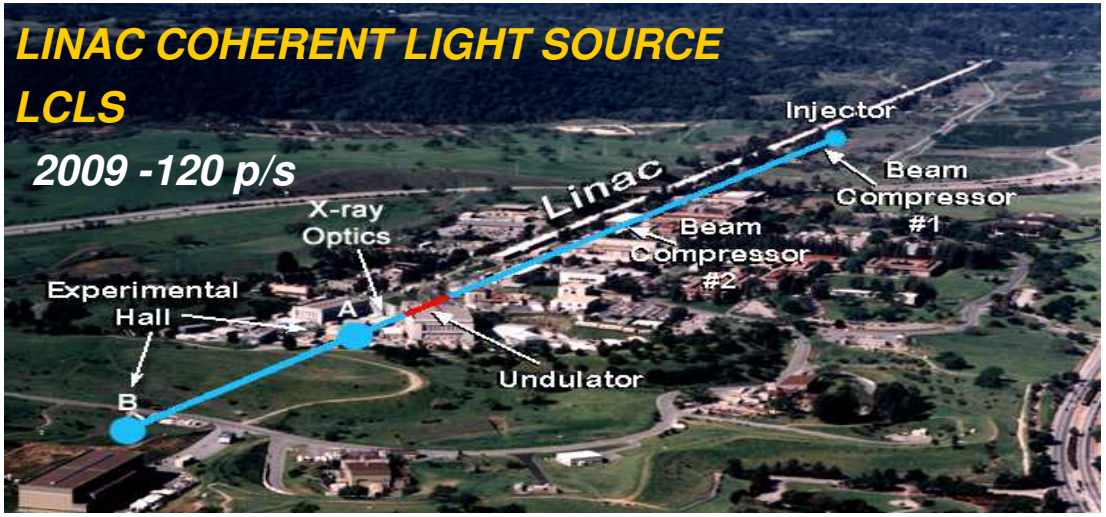
User Experiments at European XFEL

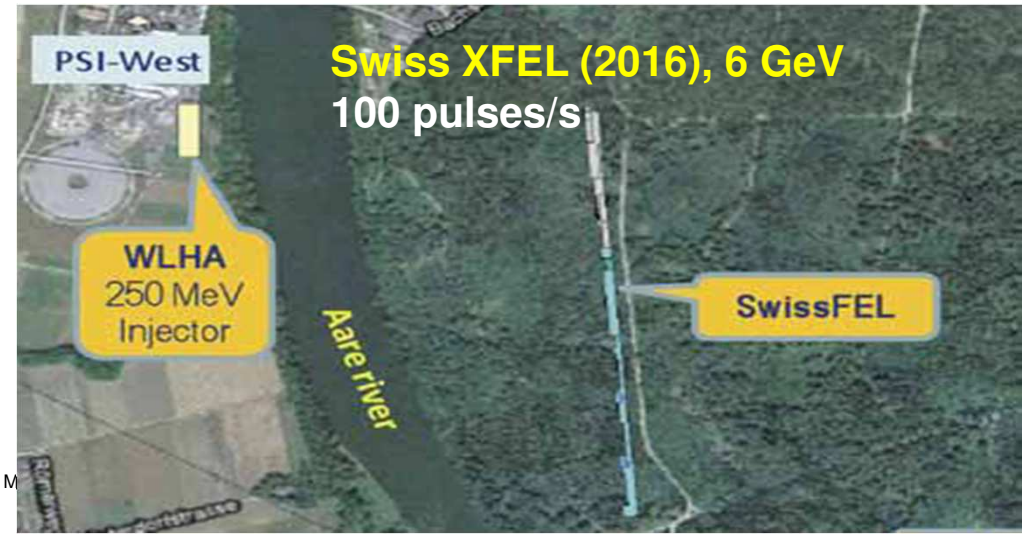
Christian Bressler

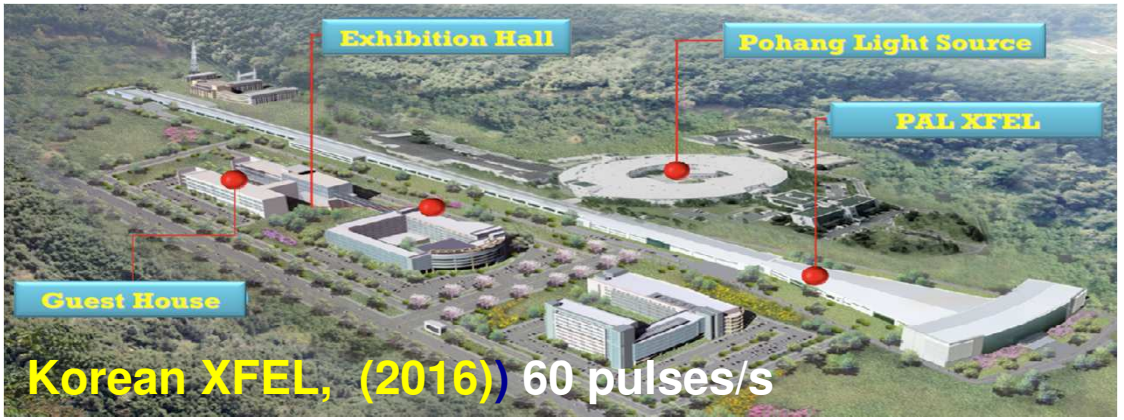
Feb 13, 2020

Beschleuniger-Betriebsseminar 2020

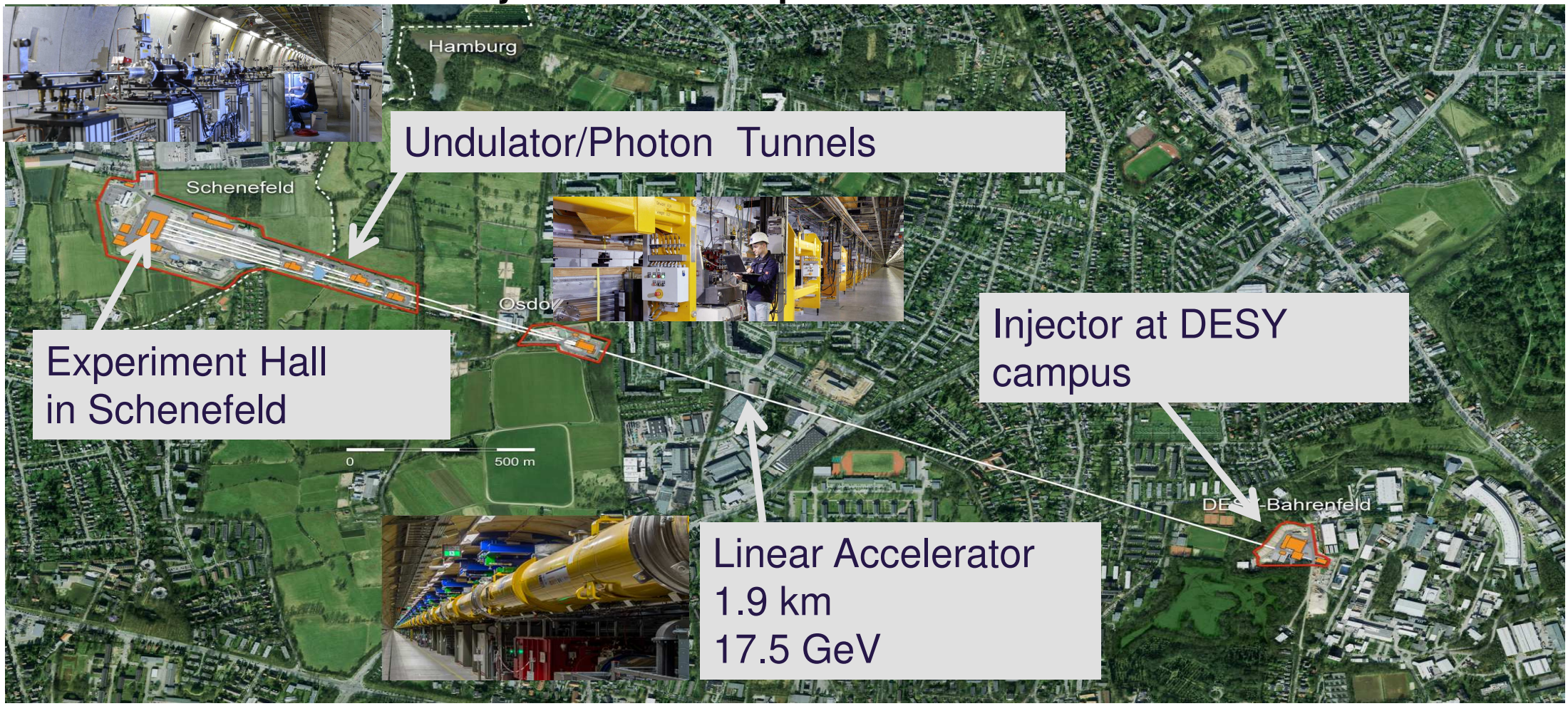
The European XFEL in the International Context : Hard X-ray FELS



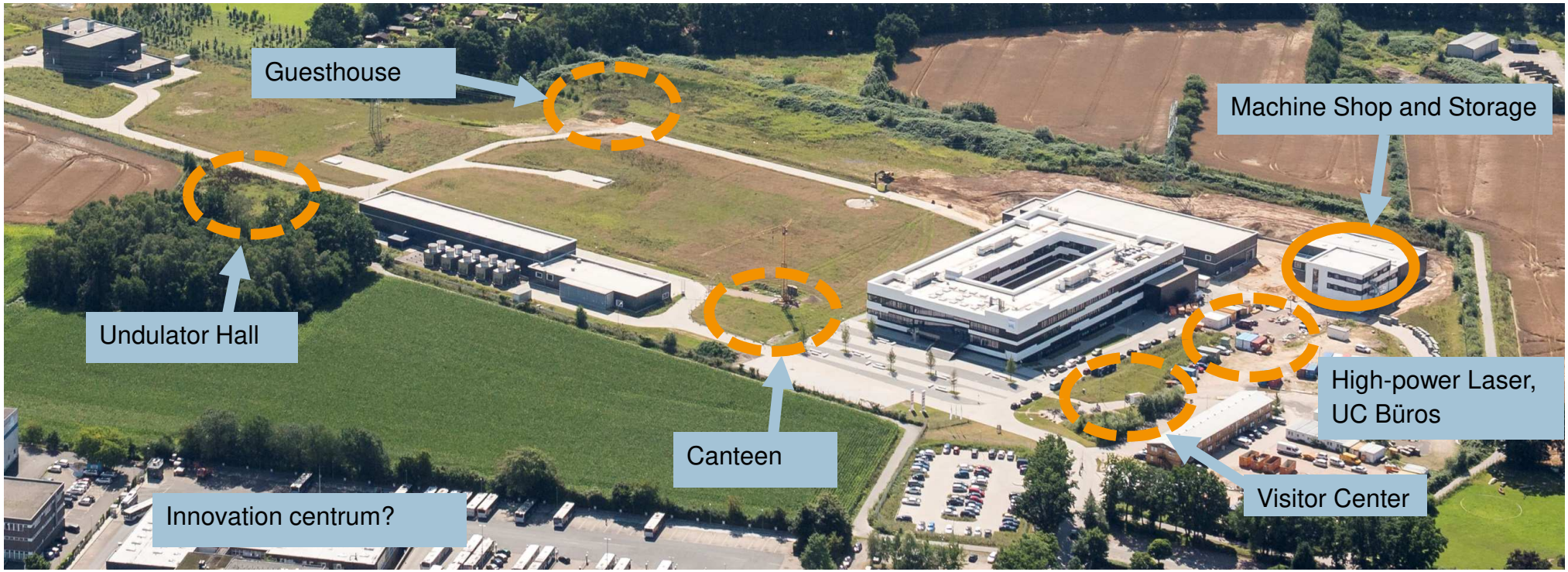




General layout of the European XFEL



Campus Schenefeld including planned Canteen und Guesthouse



Six Scientific instruments

SASE1

FXE (Femtosecond X-ray Experiments)

- Ultrafast dynamics of liquids and solid matter
- Combination of spec. & scat. techniques

SPB/SFX (Single Part., Bioimaging, & SFX)

- Coherent diffraction imaging from single part.
- Serial fs nano-crystallography

Team: A. Mancuso et al. / **SFX UC** (H. Chapman et al.)

SASE2

MID (Materials Imaging & Dynamics)

- CDI from nano-structured samples
- XPCS of nanoscale dynamics

Team: A. Madsen et al.

HED (High Energy Density science)

- Ultrafast dynamics of highly excited matter
- Combinations of scattering, diff. & spectroscopy

Team: U. Zastrau et al. / **HiBEF UC** (T. Cowan et al.)

SASE3

SQS (Small Quantum Systems)

- Ultrafast dynamics of atoms, ions & clusters
- Combination of spec. & coh. scat. techniques

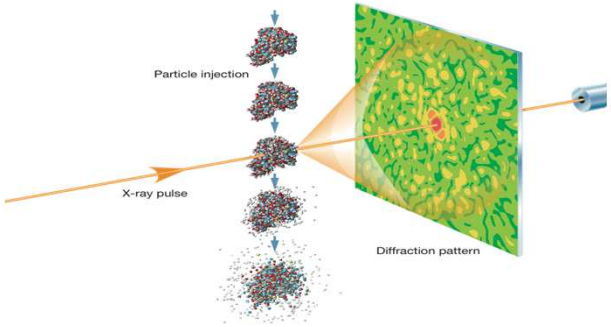
Team: M. Meyer et al.

SCS (Spectroscopy & Coherent Scattering)

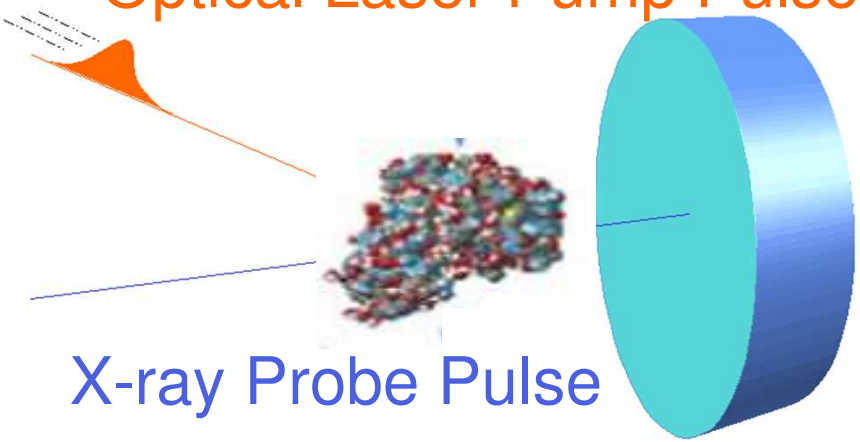
- Ultrafast dynamics of complex solids
- Combination of hr-inelastic spec. & coh.scattering

Team: A. Scherz et al. / **hRIXS** UC (A. Föhlisch et al.)

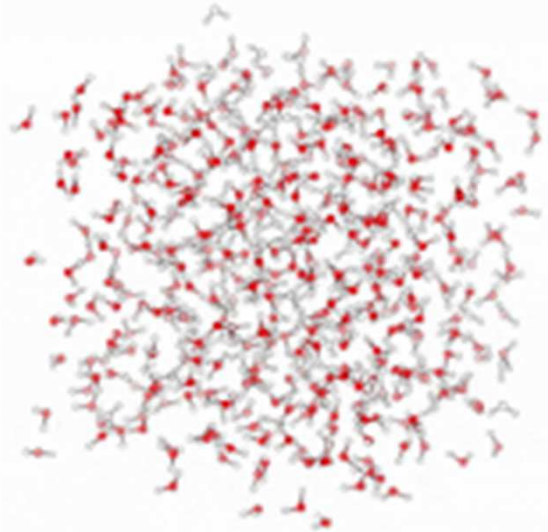
Science Case : Making Molecular Movies

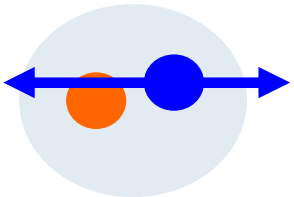


Optical Laser Pump Pulse

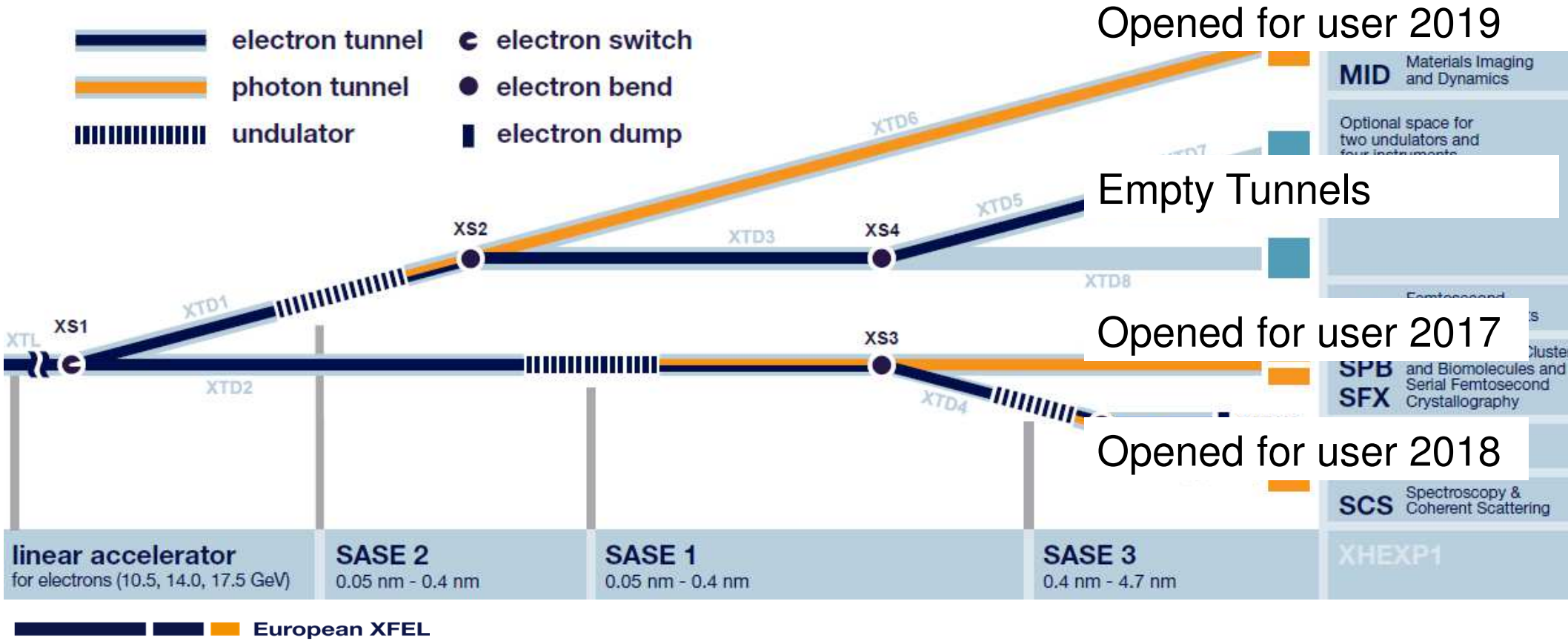


X-ray Probe Pulse

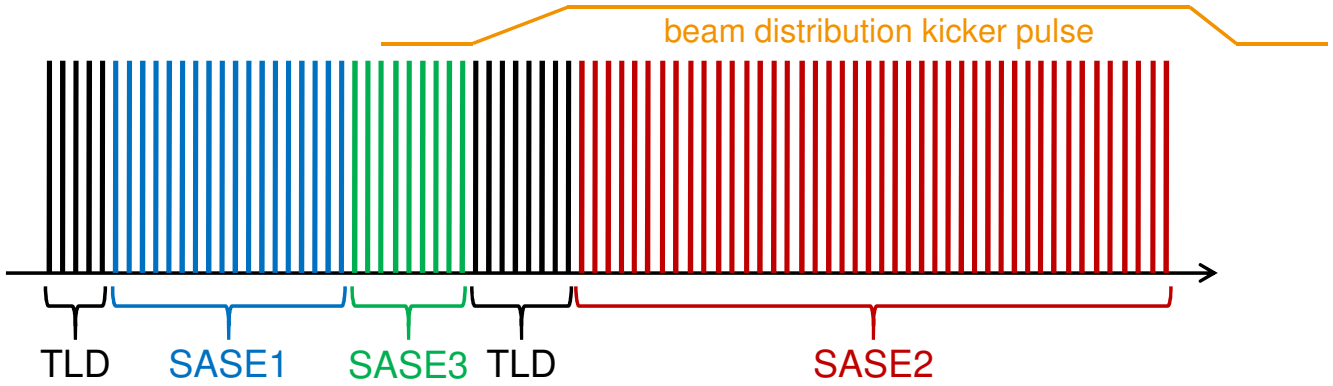


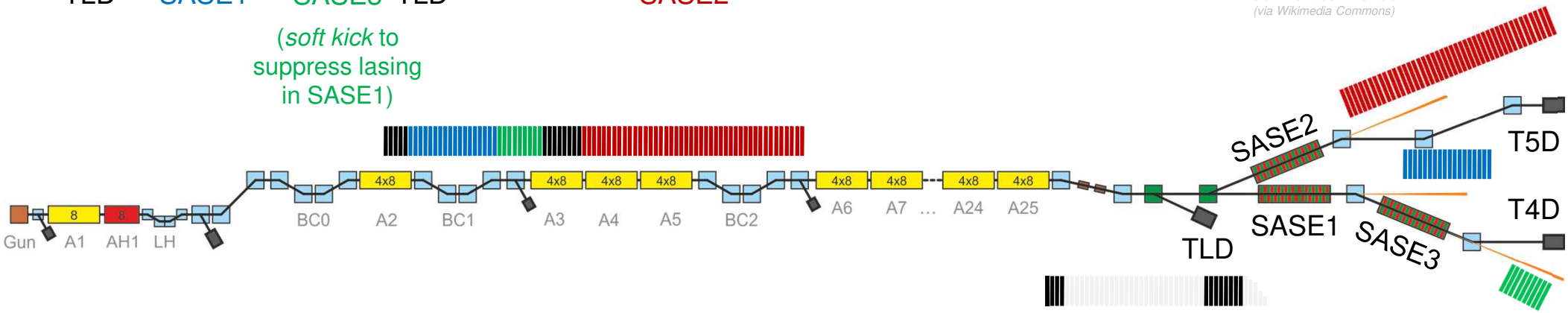


Experimental Hall



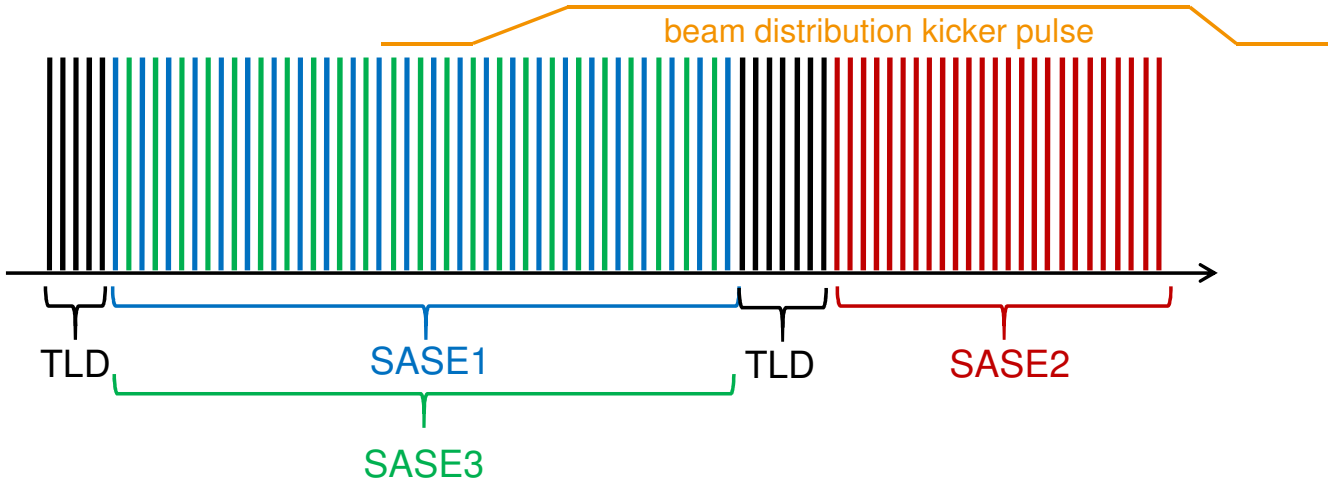
A Possible Bunch Pattern for User Operation

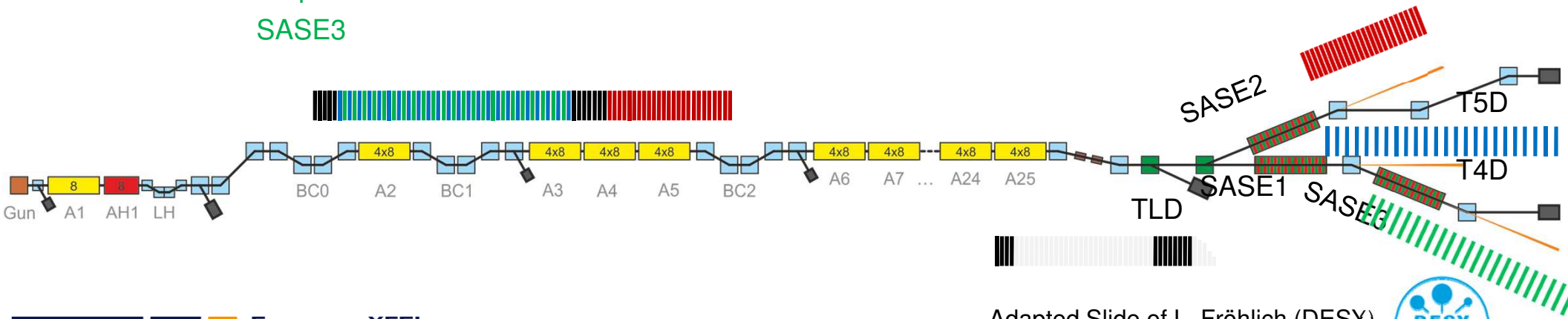




Slide by L. Fröhlich (DESY)

