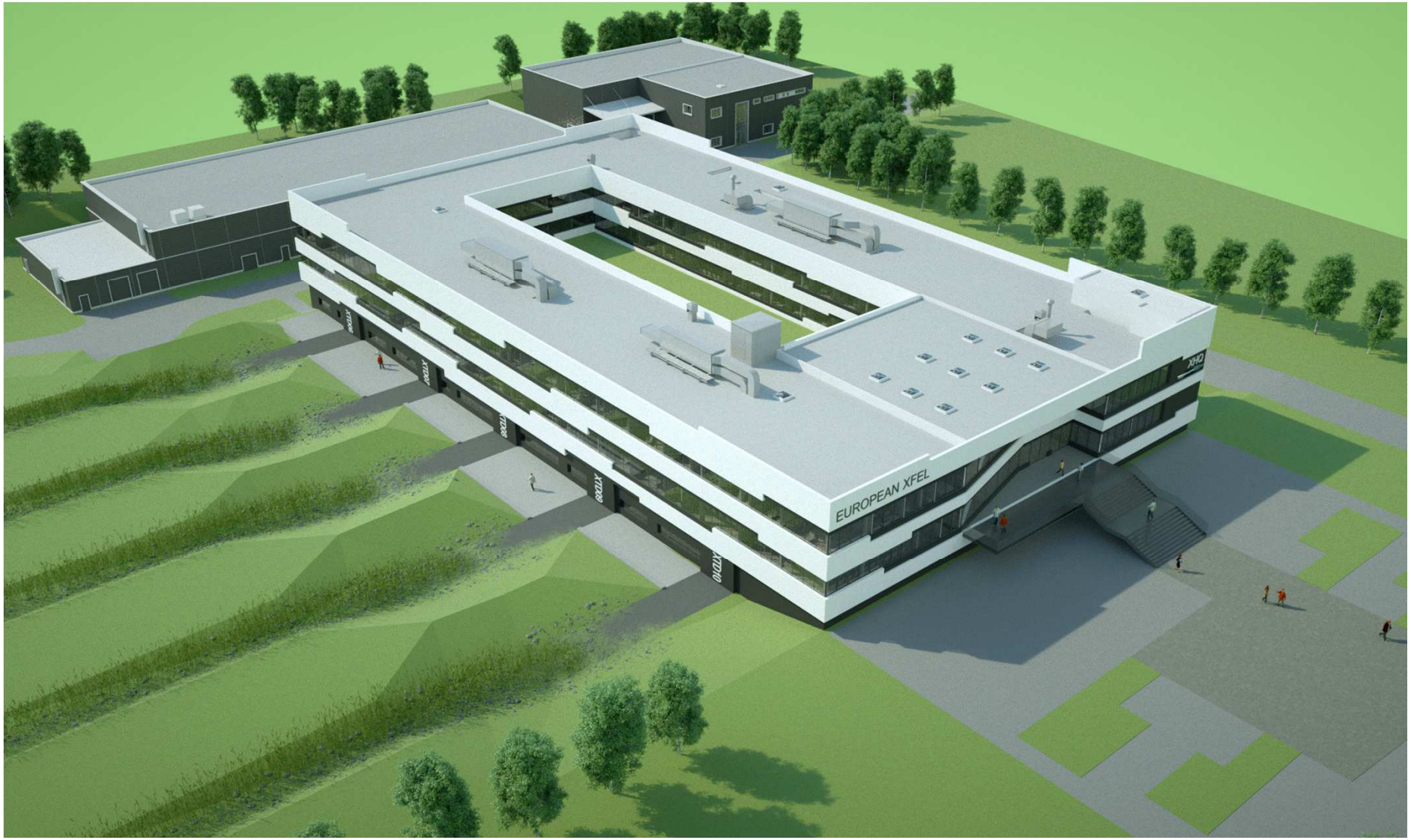


European XFEL

24.6.: MID-high quality floor was covered

European XFEL

XHQ building, construction started May 2014



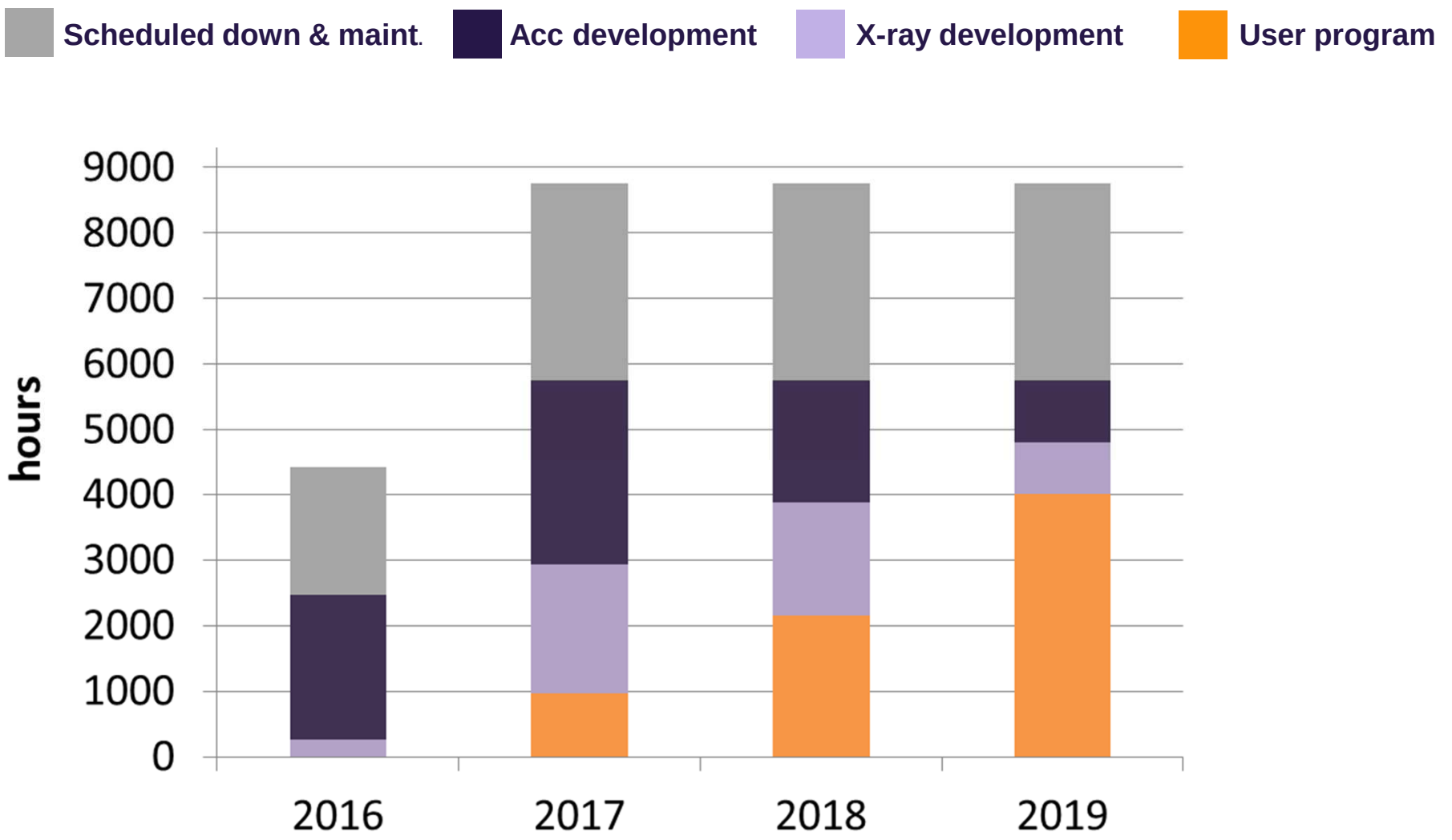
European XFEL

XHQ building, Jan. 2015

European XFEL

Coming soon: Users at the European XFEL!

This means…


Scheduled down & maint.
Acc development
X-ray development
User program
hours
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
2016
2017
2018
2019

…thank you for your attention!