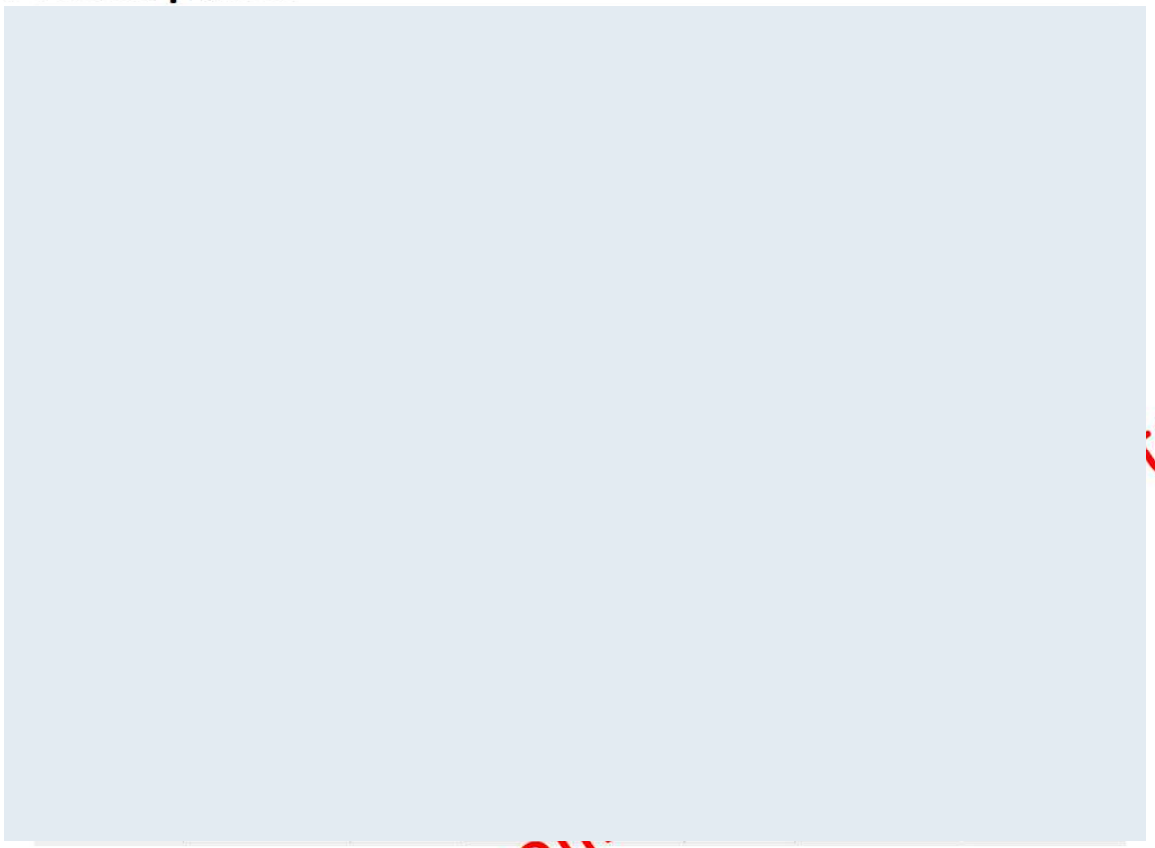
Interleaved (2.25 MHz) Bunch Pattern for 1.1 MHz at each SASE





Adapted Slide of L. Fröhlich (DESY)

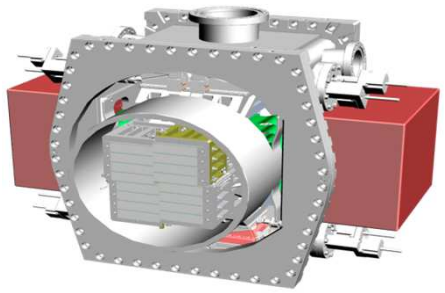
Self-seeded pulses



Following try: 9keV with 1eV BW (FWHM), up to 200 uJ

European XFEL Fast 2D Imagers

Adaptive Gain Integrating Pixel De-tector (AGIPD)



4.5 MHz

Energy Range 3 – 13 (25) keV

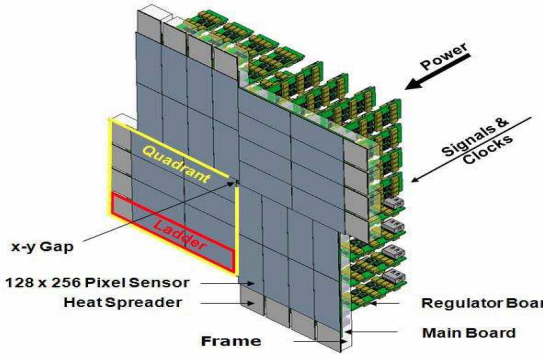
Dynamic Range 10^4 ph/px/pulse@12 keV

Single Photon Sens. Yes

Memory ≈380 images

Pixel Size 200 × 200 µm²

MiniSDD Sensor with Signal Compres-sion (DSSC)



4.5 MHz

Energy Range 0.5 – 6 (25) keV

Dynamic Range ≈100 ph/px/pulse@1 keV

Single Photon Sens. No

Memory ≈800 images

Pixel Size 236 × 236 µm²

Large Pixel Detector (LPD)

4.5 MHz

Energy Range 3 – 13 (25) keV

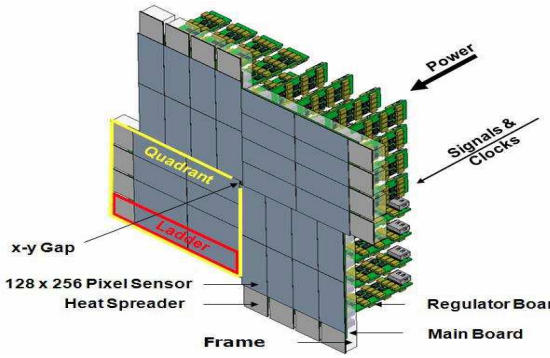
Dynamic Range 10^5 ph/px/pulse@12 keV

Single Photon Sens. Yes

Memory ≈512 images

Pixel Size 500 × 500 µm²

DePFET Sensor with Signal Compres-sion (DSSC)



4.5 MHz

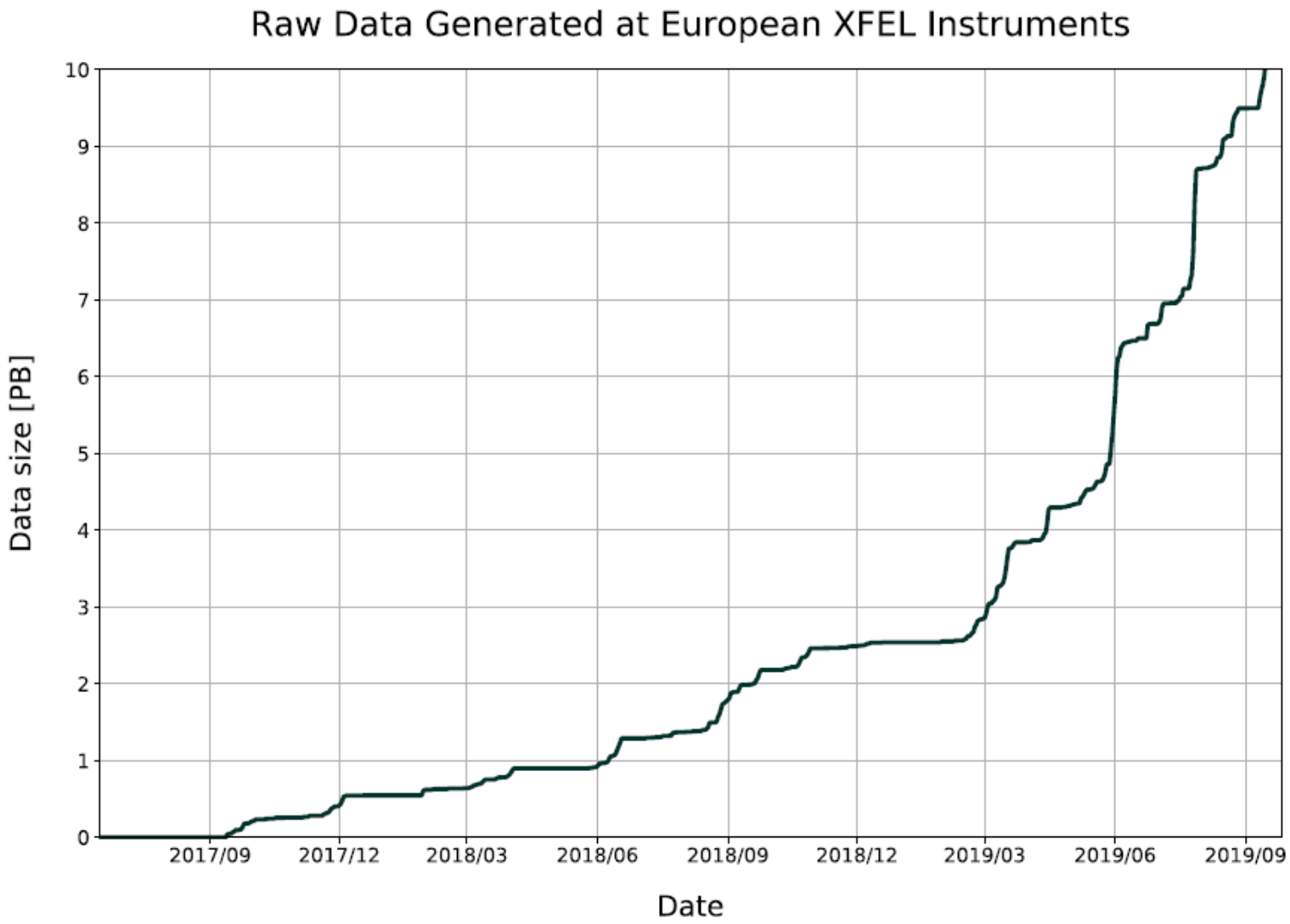
Energy Range 0.5 – 6 (25) keV

Dynamic Range 6000 ph/px/pulse@1 keV

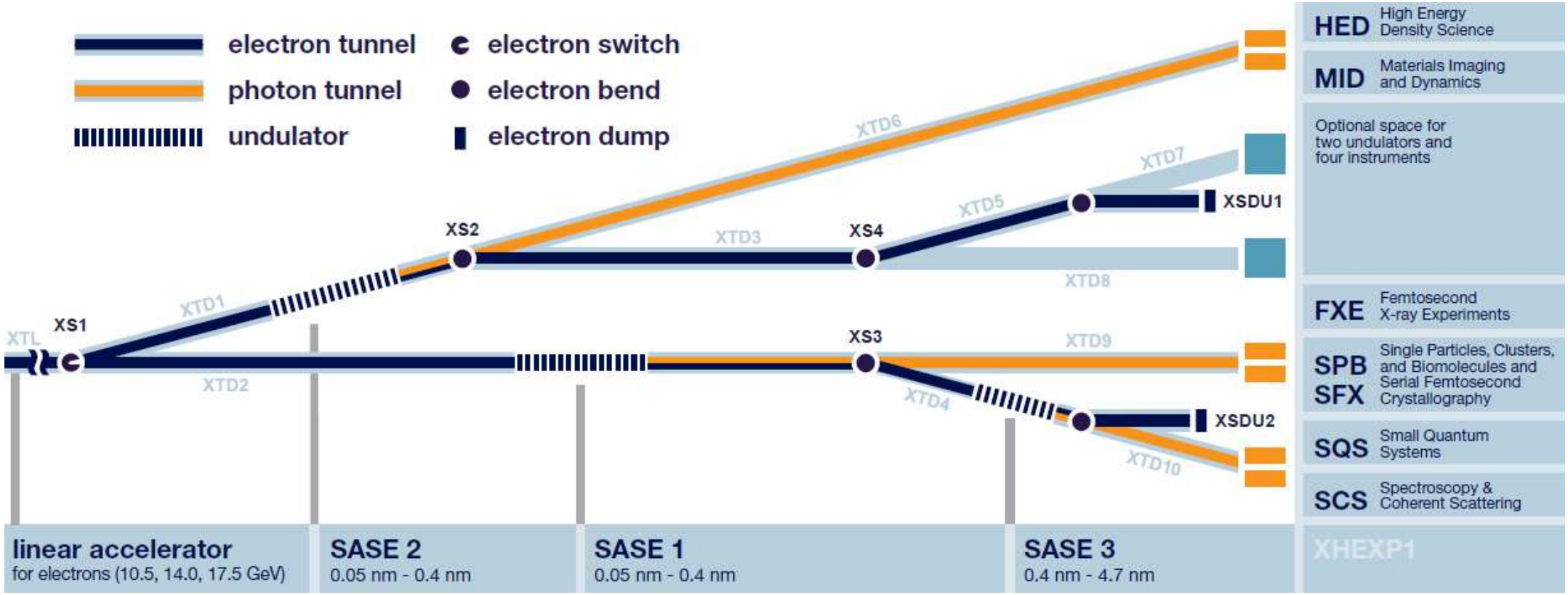
Single Photon Sens. Yes

Memory ≈800 images

Pixel Size 236 × 236 µm²


Raw Data Generated at European XFEL Instruments
Data size [PB]
0
1
2
3
4
5
6
7
8
9
10
2017/09
2017/12
2018/03
2018/06
2018/09
2018/12
2019/03
2019/06
2019/09
Date

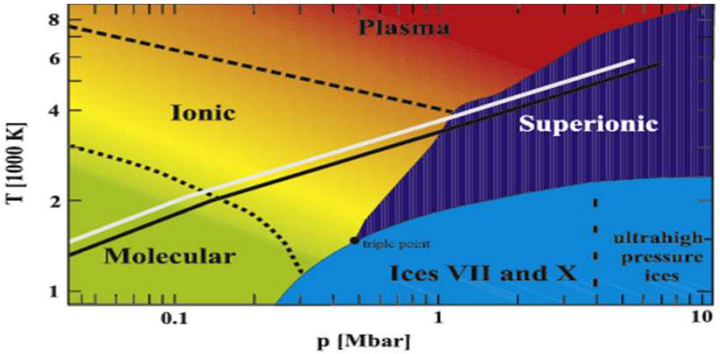
Experimental Hall



HED

Lab astrophysics informs understanding of planetary interiors, their evolution, and abundance

Experiment refines a phase diagram (here: of water)

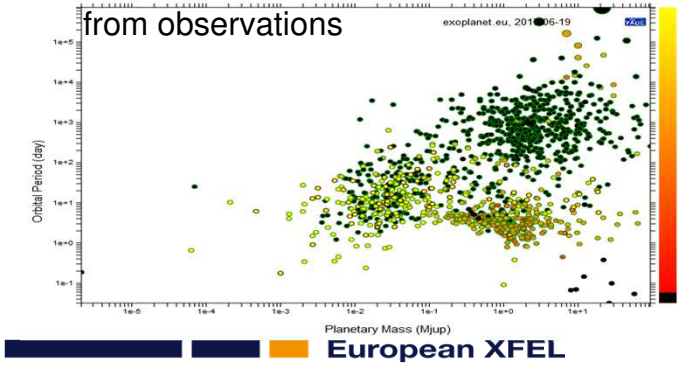


Models of planetary interiors

Redmer et al., Icarus 211 (2011)

Planet forming and evolution

Help constrain parameters from observations



Condensed Matter <> **Warm Dense Matter** <> Hot Dense Matter

$E_{therm} \sim E_{Fermi}$

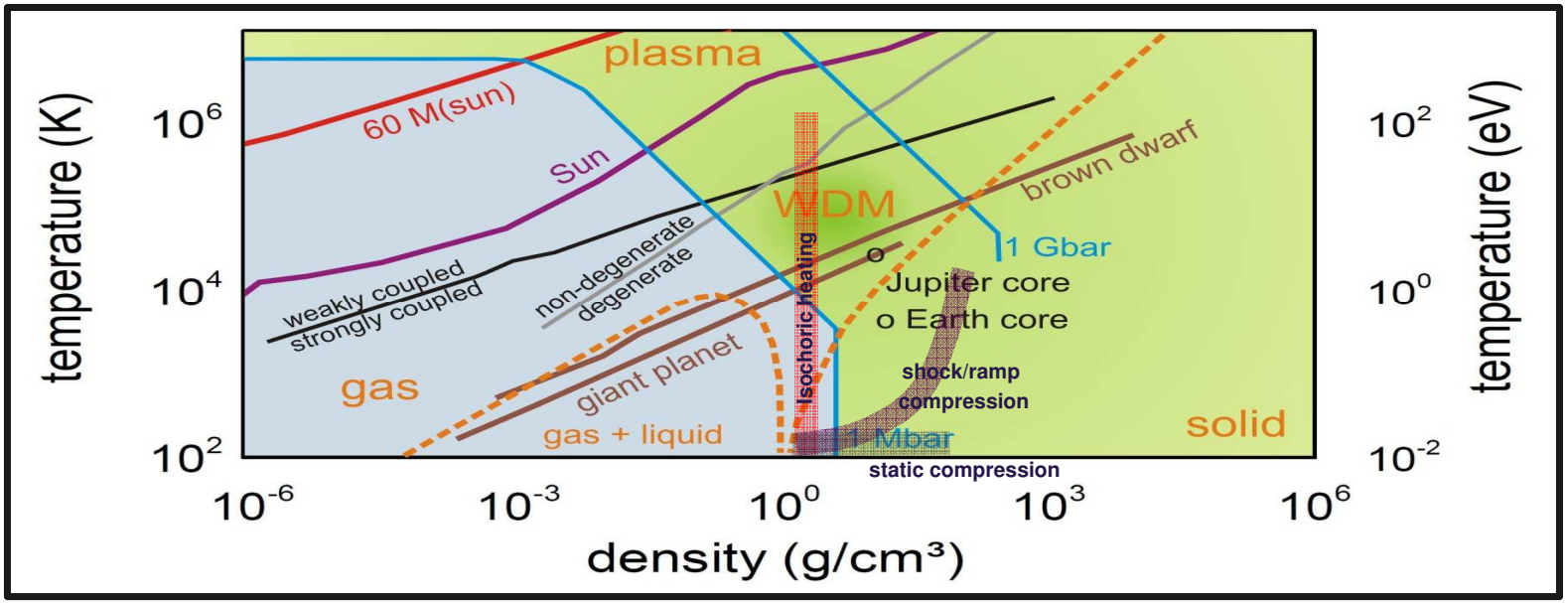
1..100 eV

$\rho_{WDM} \approx \rho_{solid}$

strong coupling

$\Gamma \geq 1$

$E_{coulomb} \sim E_{therm}$

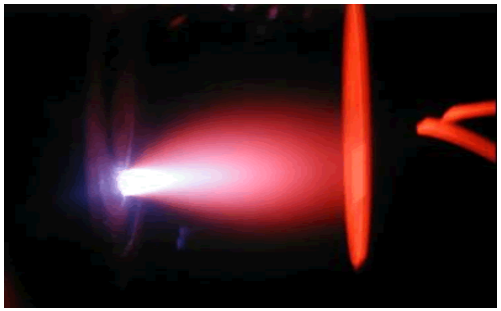


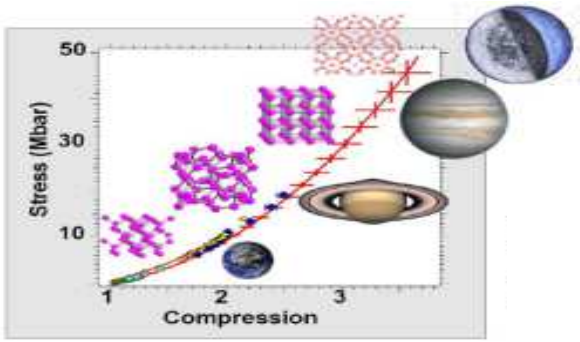
High free-electron density: penetration only up to critical density $n_c = \omega^2 \varepsilon_0 m/e^2$

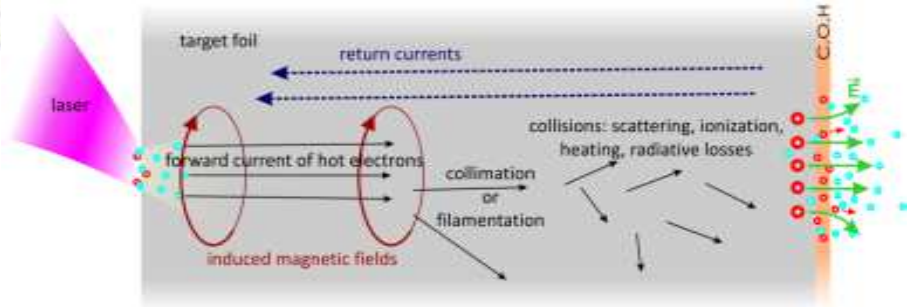
→ access to volumetric plasma parameters
only by short wavelength radiation ($\omega > \omega_P$)

High-Energy Density instrument / Ulf Zastrau

- 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)







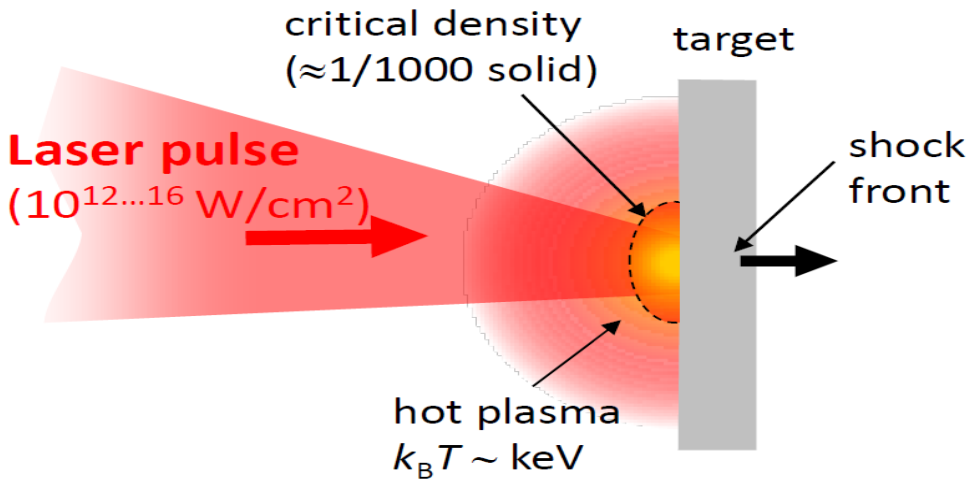
- Combination of high excitation with various X-ray techniques
  - Use of **various pump sources**: optical laser, XFEL, B-fields (60 T pulsed)
  - **Various X-ray probe techniques**: XRD, SAXS, XRTS, hrIXS, XI, XAS….

Direct laser ablation produces high pressures

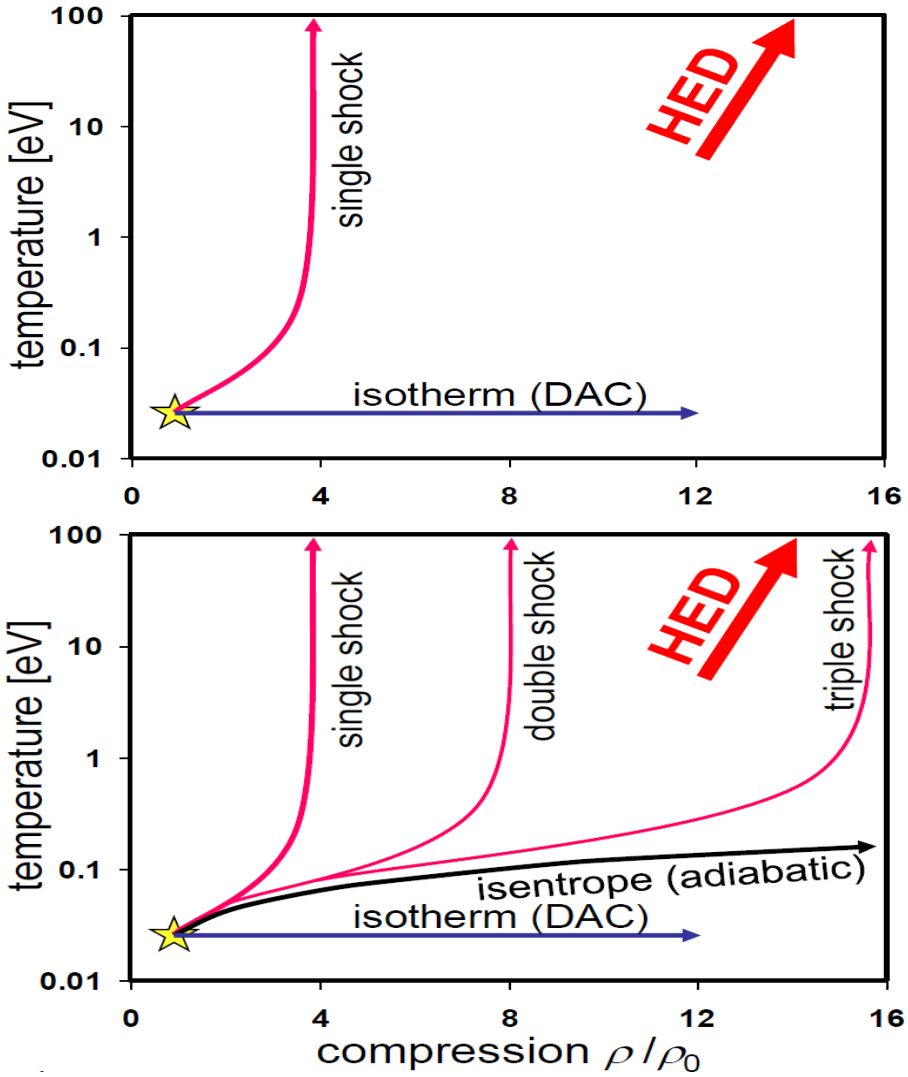
Laser radiation focused to high intensities

- Intensity $10^{12...16}$ W/cm^2

→efficient collisional absorption

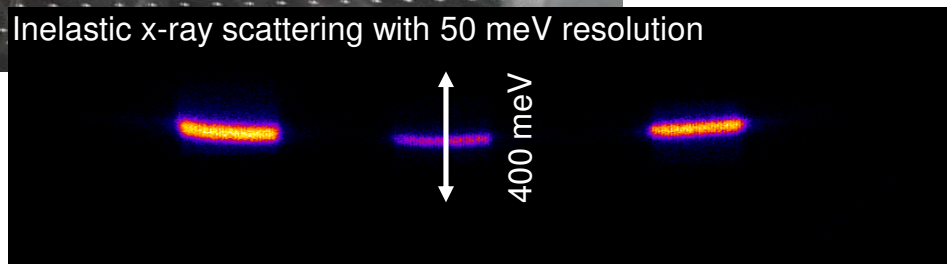


Direct laser ablation
→ pressure up to 50Mbar!



Successful first user experiment (May 15-19)

Resolving low-frequency structural dynamics (Gregori/Zastrau)



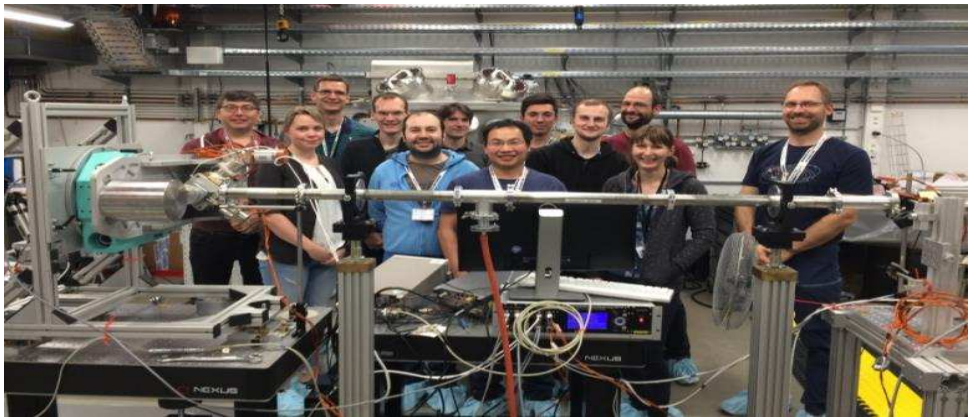
Successful first user experiment (15th – 19th May)

Resolving low-frequency structural dynamics (Gregori/Zastrau)

Community Proposal

U Oxford (UK), U Trento (IT)
U Jena, EuXFEL (Germany)
LLNL, SLAC (US), and others

Happy users at HED in 2019



Status of the large HiBEF lasers

Multi-100 TW laser (Amplitude)

Installation complete
Target shots, timing: started 2019
X-ray commissioning: 1st half of 2020
Available for Users: 2nd half of 2020
community proposal submitted

DiPOLE 100-X laser (CLF, UK)

Delivery complete
Installation at HED ongoing
Beam transport to IC1 & IC2: 2020
X-ray commissioning, VISAR: 2021
Available for Users: 2nd half of 2021

The joint HED and HIBEF team at European XFEL

Great thanks to

HP Liermann & team at ECB, DESY

HED group at HZDR


MID
MID Instrument

Materials Imaging and Dynamics Instrument

- **Materials:** MID focuses on structural studies of materials including **liquid**, glassy, amorphous and crystalline states. Connecting the nanoscale structure to the macroscopic properties of materials is at the heart of our investigations

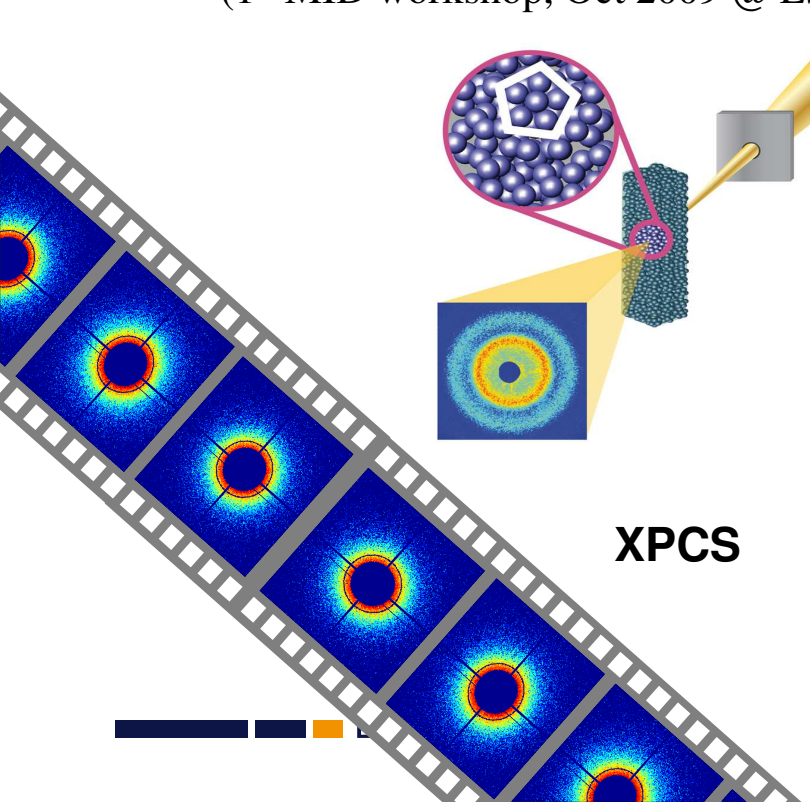
- **Imaging:** Imaging materials with X-rays is the technique used at MID. X-ray imaging can be done in many ways, e.g. using transmission and/or scattering contrast mechanisms. The coherence of the beam offers new opportunities to achieve higher spatial resolution in X-ray microscopy

- **Dynamics:** With sufficiently high time resolution in imaging experiments it will be possible to capture phenomena like phonon dynamics or atomic **diffusion**. The pulsed structure of European XFEL with MHz repetition rate of fs pulses is a unique feature

Materials Imaging and Dynamics Instrument

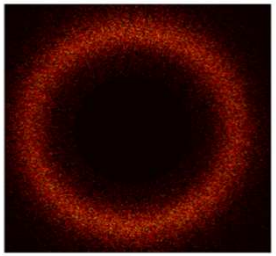
The Materials Imaging and Dynamics (MID) station aims at the investigation of nanosized **structure** and nanoscale **dynamics** using **coherent hard X-rays**. Applications to a **wide range of materials** from hard to soft condensed matter and biological structures are envisaged

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

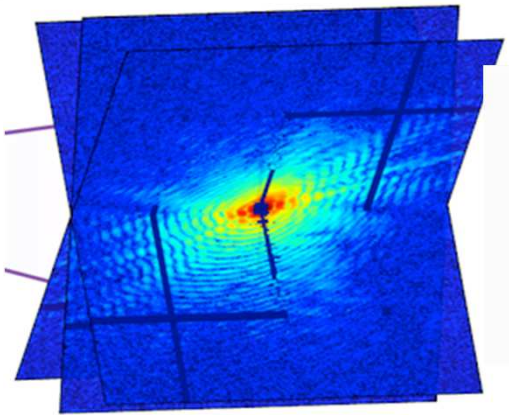


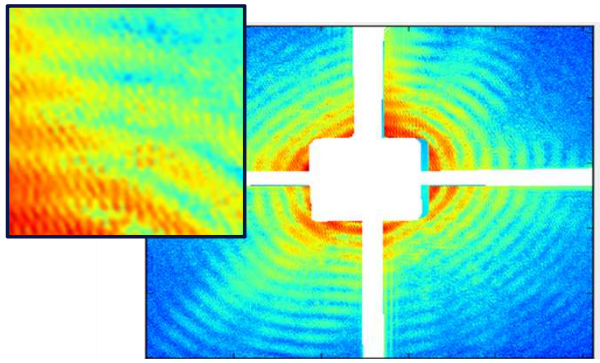
XPCS

XCCA



CDI

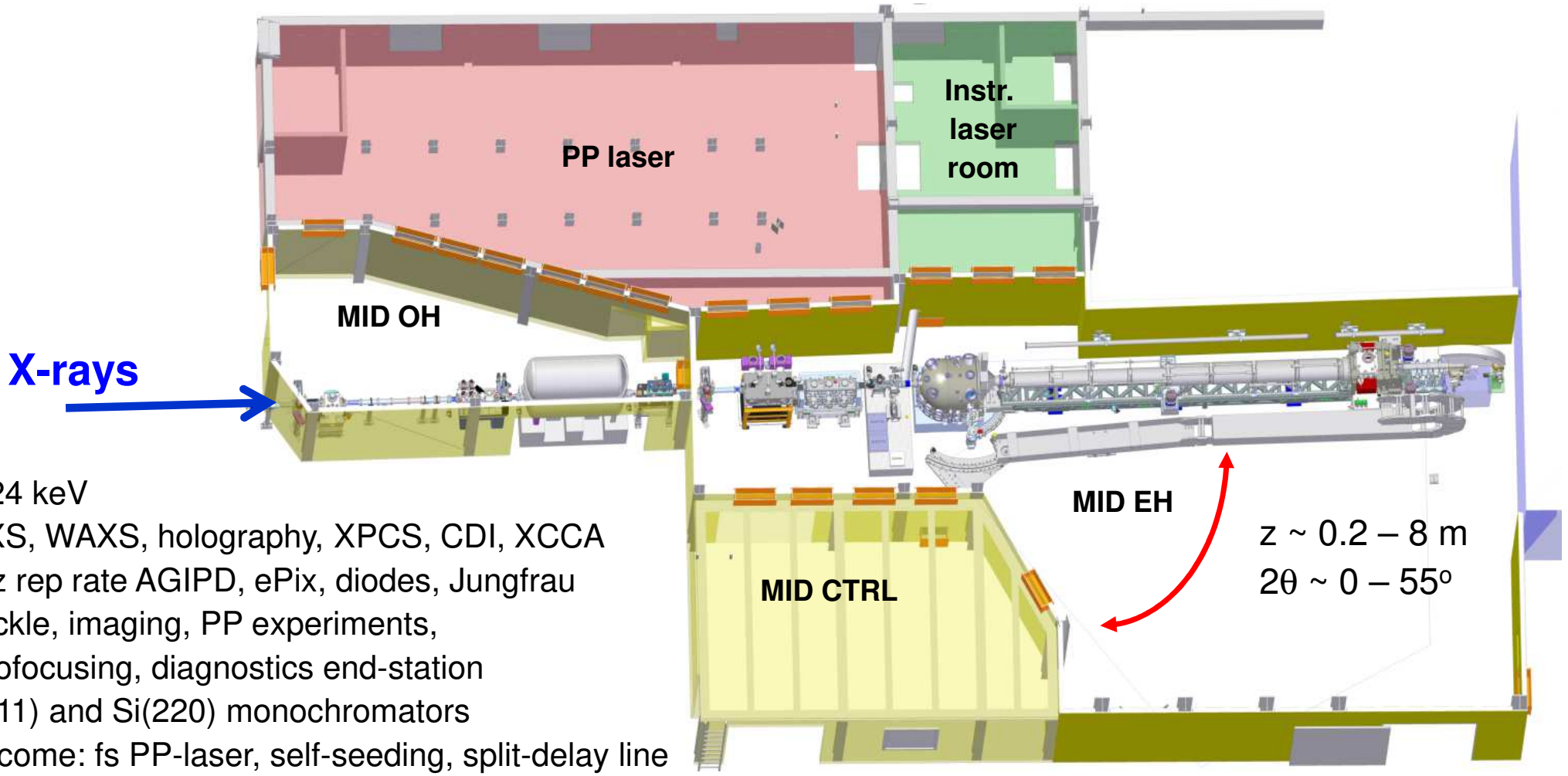




Holography

in combination with:
- External pump
- Spectroscopy
- Nano-focusing
- Split-delay techniques

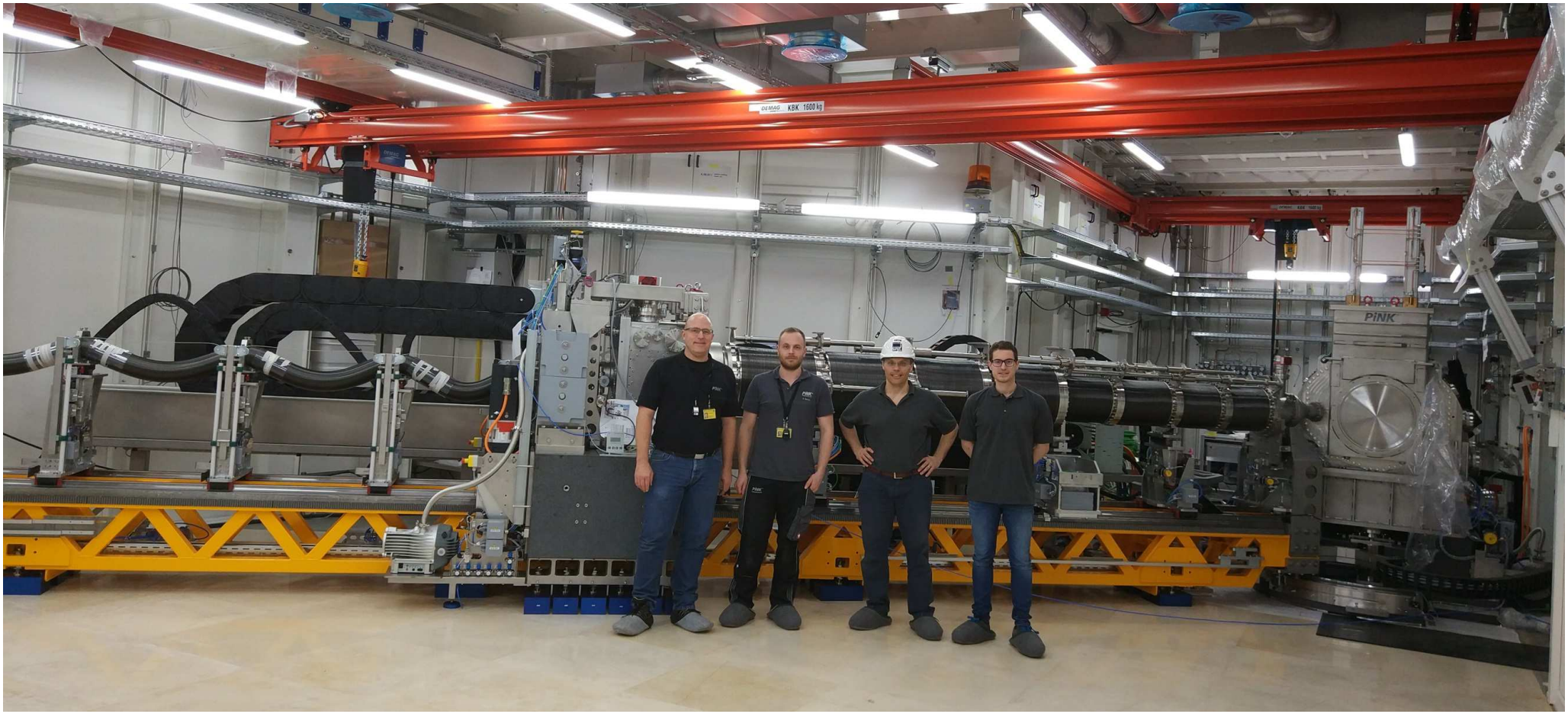
Materials Imaging and Dynamics Instrument



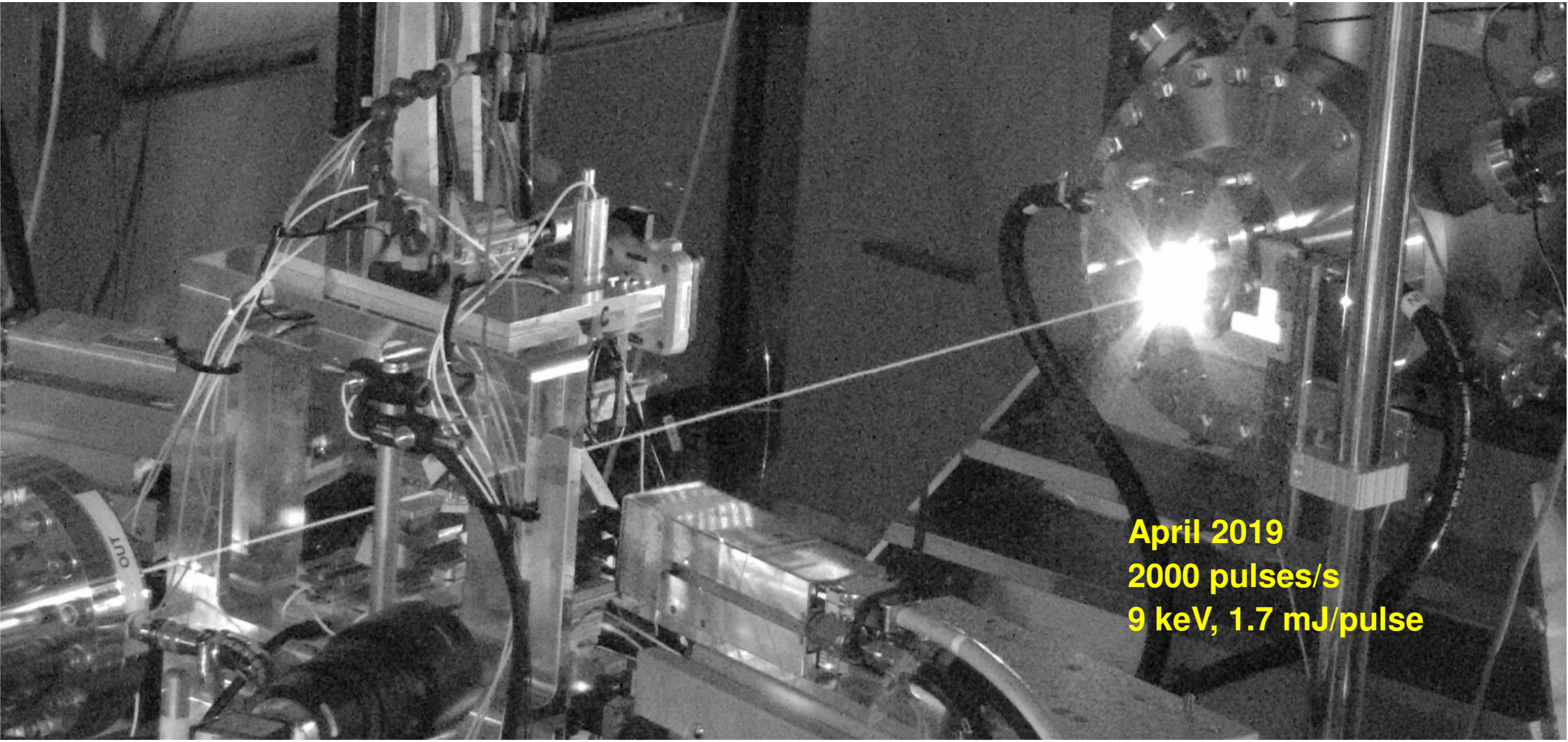
- 5 - 24 keV
- SAXS, WAXS, holography, XPCS, CDI, XCCA
- MHz rep rate AGIPD, ePix, diodes, Jungfrau
- speckle, imaging, PP experiments,
- nanofocusing, diagnostics end-station
- Si(111) and Si(220) monochromators

Still to come: fs PP-laser, self-seeding, split-delay line

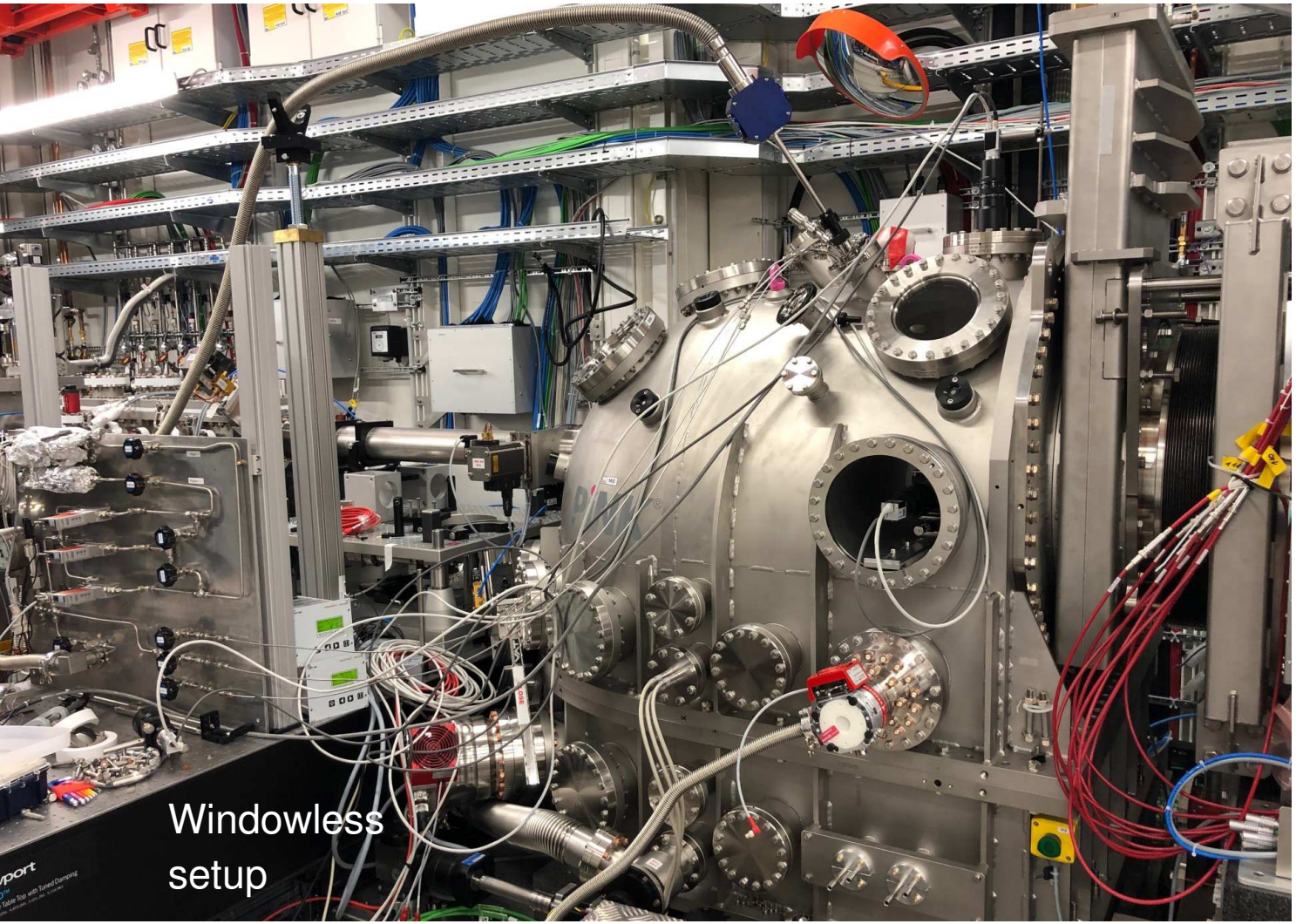
Materials Imaging and Dynamics Instrument



MID commissioning



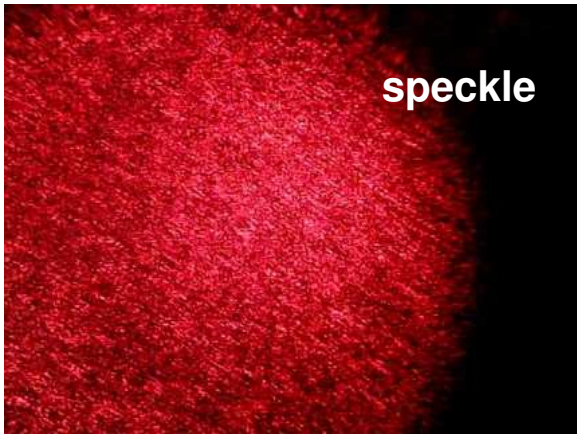
Capturing the early stages of crystallization (#2272 and 2542)

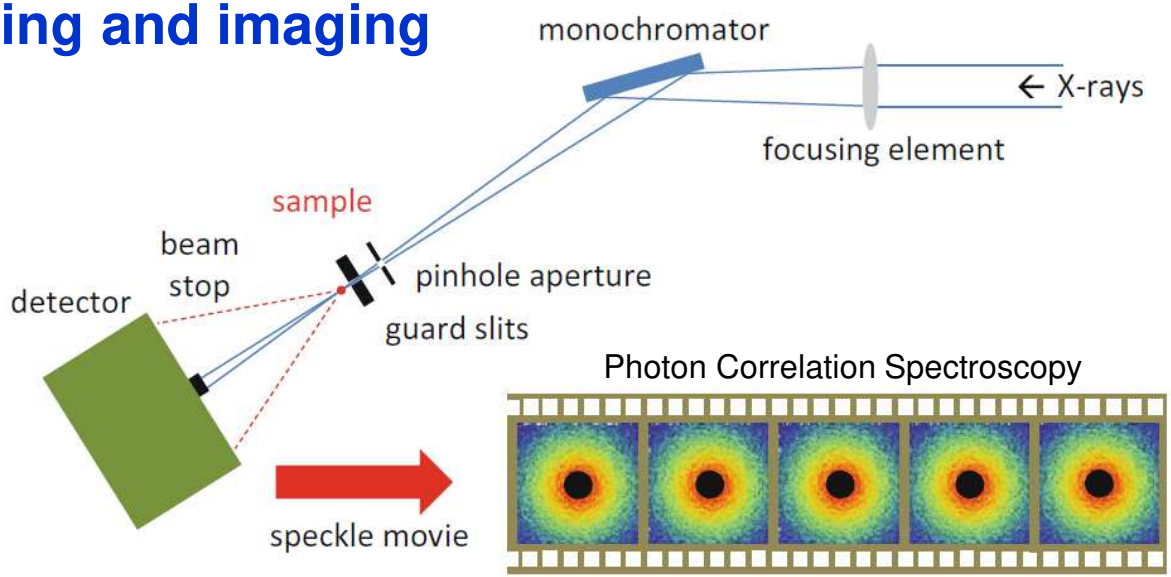


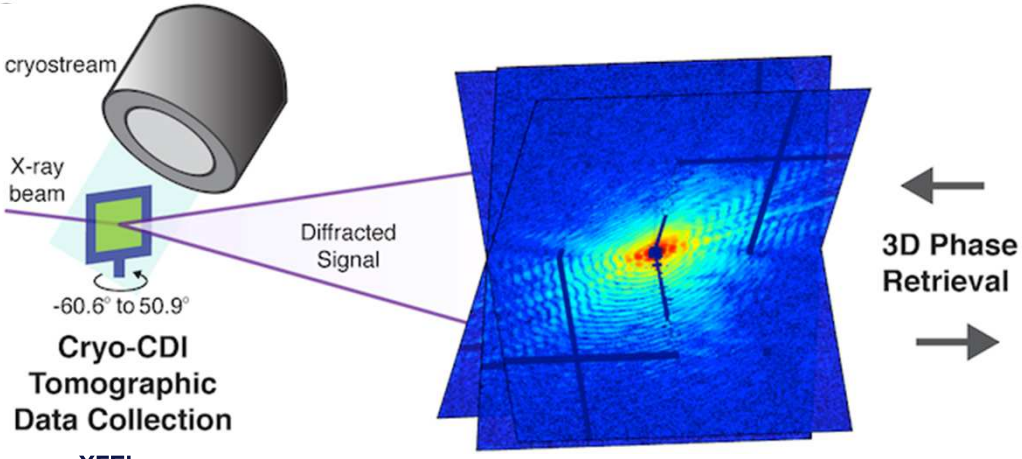
1st users at MID (#2272)
20-24 March 2019

Alexander Schottelius,
Robert Grisenti,
Anton Kalinin, et al.
Uni. Frankfurt and GSI

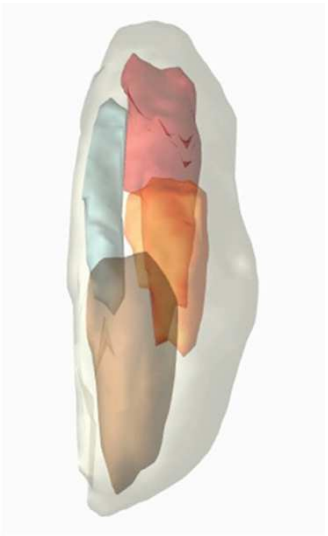
Examples: Coherent scattering and imaging







3D Phase Retrieval

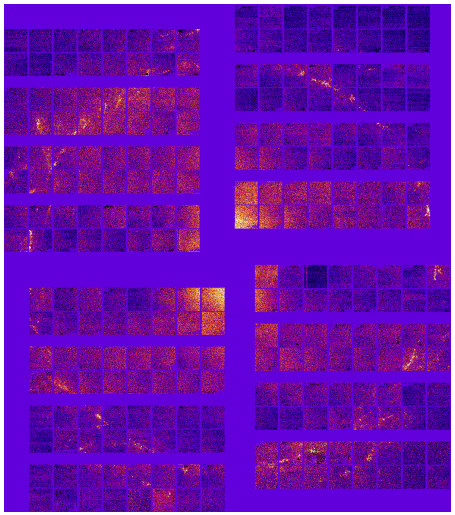


Coherent Diffraction Imaging

Capturing the Early Stages of Crystallization

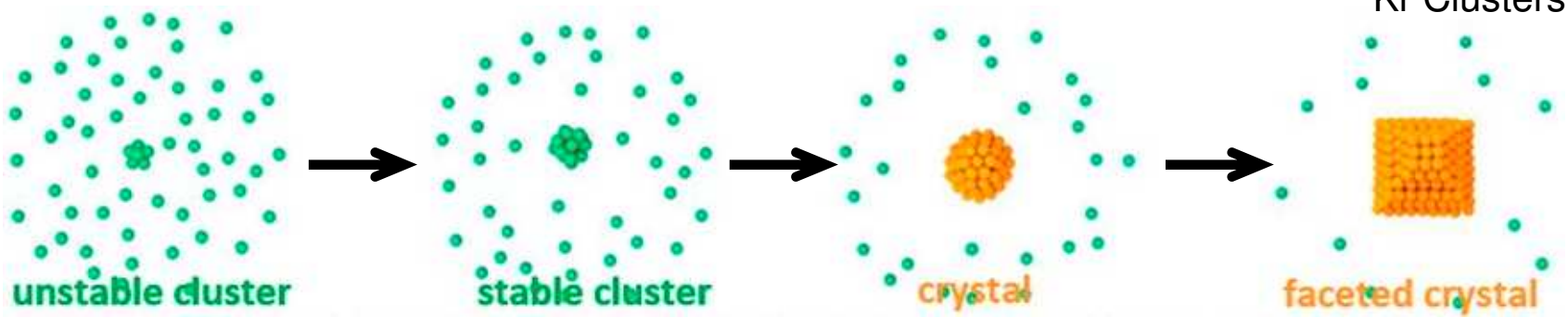
Investigating short-range ordering in freezing liquids

- Need short pulses to capture short-lived structures
- Need correlation analysis (XCCA*) to see weak structural order (clusters) prior to crystallization occurring



Kr Clusters (MID)

Classical view: crystallization as a two-step process

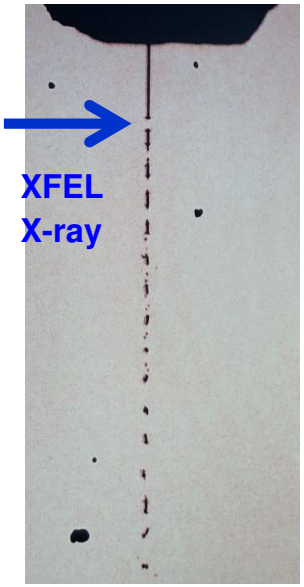


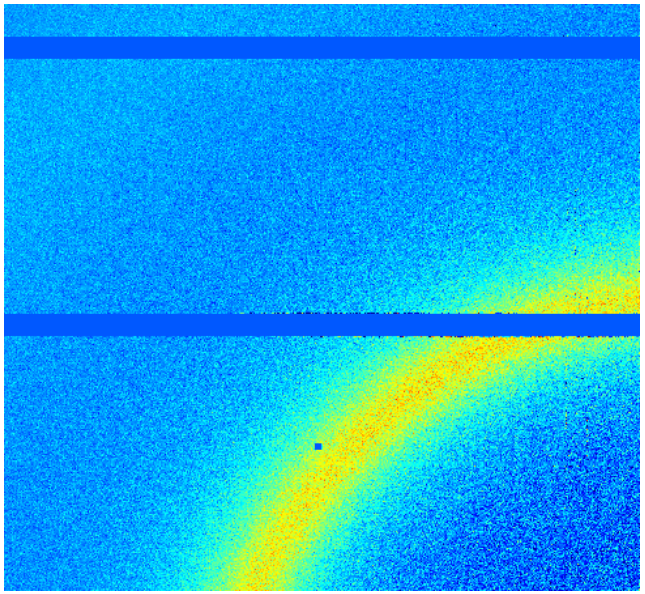
Homogeneous nucleation **Growth**

*XCCA: X-Ray Cross-Correlation Analysis

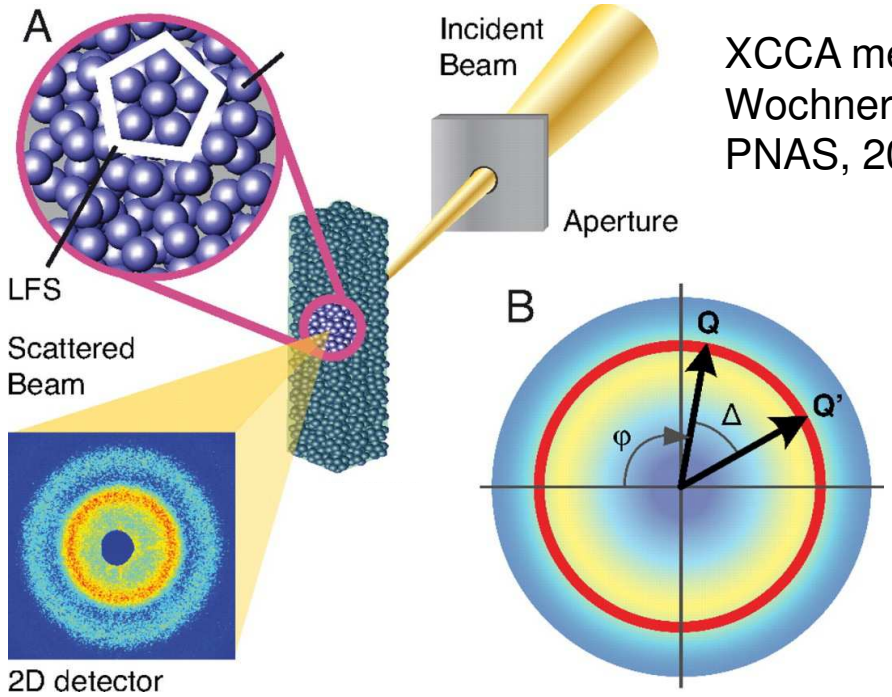
Capturing the Early Stages of Crystallization

XCCA:
X-ray Cross-Correlation Analysis





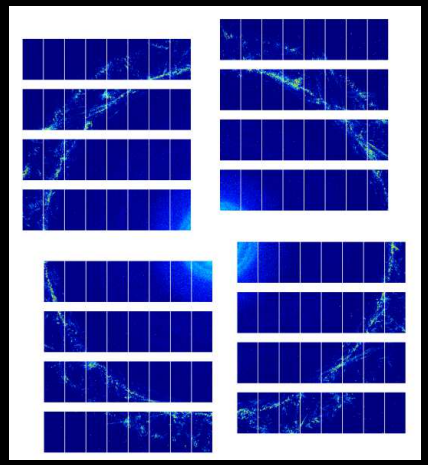
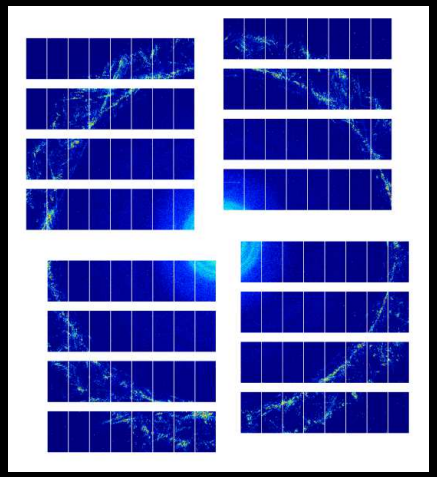
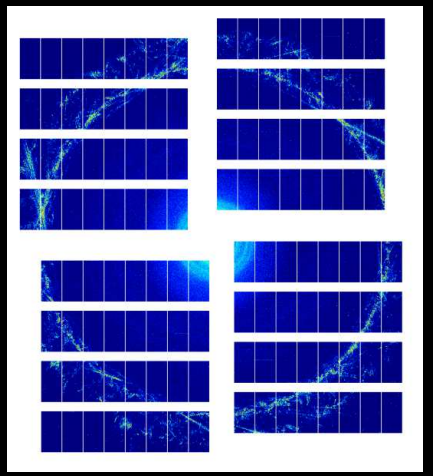
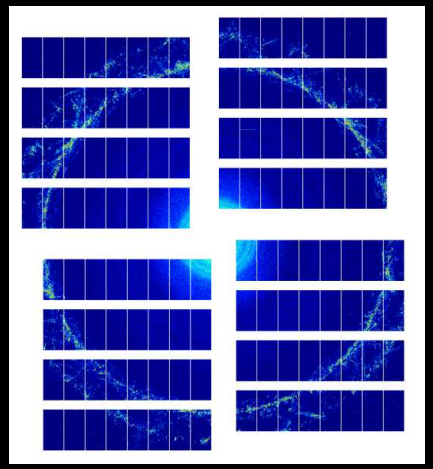
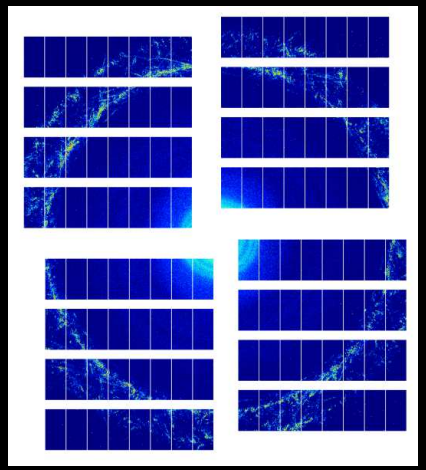
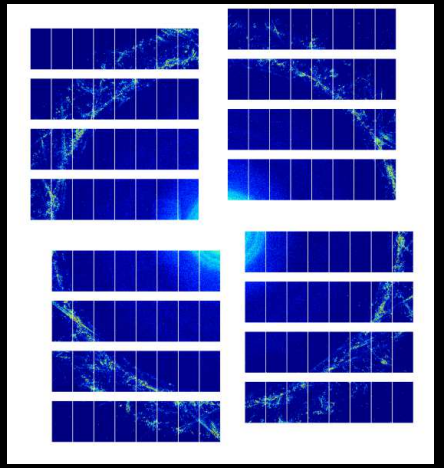
Extend scattering pattern to
φ = 360° with AGIPD detector



XCCA method:
Wochner *et al.*
PNAS, 2009

$$\left\langle C^{i,j}(q,\Delta)\right\rangle_M = \left\langle \left\langle I^i(q,\varphi) I^j(q,\varphi+\Delta)\right\rangle_\varphi \right\rangle_M$$

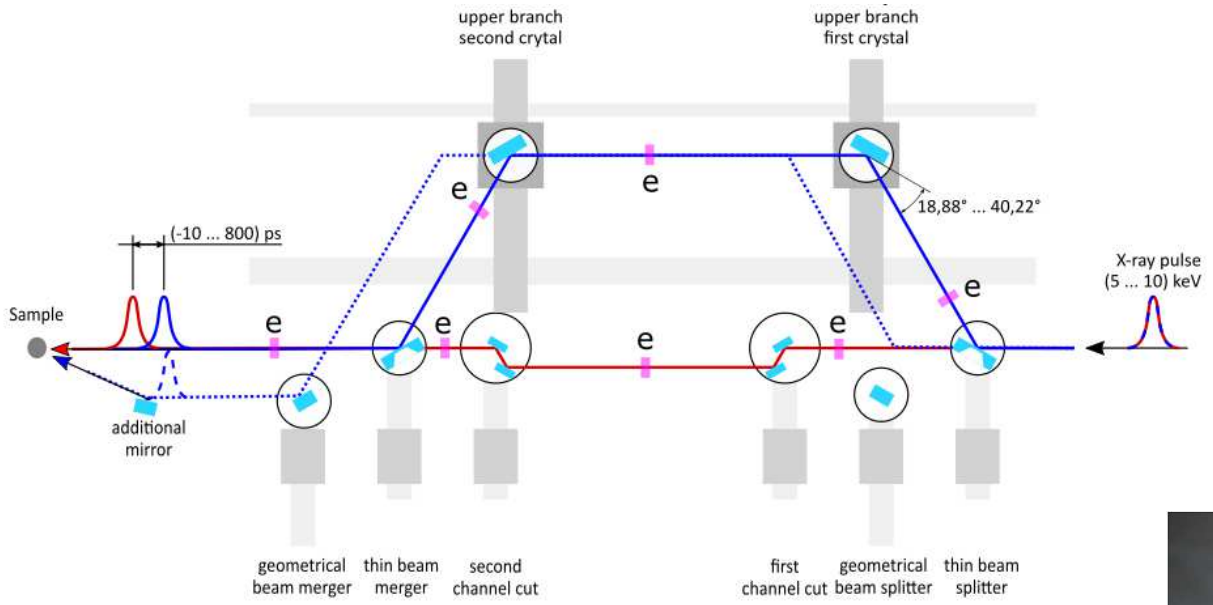
Capturing the early stages of crystallization (#2272 and 2542)

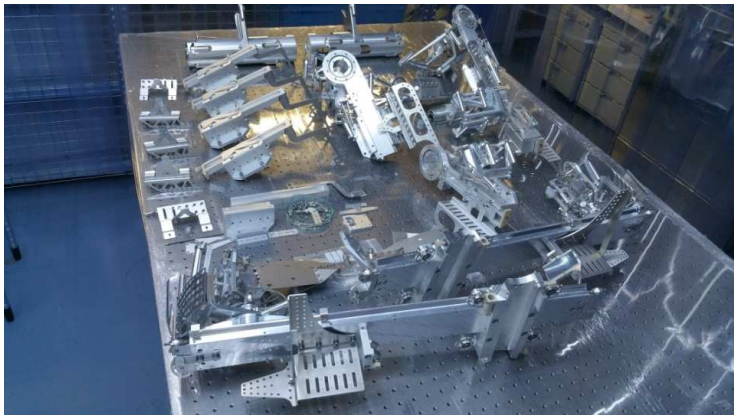
XCCA analysis in progress

R. Grisenti *et al*

Split-Delay line at MID



Inner mechanics

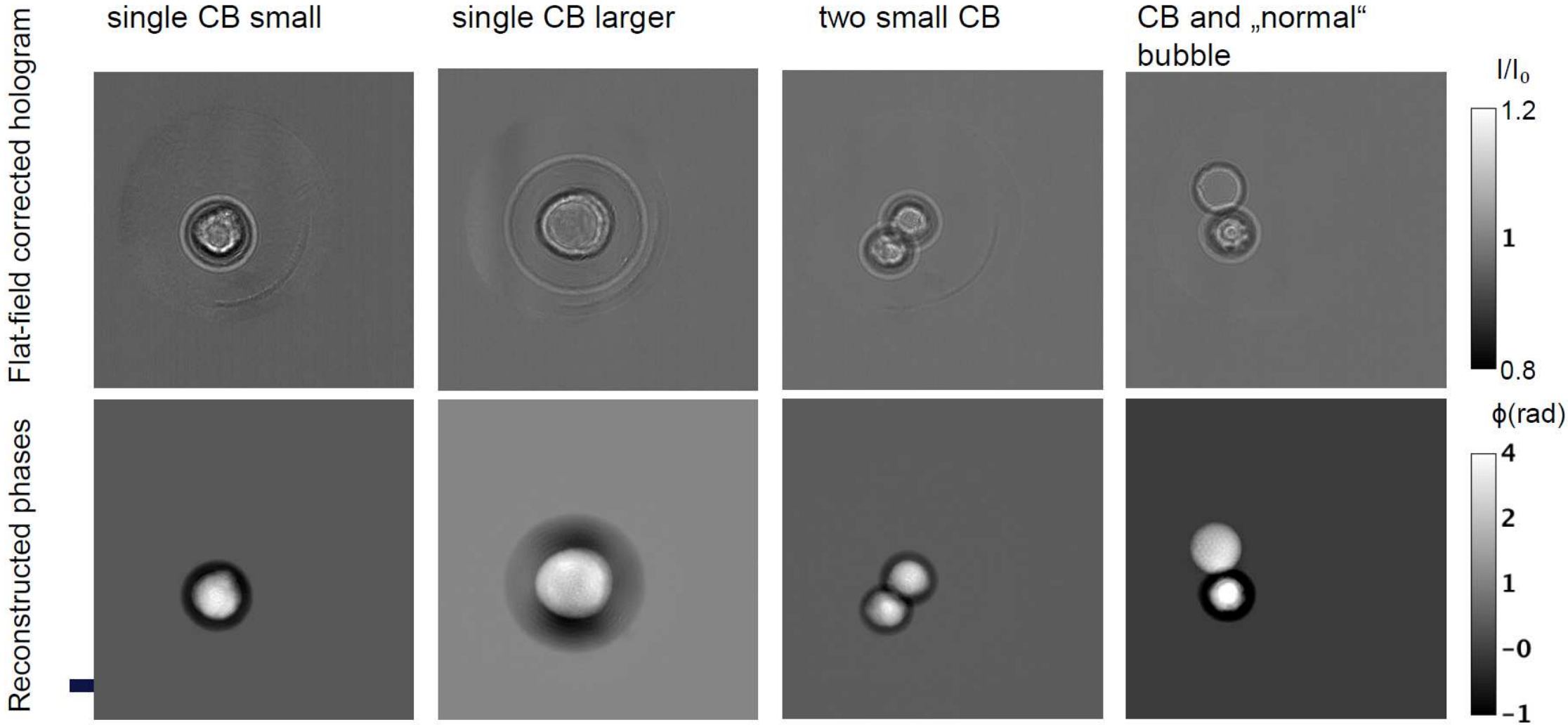


Max Born Institute
Eisebitt group

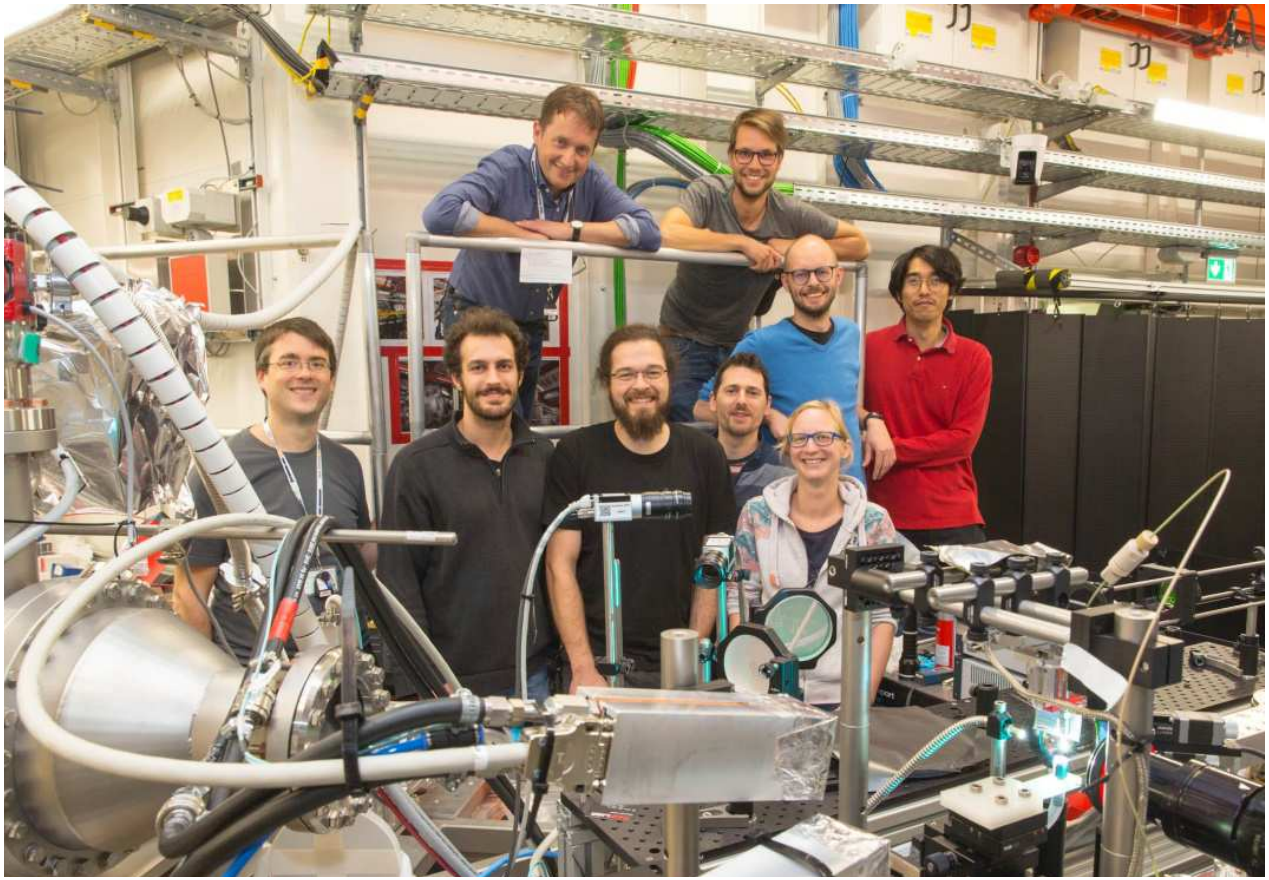
Capturing the early stages of crystallization (#2272 and 2542)

Busy control room

MID **2207 Salditt & Hagemann - Time-resolved in-line holography – cavitation dynamics**



Time-resolved (ns) in-line holography of cavitation dynamics (#2207 & #2544)



T. Salditt, J. Hagemann et al.

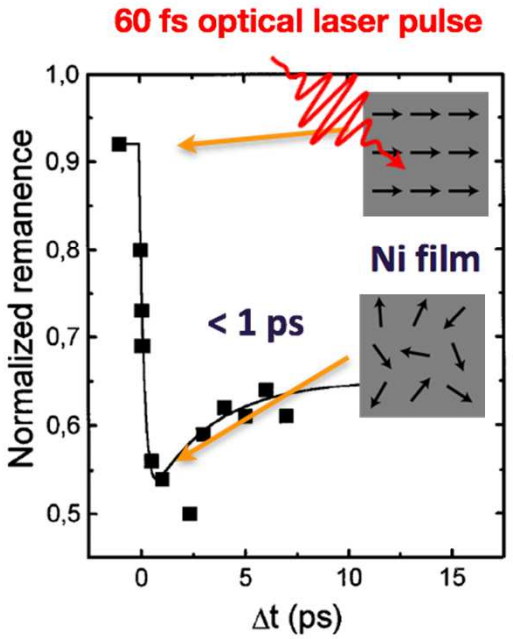
GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN

DESY.


SCS Instrument
SCS

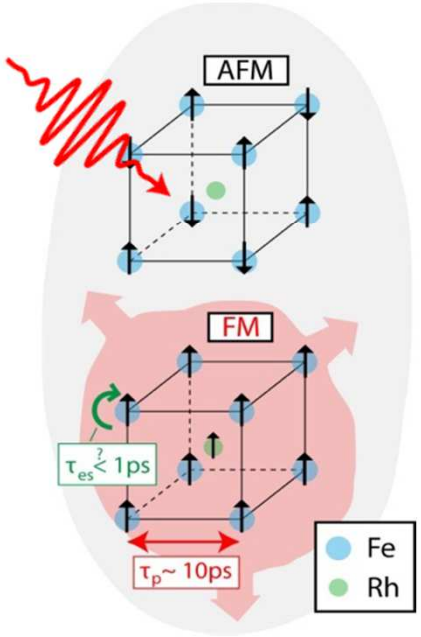
SCS: Manipulation of spins with femtosecond light pulses

Ultrafast Demagnetization (Disordering of Magnetization)

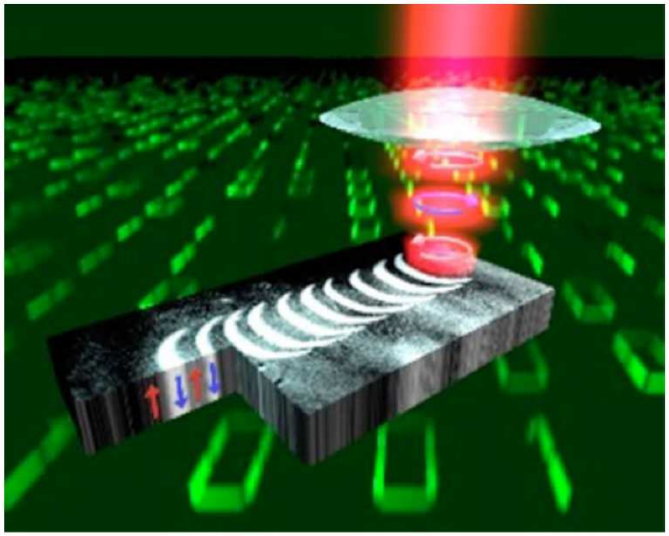


Beaurepaire *et al.* PRL **76**, 4250 (1996)

Ultrafast Remagnetization (Generation of Ferromagnetic ordering)



All-optical magnetization reversal



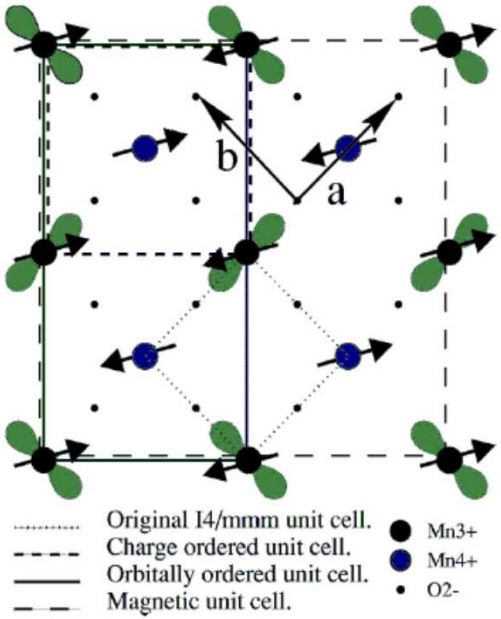
Courtesy from Rasing group, Nijmegen

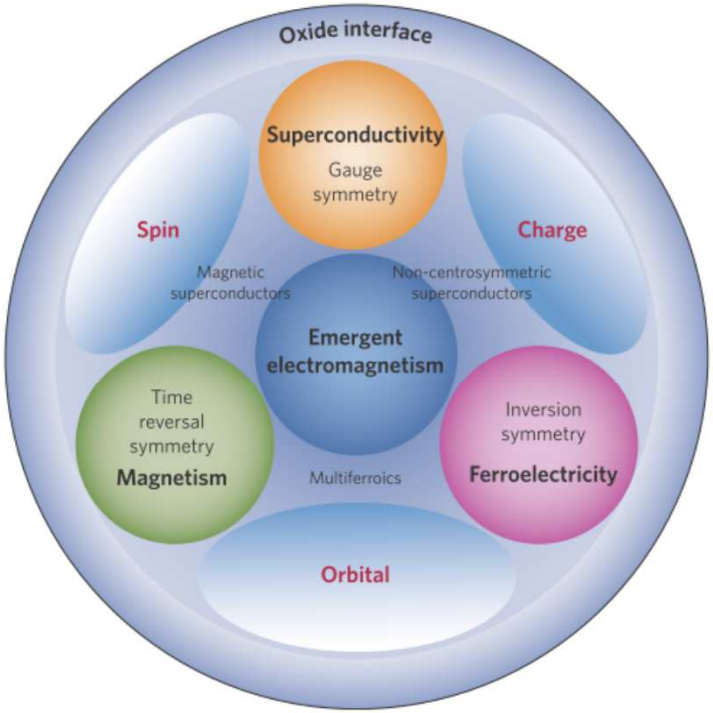
Stanciu *et al.* PRL **99**, 047601 (2007)

Vahaplar et al. PRL **103**, 117201 (2009)

SCS: Physics of complex materials by nuclear, charge, spin, and orbital degrees of freedom and their interplay

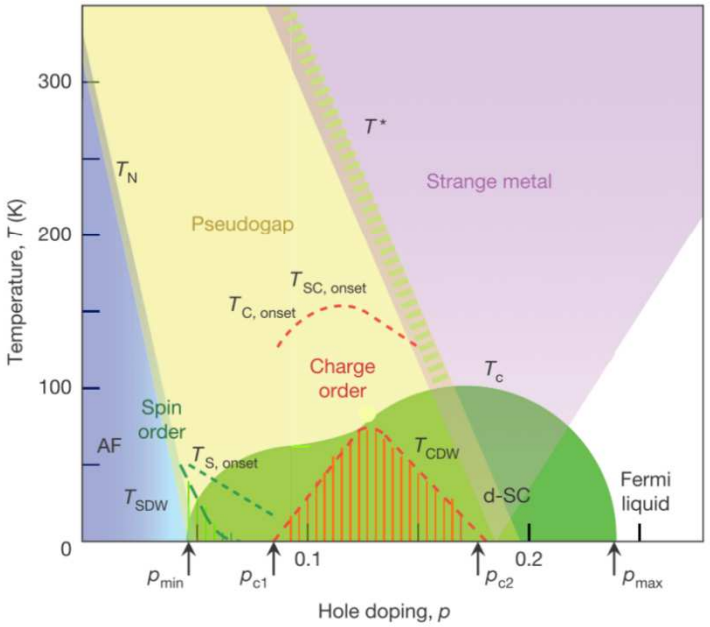
C.W.M. Castleton and M Altarelli,
Phys. Rev. B 62, 1033 (2000)



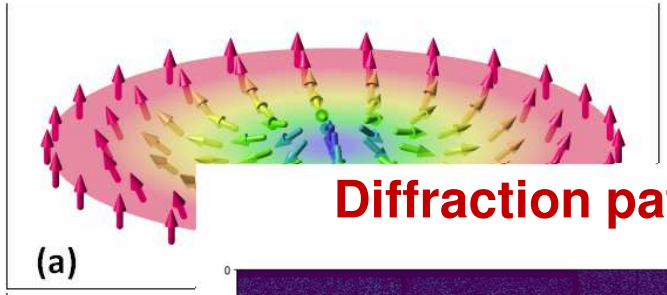


H.Y. Hwang et al.,
Nature materials 11, 103 (2012)

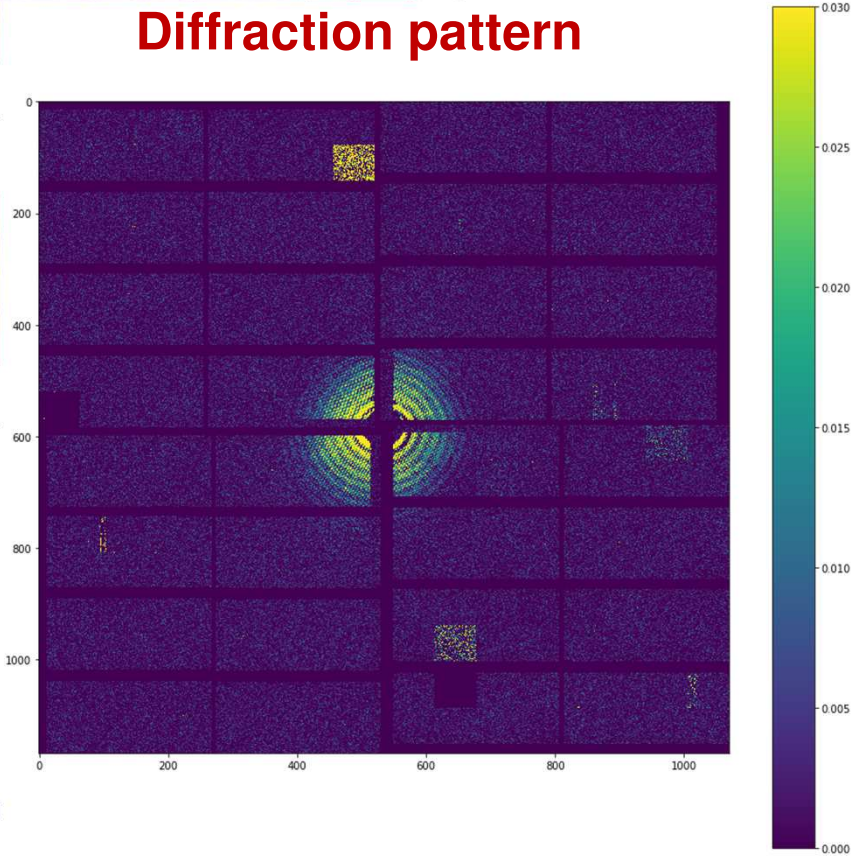
B. Keimer et al.,
Nature 518, 179 (2015)



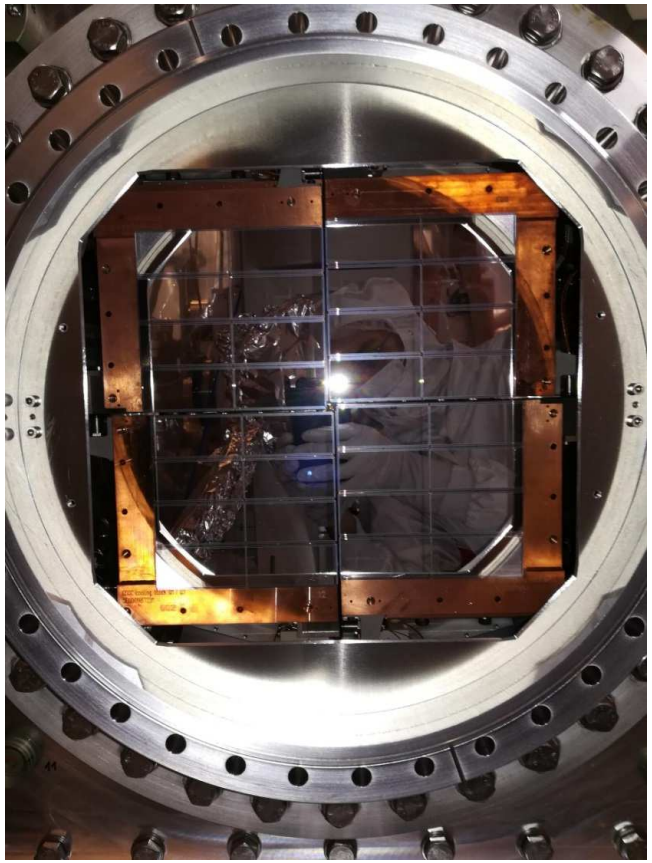
Dynamics of Magnetic skyrmions, experiment #2222 University of Stockholm



Diffraction pattern

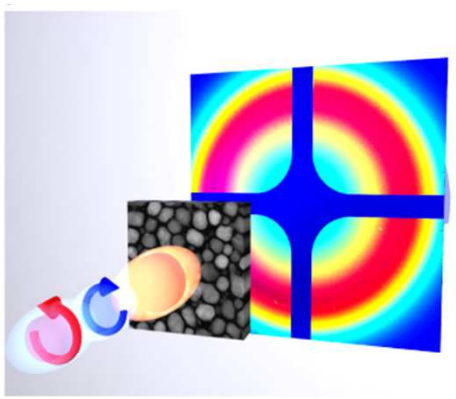


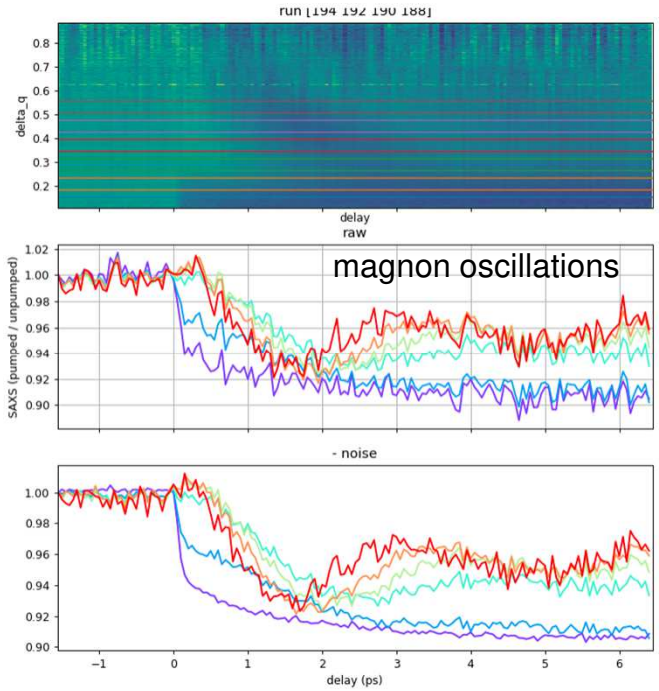
DSSC detector in use for the first time



Non-equilibrium pathways for energy and angular momentum transfer

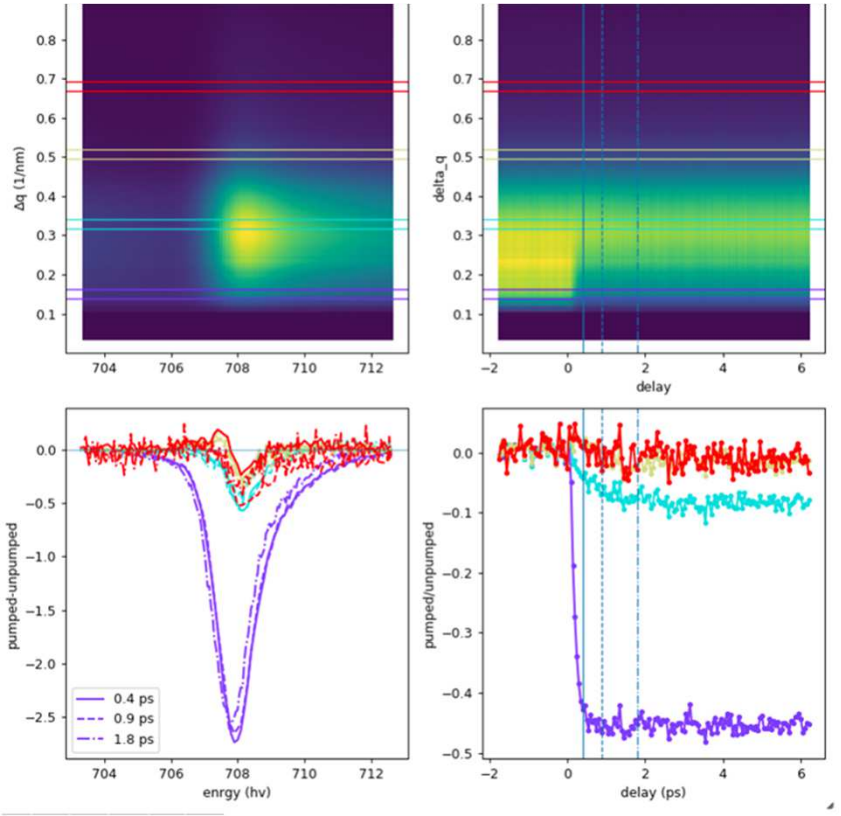
SAXS on free-standing sheet (50-100 um) of 16nm FePt nanoparticles embedded in carbon





FePt dynamic response to laser-induced electronic and phononic stresses by the instantaneous repopulation of electrons and phonons.

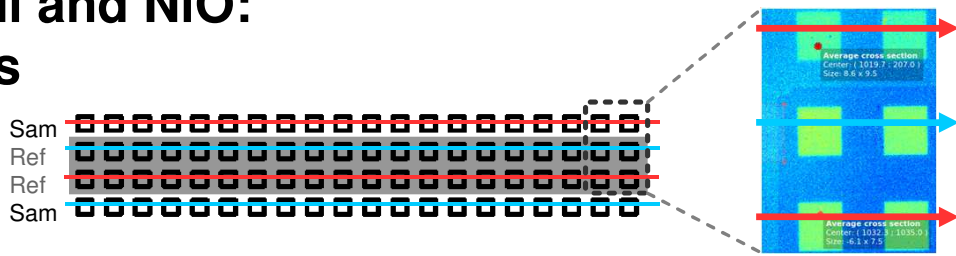
State and momentum-resolved electron dynamics

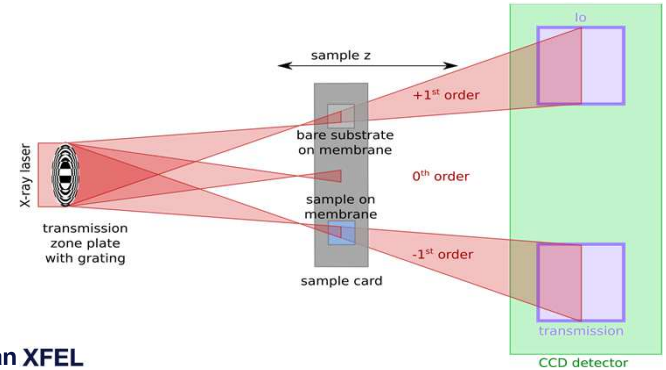


H. A. Dürr et al, UP2280, Sep 2019.

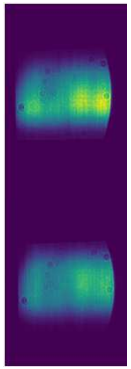
Single-shot X-ray absorption spectroscopy on Ni and NiO: from nonperturbing fluences to nonlinear effects

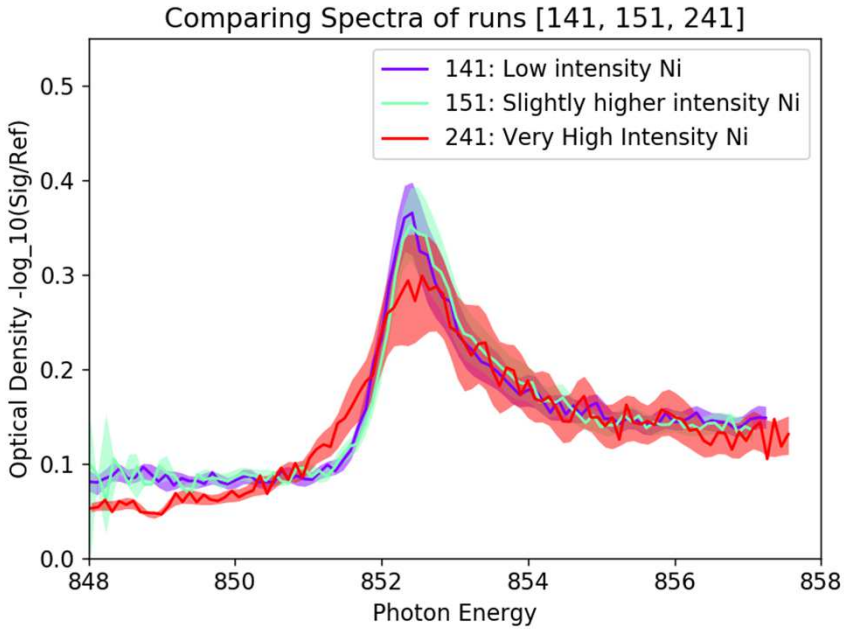
Martin Beye (DESY), et al, Open community proposal





fCCD





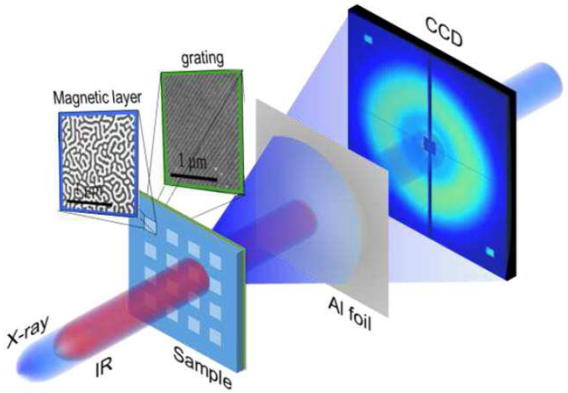
Preliminary results !

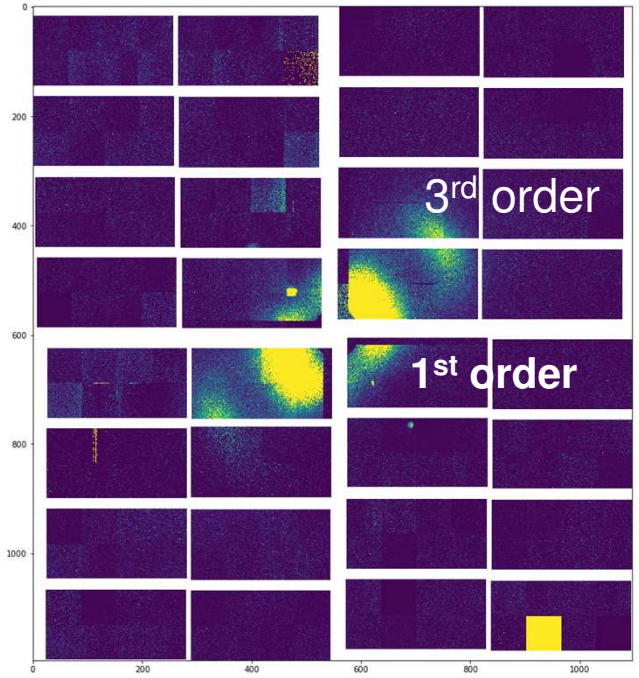
Time-resolved magnetic SAXS:

Ultrafast spin transport in laser-driven magnetization reversal

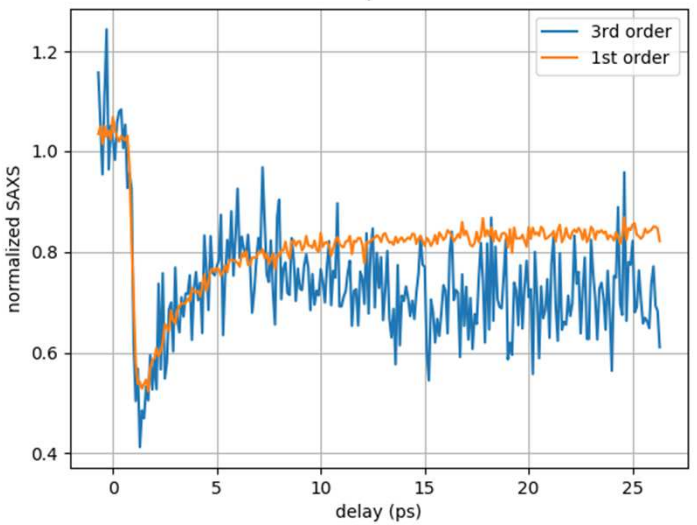
Emmanuelle Jal (U Sorbonne), et al., Open community proposal

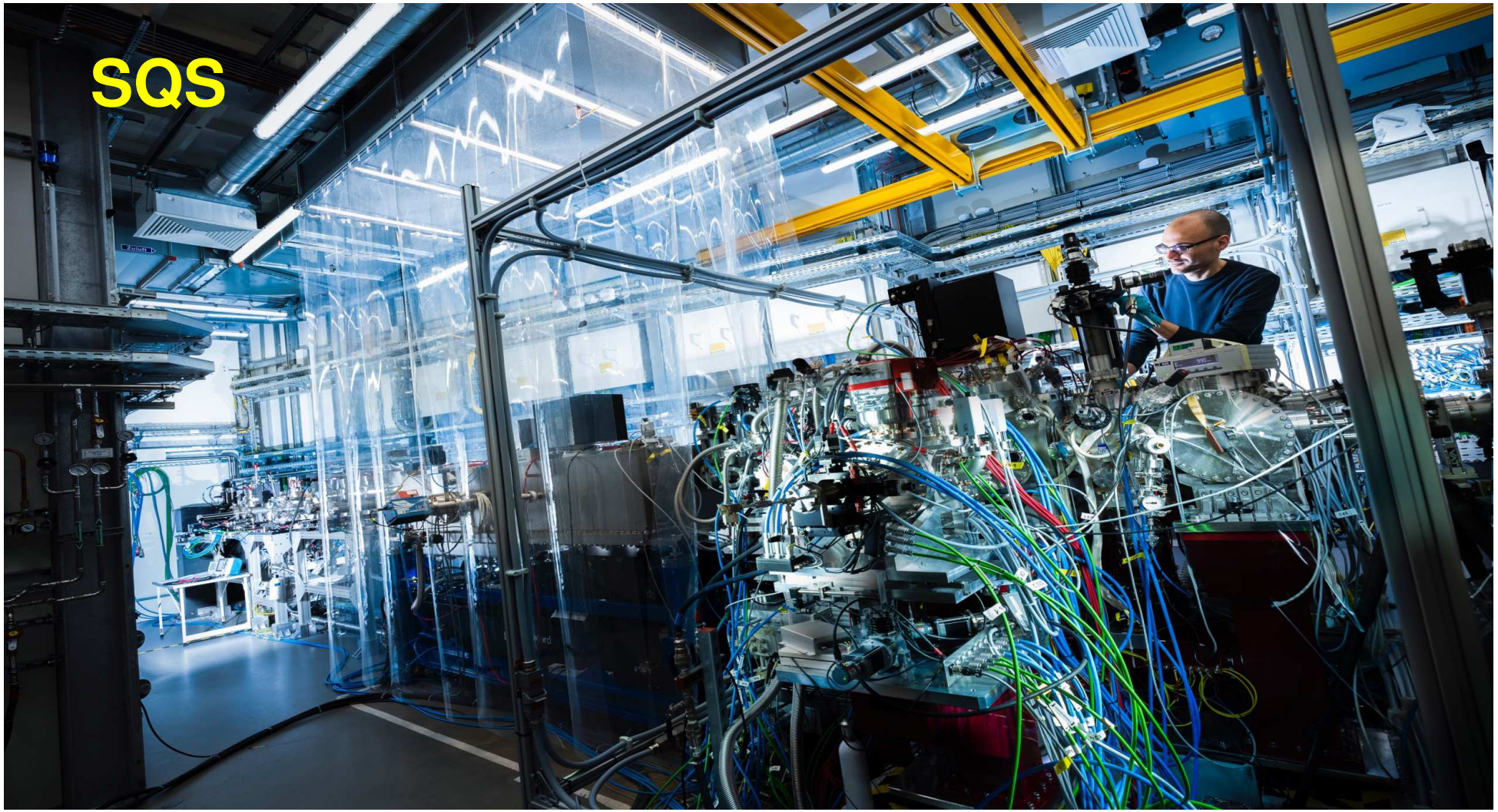
First experiments using
SA3 PP laser (mid Aug 2019)
800 nm, 50fs, 1.1 MHz





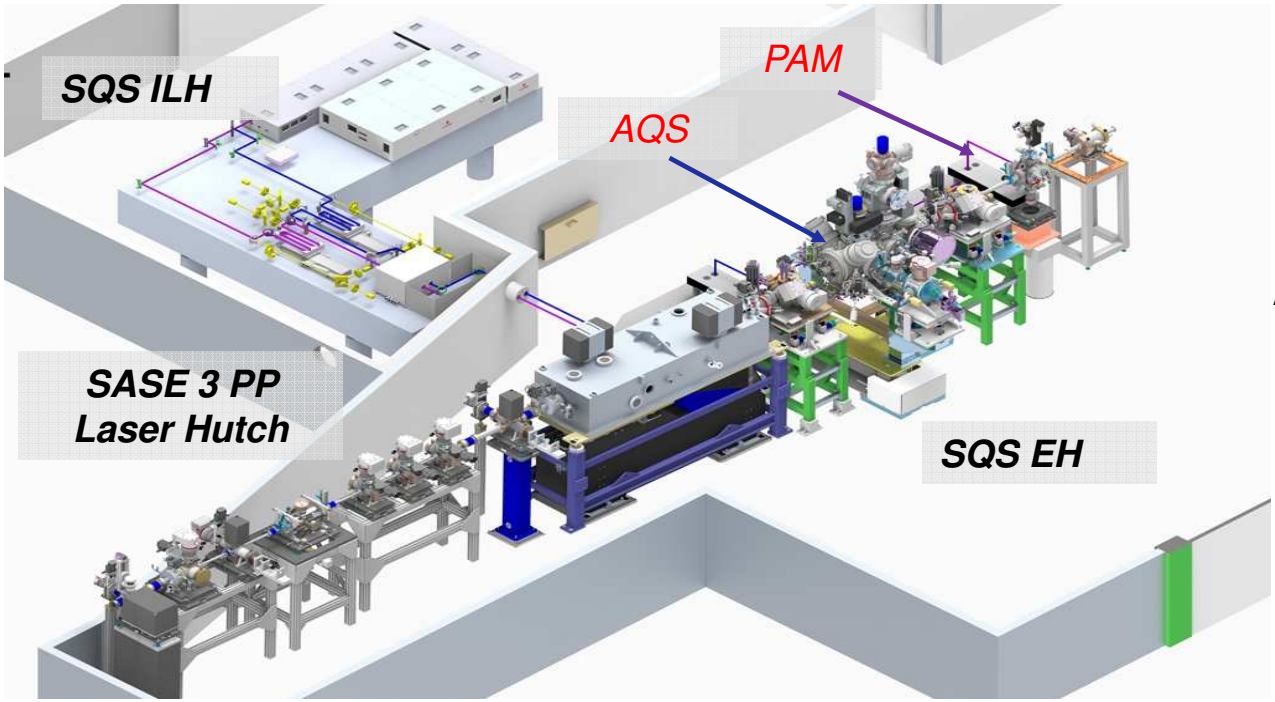
Co/Pt multilayers in stripe domain pattern




SQS

PP laser infrastructure at SASE 3 for the SQS instrument

SASE3 PP Laser available > Q3/2019



Installation Q1/2019

INTERIM SOLUTION:

Fiber-based pump probe laser for day 1

Active Fiber Systems 200W laser amplifier

Parameter	Unit	Value
Wavelength	nm	1030
Pulse duration (FWHM)	fs	300 (40)
Repetition rate	MHz	0.1 – 20
Pulse energy	mJ	2 @ 0.1 MHz
Polarization		variable
Focus size	μm	30 $(1/e^2)$

http://www.afs-jena.de/

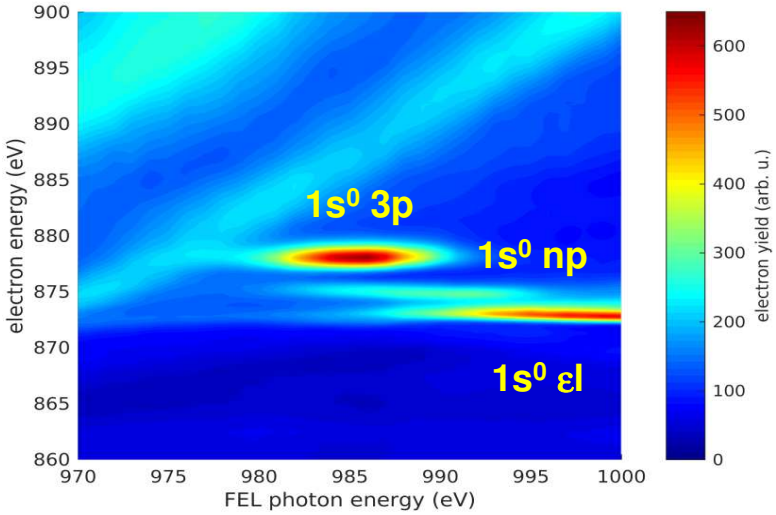
SQS (Small Quantum Systems)

All experimental stations are operational !!!

AQS
(multi-photon spectroscopy)

Non-linear electronic interaction of atoms with x-rays

PI: T. Mazza et al. (SQS)

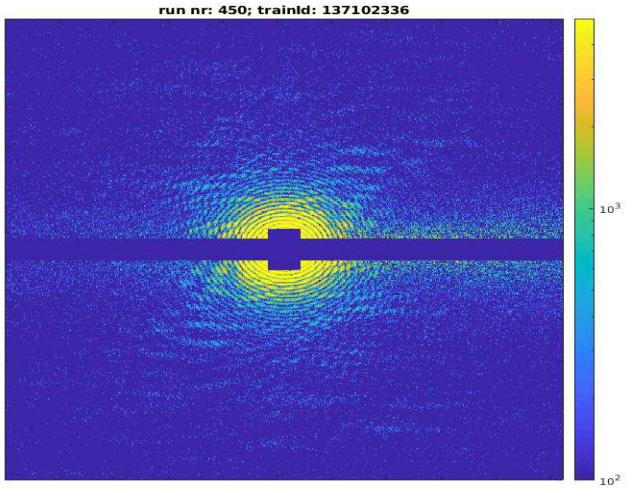


Neon

NQS
(imaging)

Doped He nanodroplets imaging

PI: R. Tanyag, D. Rupp (TU/MBI Berlin)

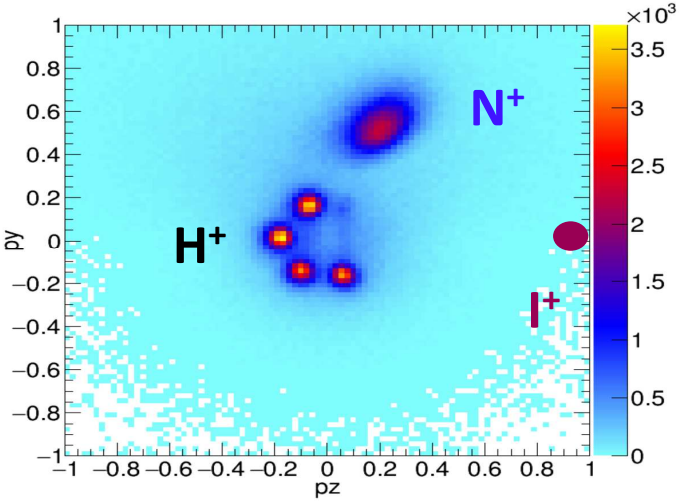


Xe-doped He droplet

SQS-REMI
(coincidences)

Charge transfer and Coulomb explosion initiated by fs X-ray pulses

PI: R. Boll et al. (SQS)



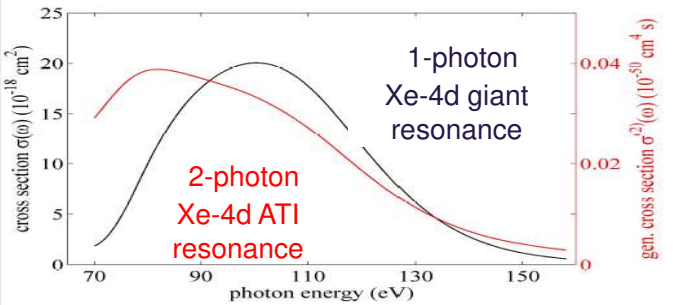
Iodopyridine

Science @ SQS (Small Quantum Systems)

(M. Meyer)

Non-linear phenomena

Intensity > 10^{18} W / cm^2

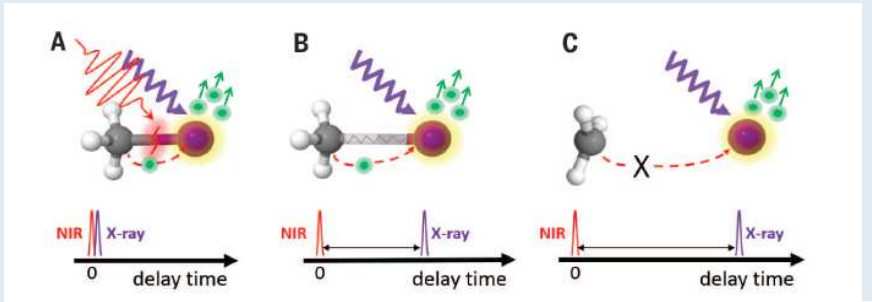


Multi-photon processes

Mazza *et al.* (2015)
Nat.Comm. **5** 36845

Time-resolved studies

Pulse durations: 2 - 100 fs

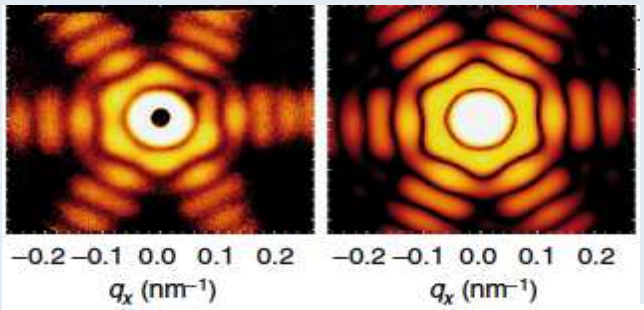


Dissociation dynamics

Erk *et al* (2014)
Science **345** 288

Imaging experiments

Spatial coherence

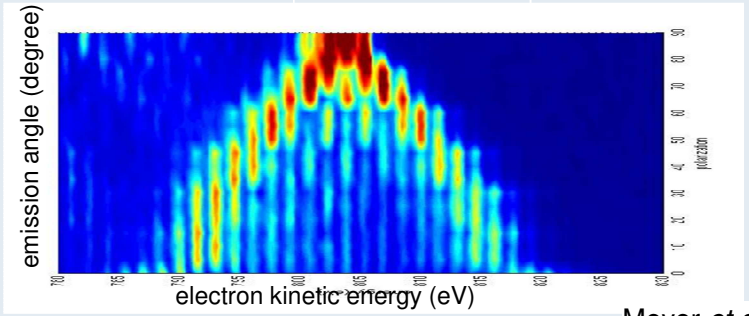


Size and shape selection

Barke *et al.* (2015)
Nat.Comm. **6** 6187

Strong field phenomena

Synchronized intense NIR laser



Electron dynamics

Meyer *et al.* (2012)
PRL **108** 063007

NQS “Nano-size Quantum Systems”

pnCCD detector (10 Hz)

(coherent diffraction imaging)

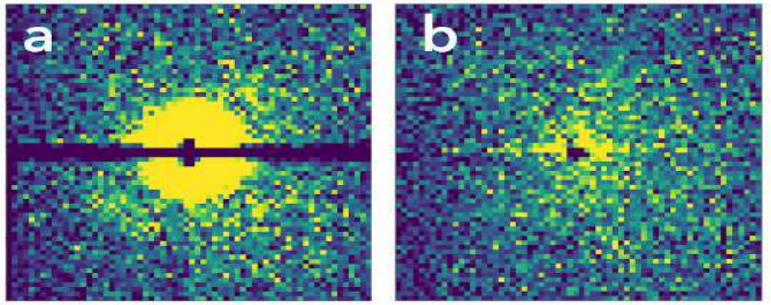
Single Protein Imaging

PI: F. Maia (Uni Uppsala)

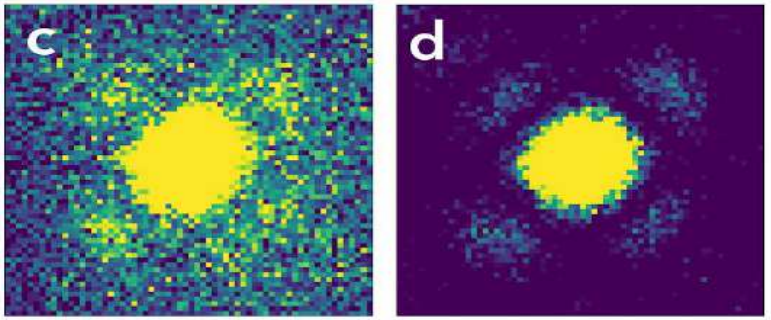
GroEL from E. Coli

Exp.

1.2 keV
6 mJ



Sim.

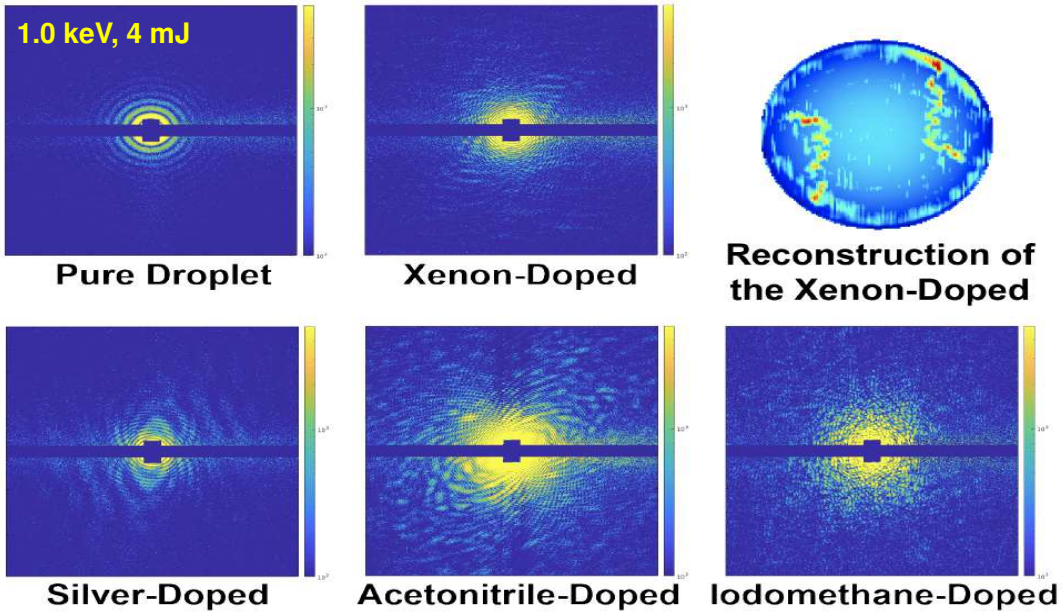


Diffraction images from a 14 nm protein !!

Single Particle (nano-droplets) Imaging

PI: R. Tanyag, D. Rupp (TU/MBI Berlin)

Doped He nanodroplets

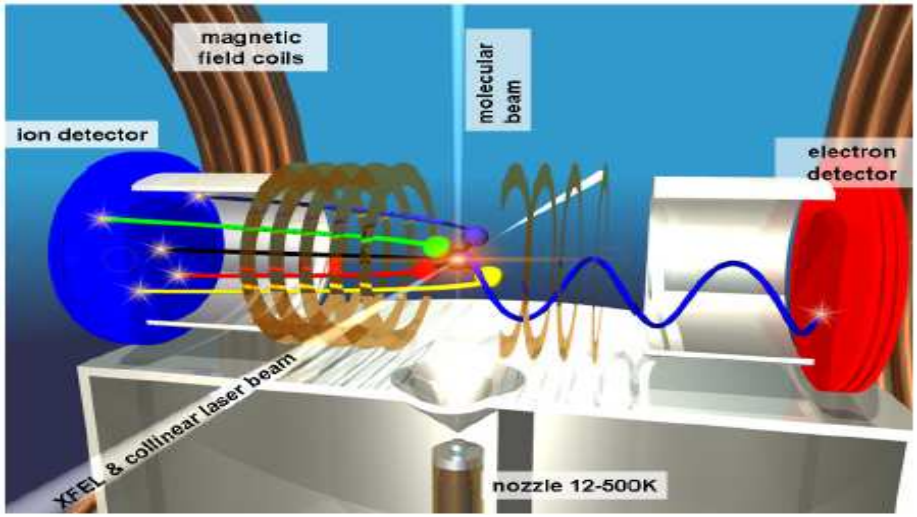


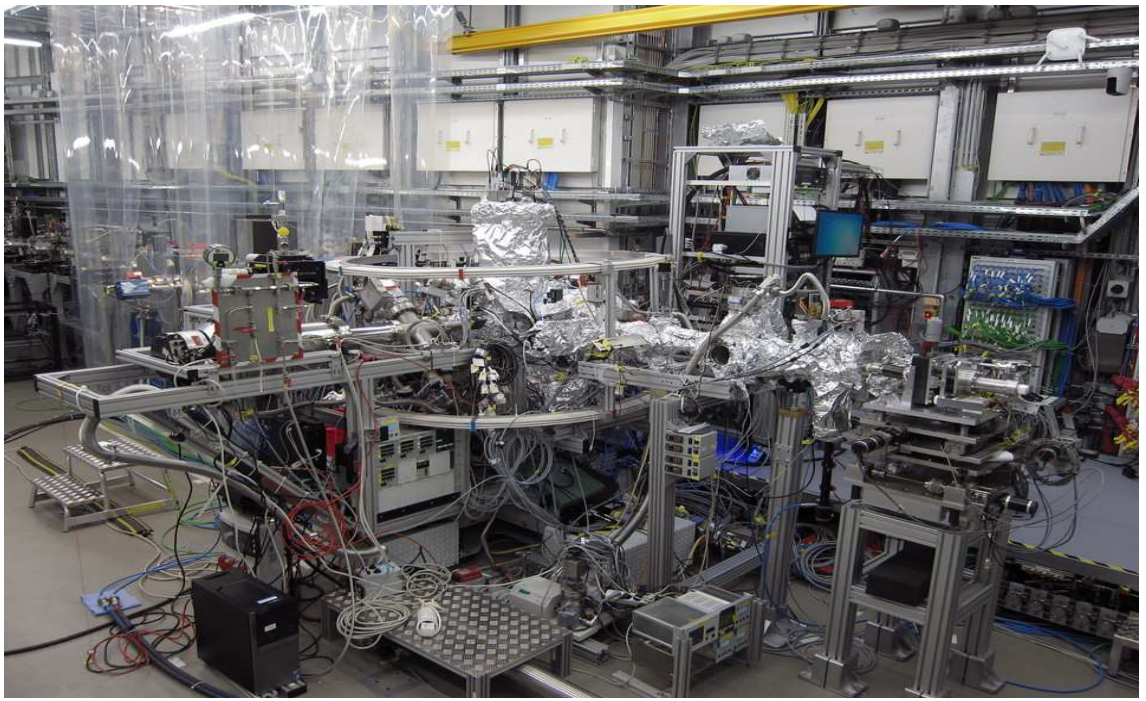
→ Talk Rico Tanyag 30.01., 11h30

SQS-REMI in collaboration with Uni. Frankfurt (R. Dörner et al.)

REMI: Reaction Microscope
U. Frankfurt (R. Dörner et al.)

Angle- and energy-resolved
electron and ion spectra
in coincidence





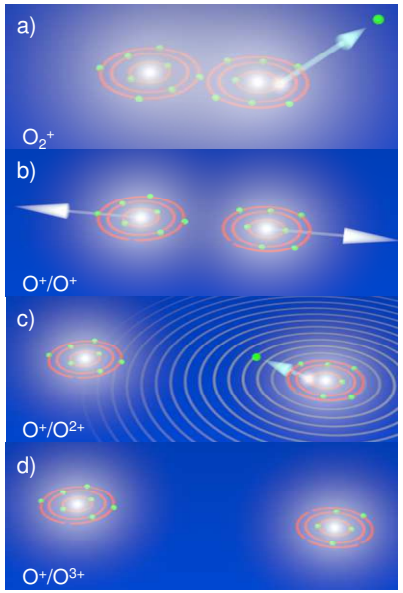
Start of Commissioning : February 12, 2019

Start of User Operation : February 26, 2019

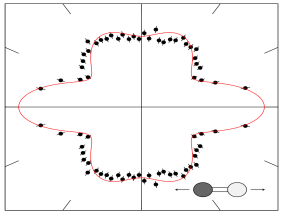
SQS - Reaction Microscope (electron – ion coincidences)

Photoelectron diffraction imaging of a molecular breakup (O_2)

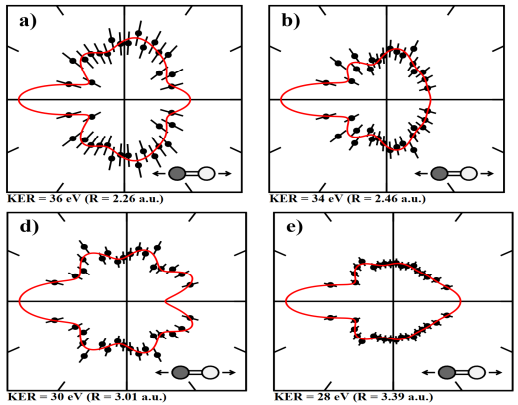
PI: T. Jahnke (U. Frankfurt)



1st electron



2nd electron

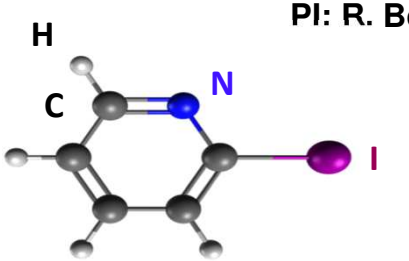


Electron angular distributions monitor the fragmentation process

Charge transfer and Coulomb explosion initiated by fs X-ray pulses

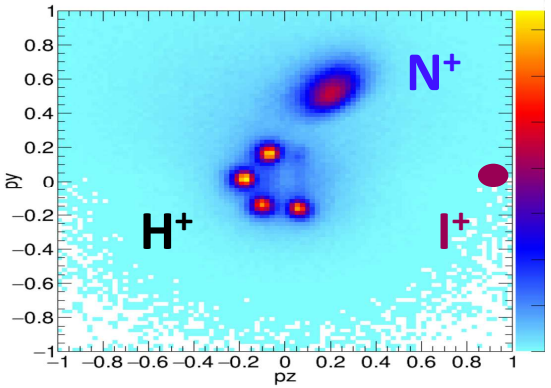
PI: R. Boll et al. (SQS)

→ Talk 14h30

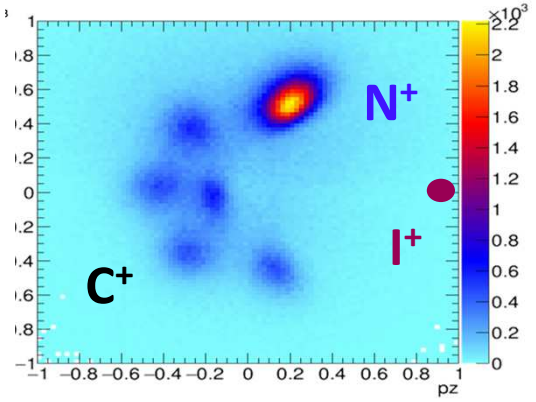


Iodopyridine
C_5H_4NI

I+ / N+ / H+ coinc.



I+ / N+ / C+ coinc.



Ion images visualize the molecular structure

REMI-chamber in collaboration with U. Frankfurt (R. Dörner et al.)

Next upgrades for SASE3 / SQS

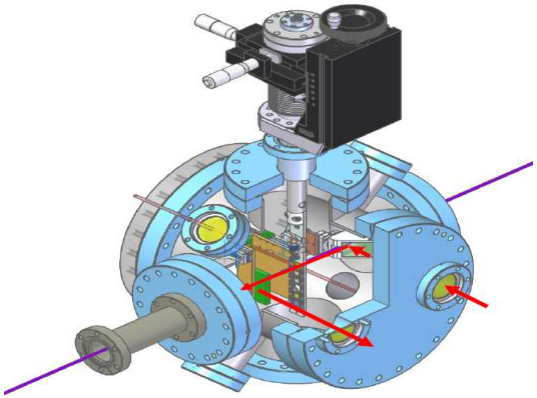
Two color lasing (2CPP)	→	**2020 summer**	**installation**
	→	**2020 Q3/Q4**	**commissioning**
	→	**2021 Q1/Q2**	**operation**
Spectral diagnostics	→	**2020 Q2**	**installation**
	→	**2020 Q3/Q4**	**commissioning**
Controlled adjustment of pulse duration			
	→	**2020 Q1/Q2**	**commissioning**
	→	**2020 Q3/Q4**	**operation**
Circular polarization	→	**2021 Q1/Q2**	**test**
	→	**2021 Q3/Q4**	**operation**

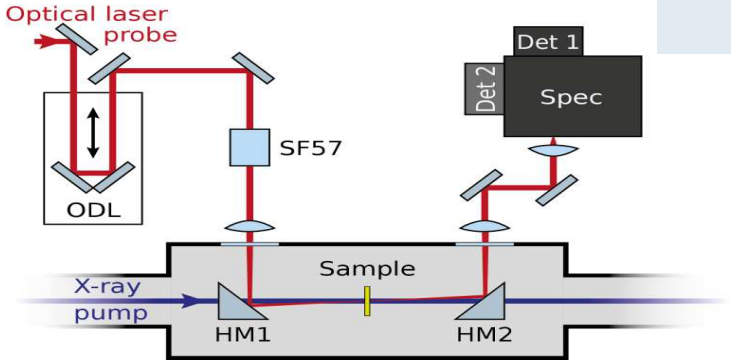
SPB/SFX

Adrian Mancuso
for the SPB/SFX team
4th November 2019

SASE / PP Laser timing with Photon Arrival Monitor

- Sato et al. submitted

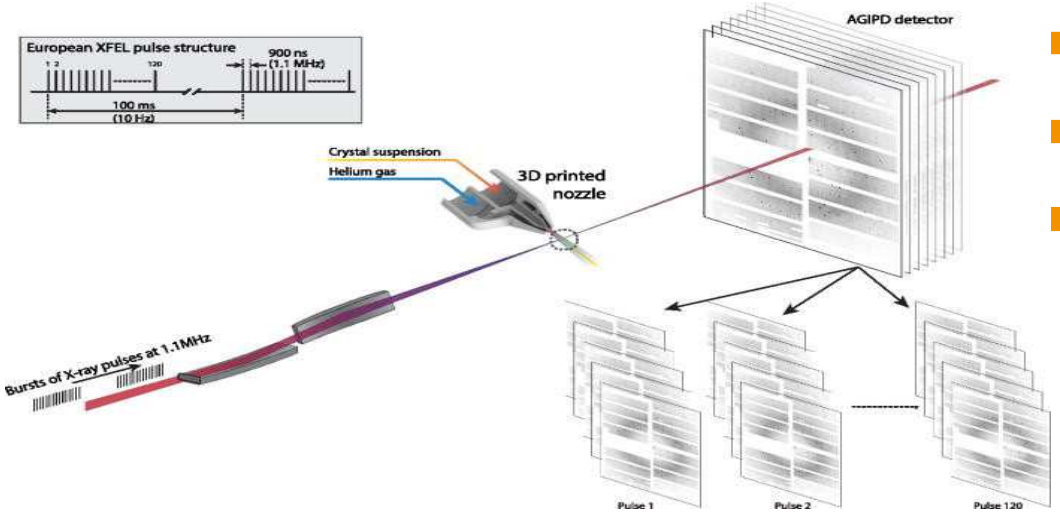


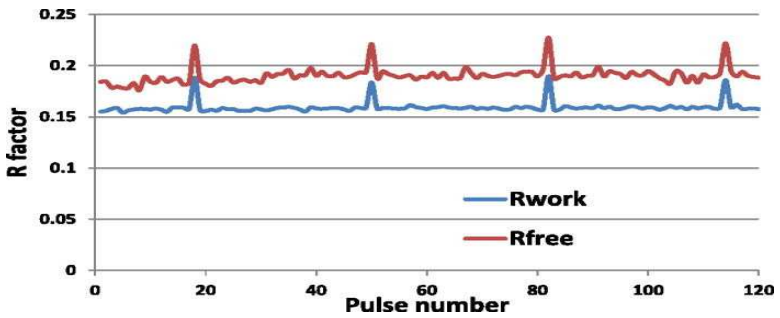


- Timing jitter measured over 2 hours (approximately 70000 pulse trains)
- distribution of nominal delay for the entire measurement with RMS jitter of 31.9 fs.
- Submitted for publication

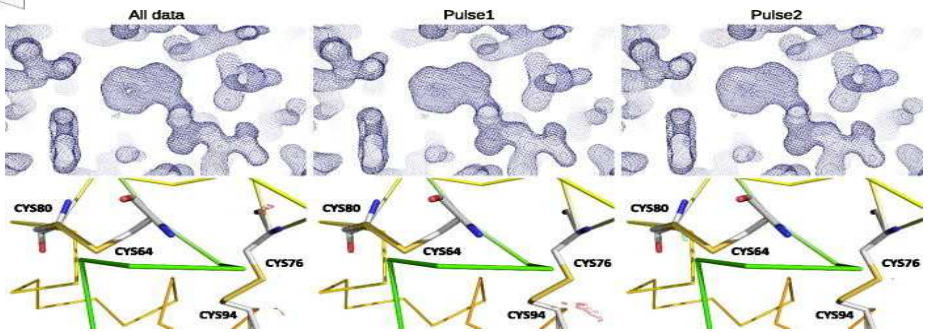
SFX structure determination with MHz pulse trains

- Yefanov, Oberthuer et al. Structural Dynamics **6**, 064702 (2019)





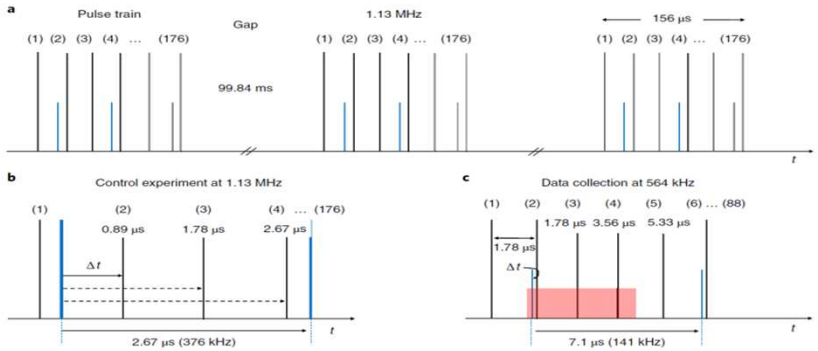
- Full data sets collected for every pulse position in 120 pulse train pattern @ 1.1MHz intra-train rate
- No discernable loss of data quality for any individual pulse position within the train
- Data from all pulses can be merged to generate high fidelity data sets: 1.3 million indexed patterns, SNR of 48

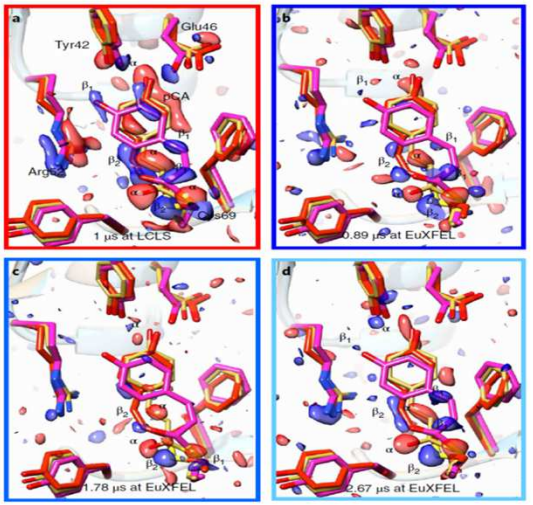


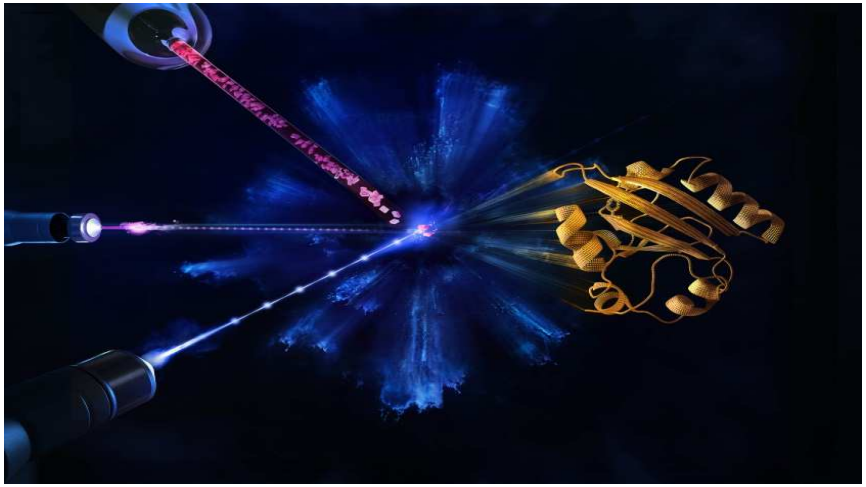
TR-SFX of PYP with custom filled MHz pulse trains

- Pandey, Bean et al. Nature Methods, volume 17, 73–78 (2020)

- X-ray and PP-laser schemes matched to excitation cycle and sample behaviour
- Pulse trains generate excitation cycle data from multiple points and control sets in single data runs
- Pathway to study entire excitation cycle in a single beamtime under the same conditions



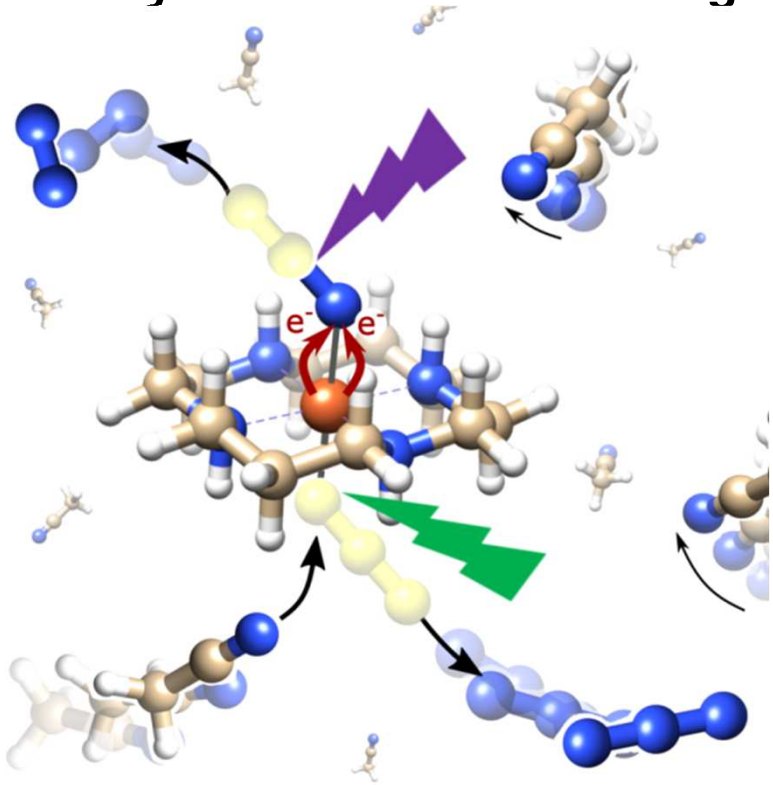





FXE

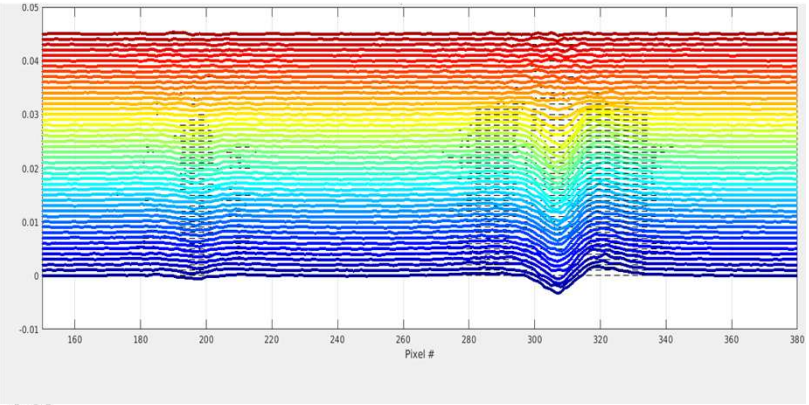
FXE scientific instrument

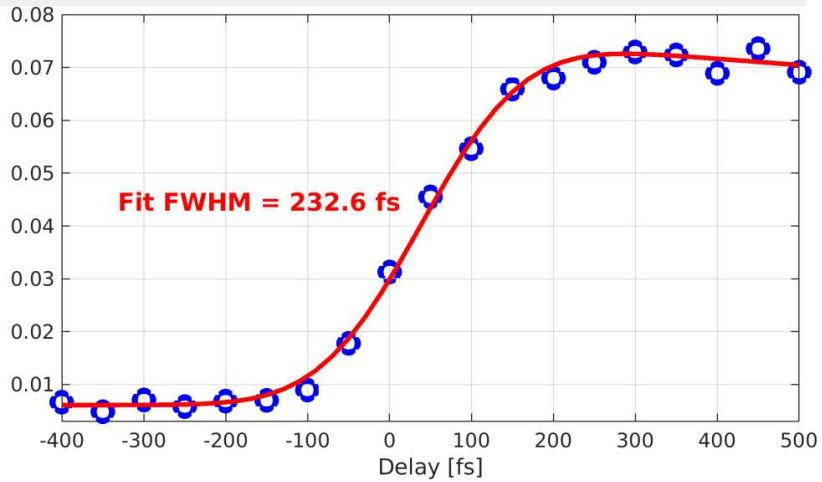
Motivation: can we possibly ever record a meaningful molecular movie?



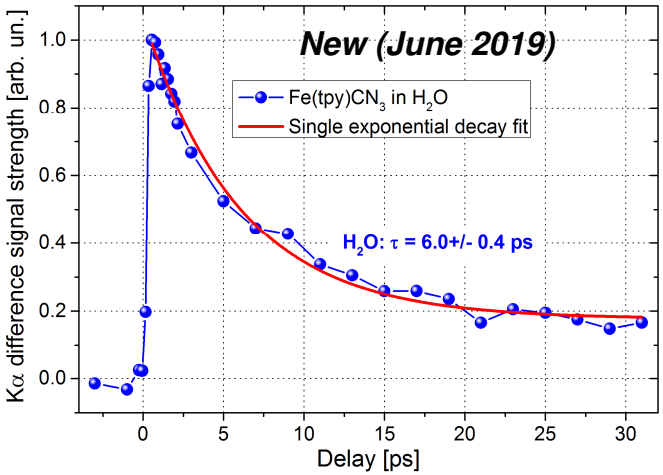
Online Monitor of pp signals allows to optimise the signal

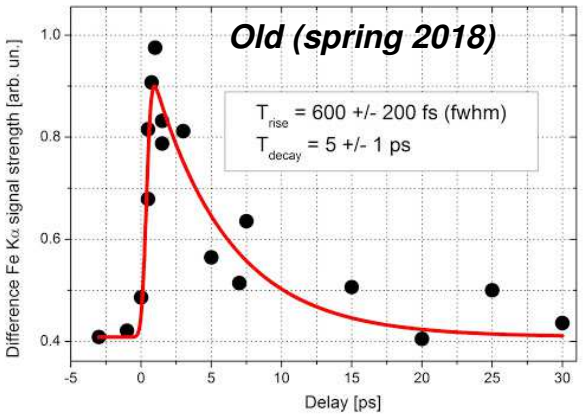
Sub-picosecond resolved XES measurements
(both Kα and Kβ emission lines)

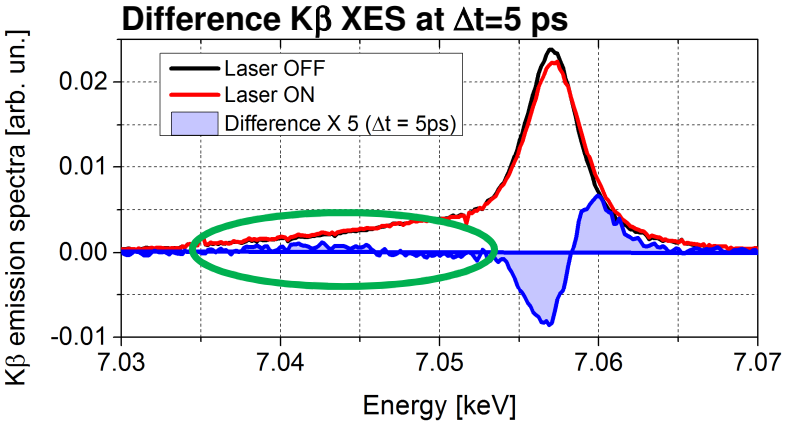




agrees with intermediate spin state lifetime via
(TD-)DFT and femtosecond optical spectroscopy

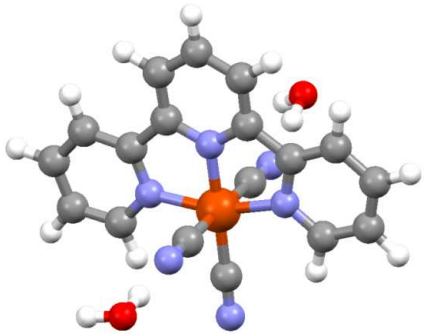






Mixture of triplet and quintet states, but <u>mostly</u> triplet

$[Fe(terpy)(CN)_3]^-$ in water



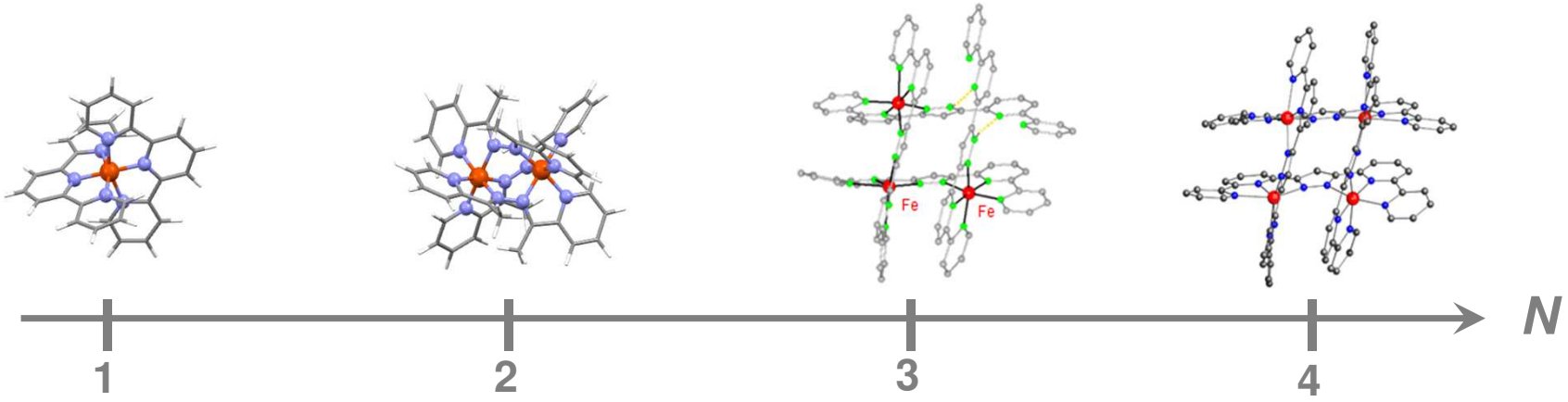
G. Vankó, *et al*; *J. Phys. Chem. C*, (2015)

European XFEL

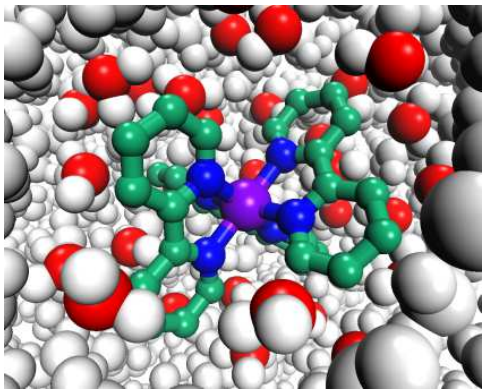
FXE : Controlling spin-state switching in the condensed phase (Experiment #2050)

30.11. – 04.12.2017 PI: Sophie Canton (DESY/ELI)

- **Characterizing the fs spin and structural dynamics as function of *N***



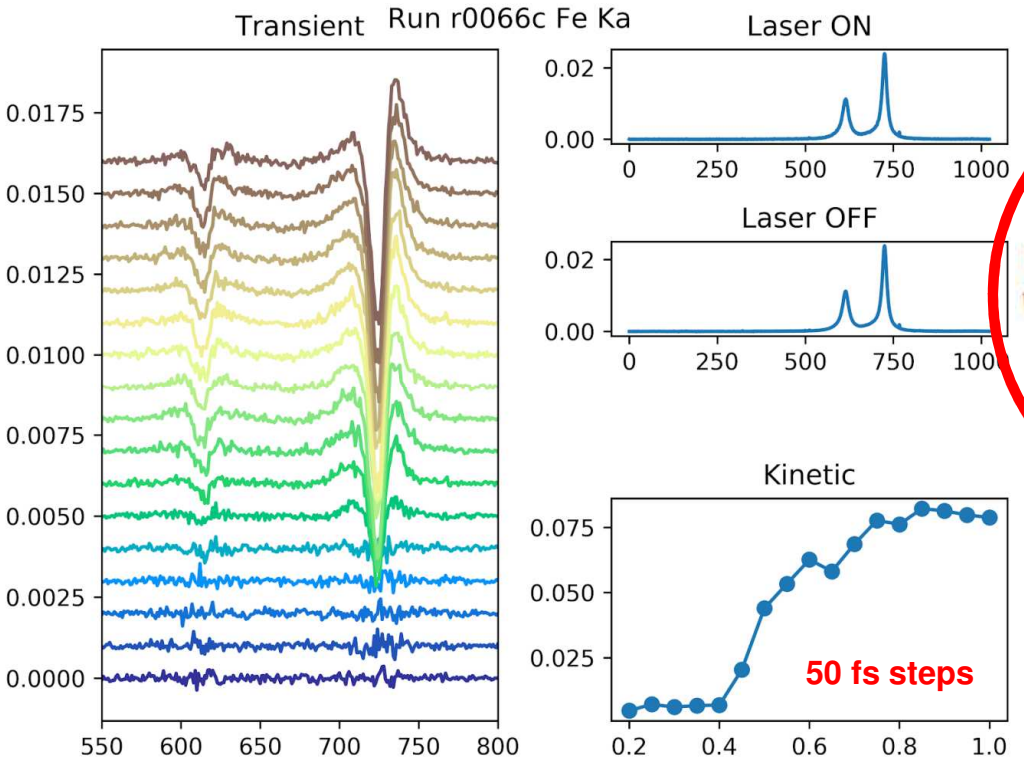
- **What is the role of the solvation shell ?**

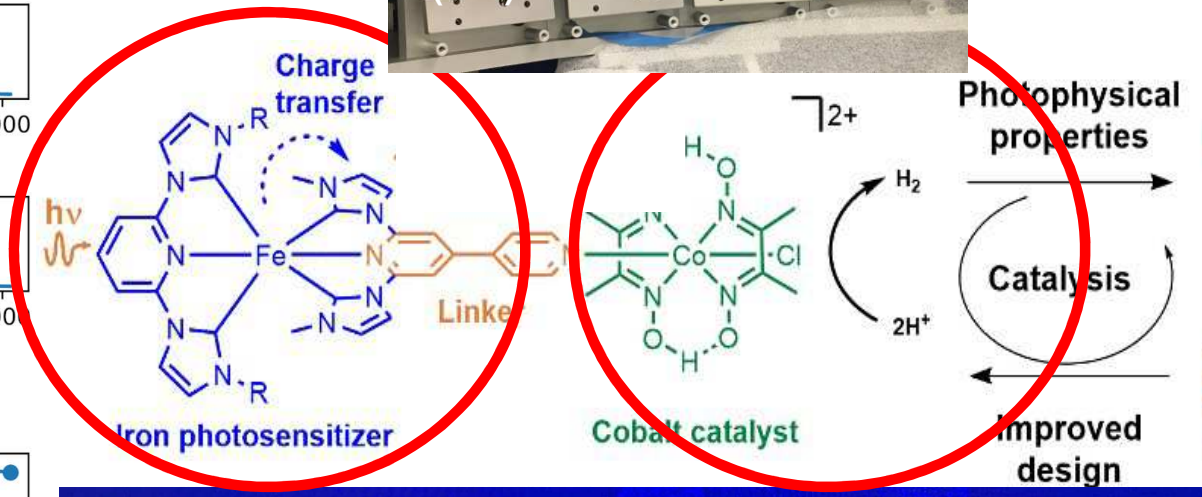


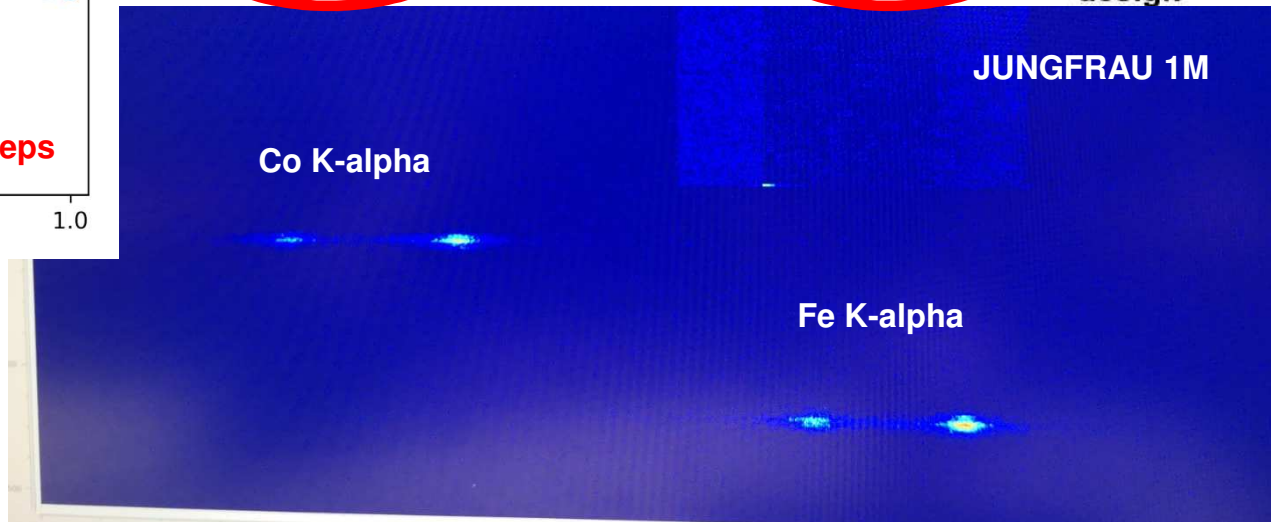
Implications

Molecular electronics, quantum information
Energy management in multichromophoric systems

September 2019 (Matthias Bauer, Uni Paderborn)



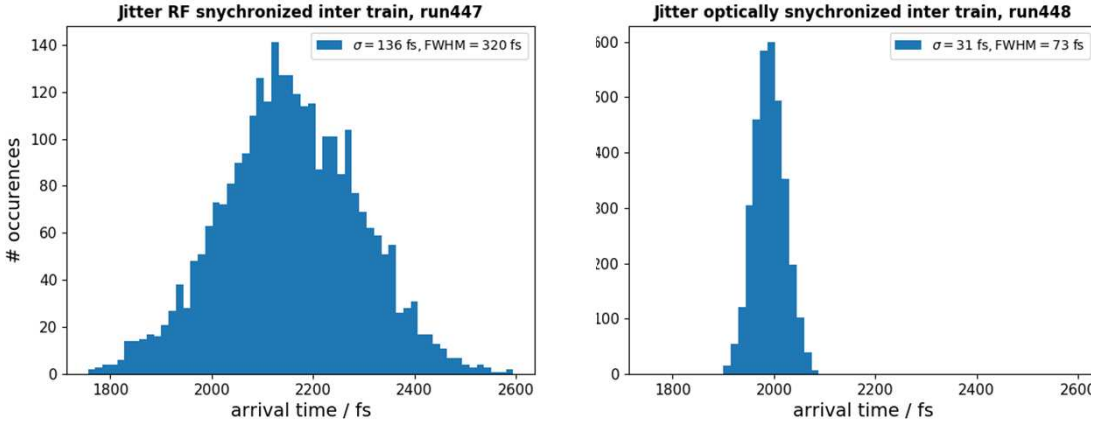




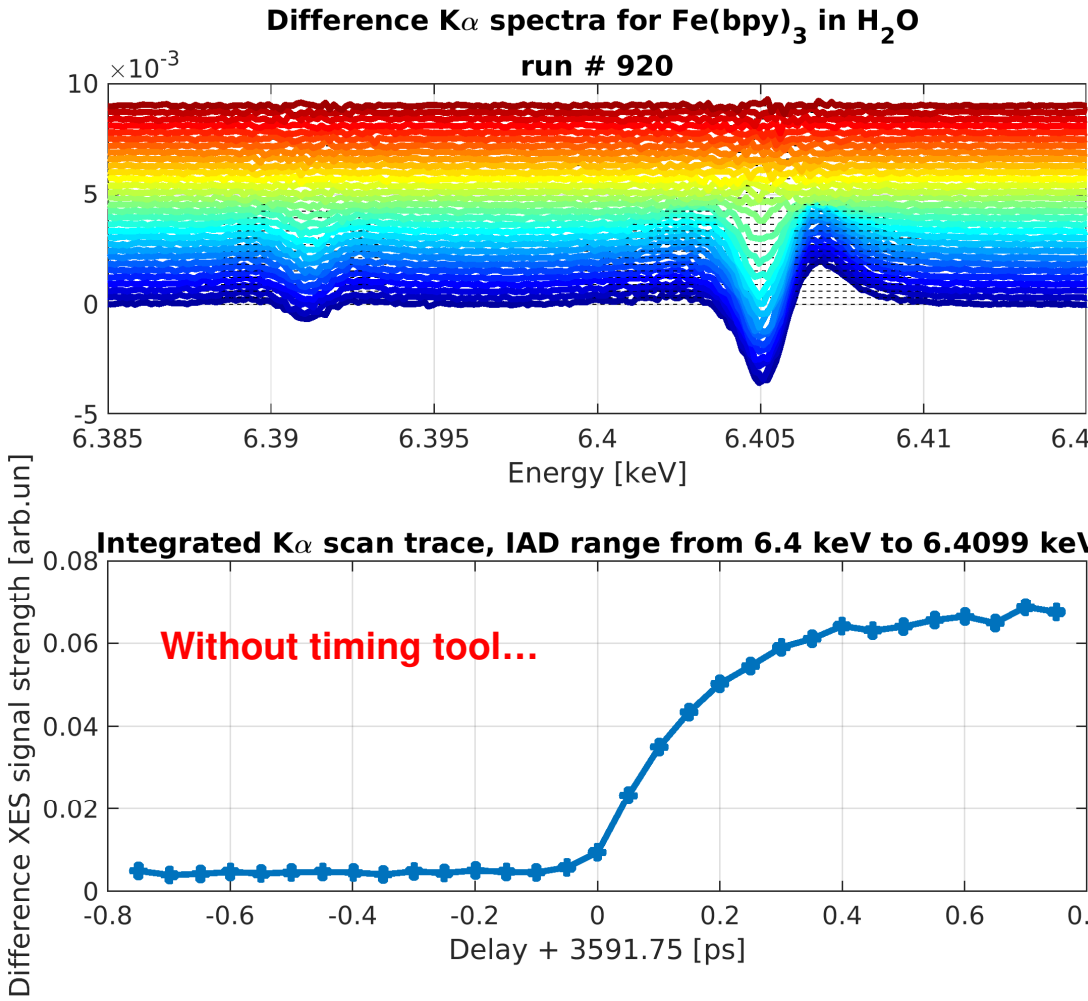
Instrumentation and detectors at FXE

Timing-tool

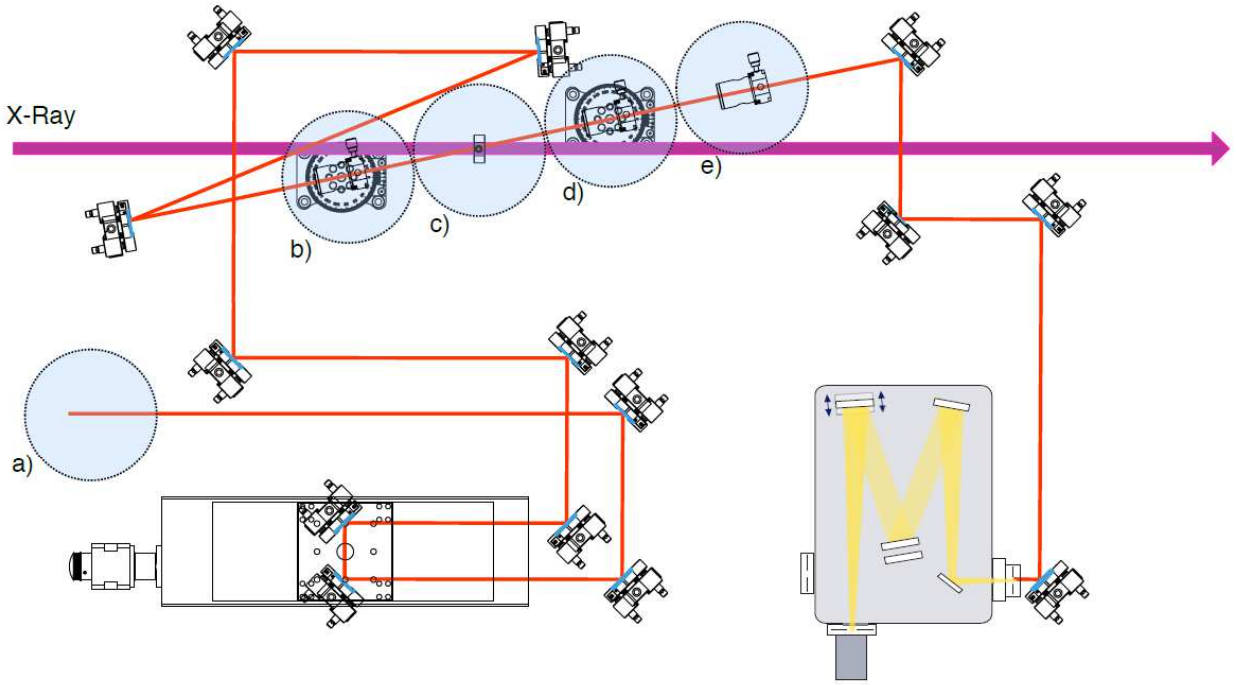
- first tests at the sample position: RF/optcial synchronization around 320/70 fs jitter (FWHM) jitter
- a non-invasive timing-tool near the sample position still needs to be implemented
- not highest priority according to user demands and current accuracy (< 100 fs, right figure)

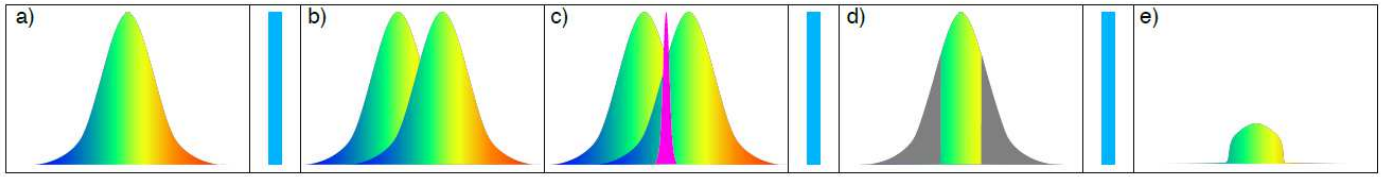


single shot @ 564 kHz detector frame rate (1.1 MHz machine)



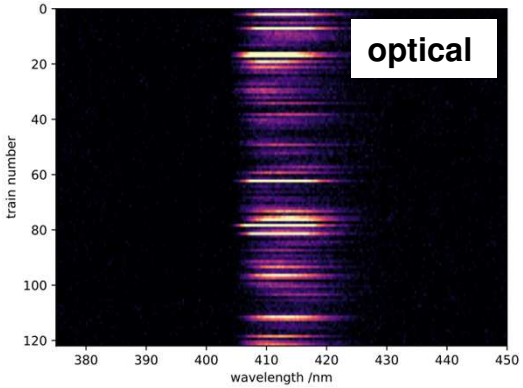
Interferometric Timing Tool Setup (M. Diez, A. Galler et al.)

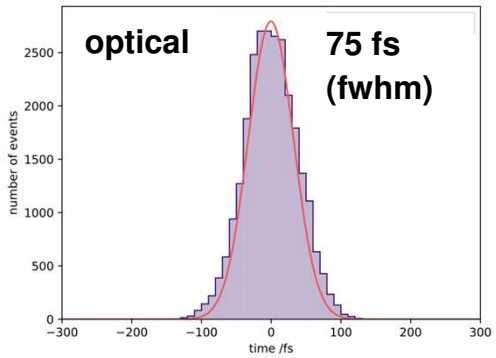


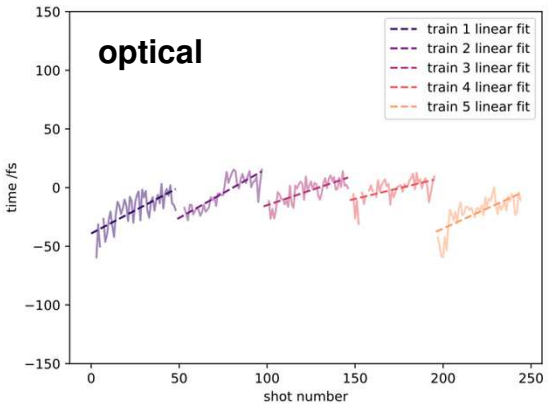


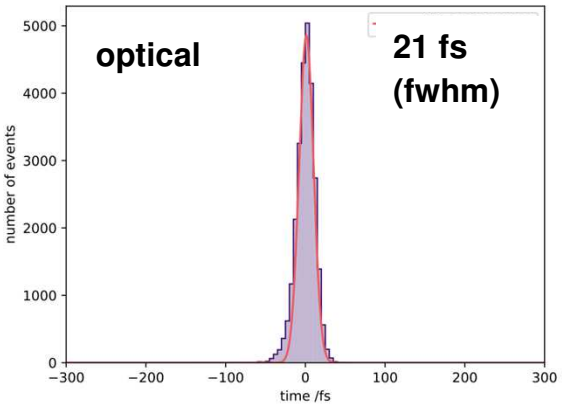
M. Diez *et al., to be published (2020)*

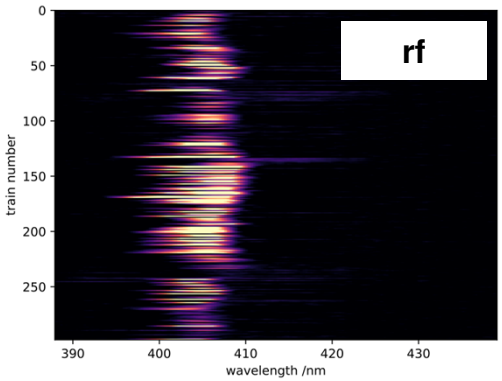
Interferometric timing tool: optical vs rf synchronization (M. Diez, A. Galler et al.)

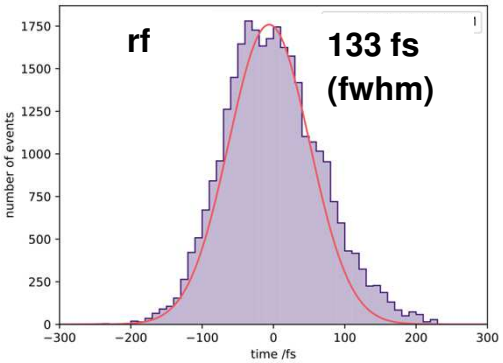


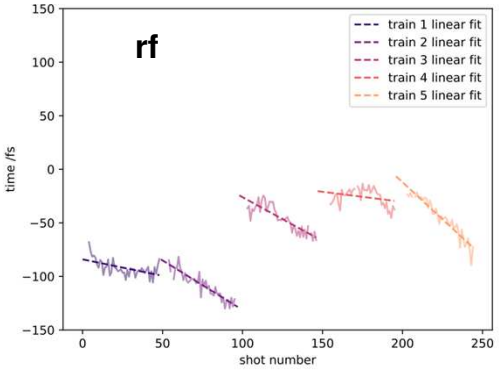


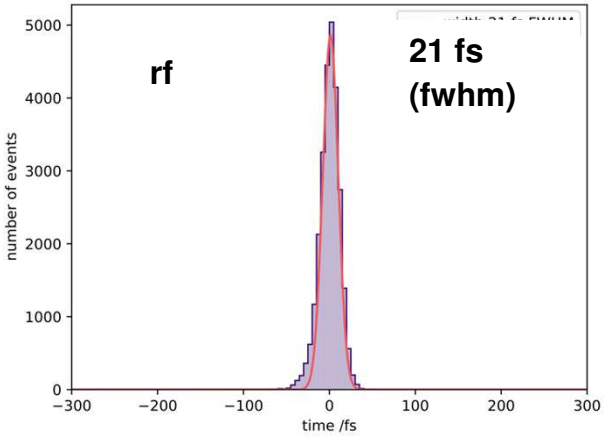






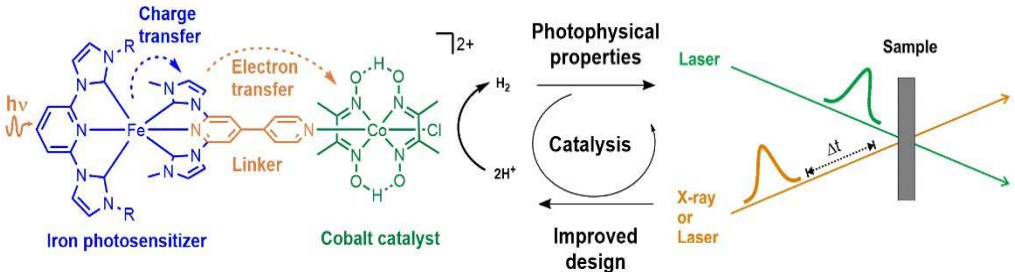






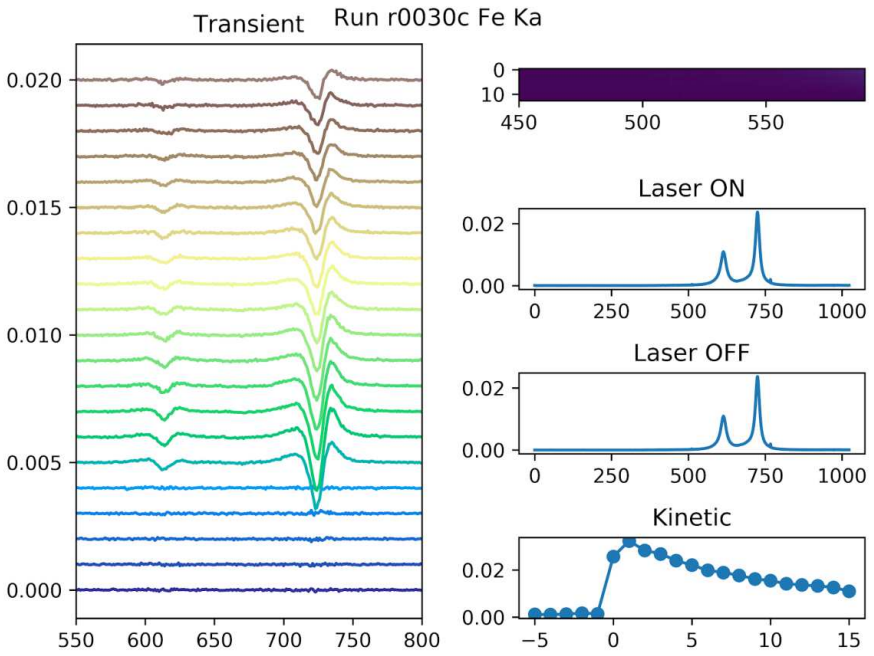
M. Diez *et al., to be published (2020)*

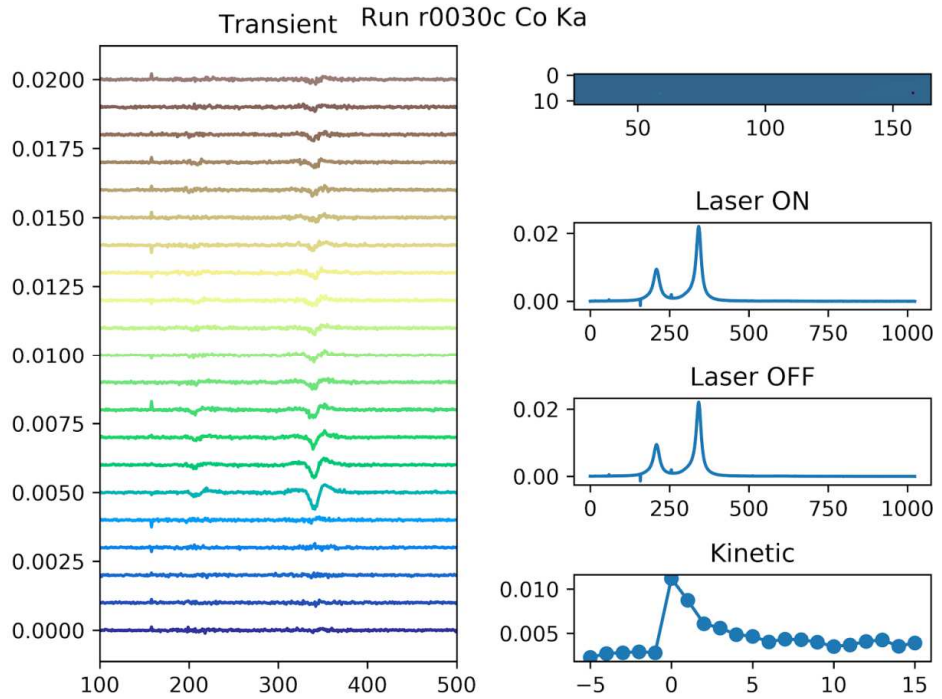
September 2019 (Matthias Bauer, Uni Paderborn)



This shows our world class signal quality with 1200 pulses/sec at 2 mJ!

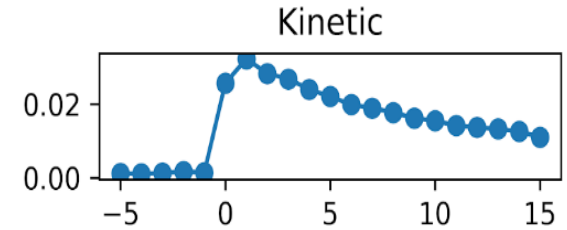
Long MLCT lifetime = efficient charge transfer?



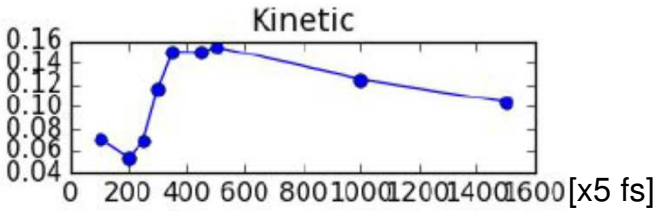


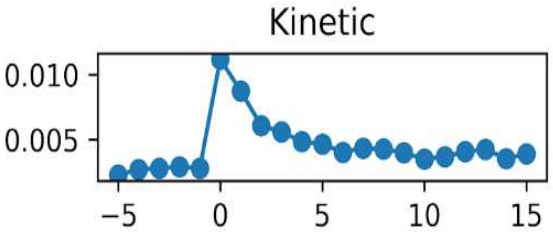
Noble-metal free dyads with Fe^{II} photosensitzer

Matthias Bauer (University of Paderborn)

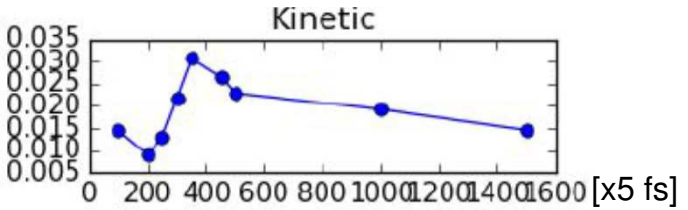


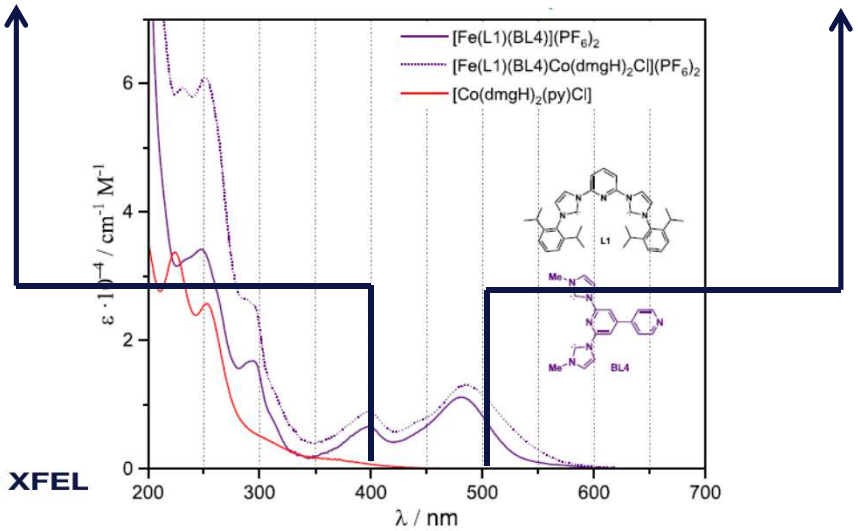
Fe Kα

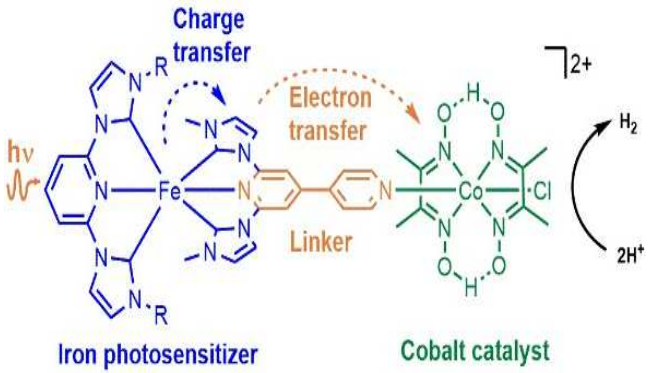




Co Kα







Acknowledgement to the fantastic European XFEL staff

Thanks to all the XFEL staff for their hard work and for their commitment.

And to the fantastic Accelerator Staff