Introduction & Scientific Trends for Different Photon Energies

"Shaping the Future of the European XFEL: Options for the SASE4/5 Tunnels"
06 - 07.12.18, Schenefeld

Serguei Molodtsov
European XFEL, Scientific Director

European XFEL inauguration (Sept. 1, 2017)

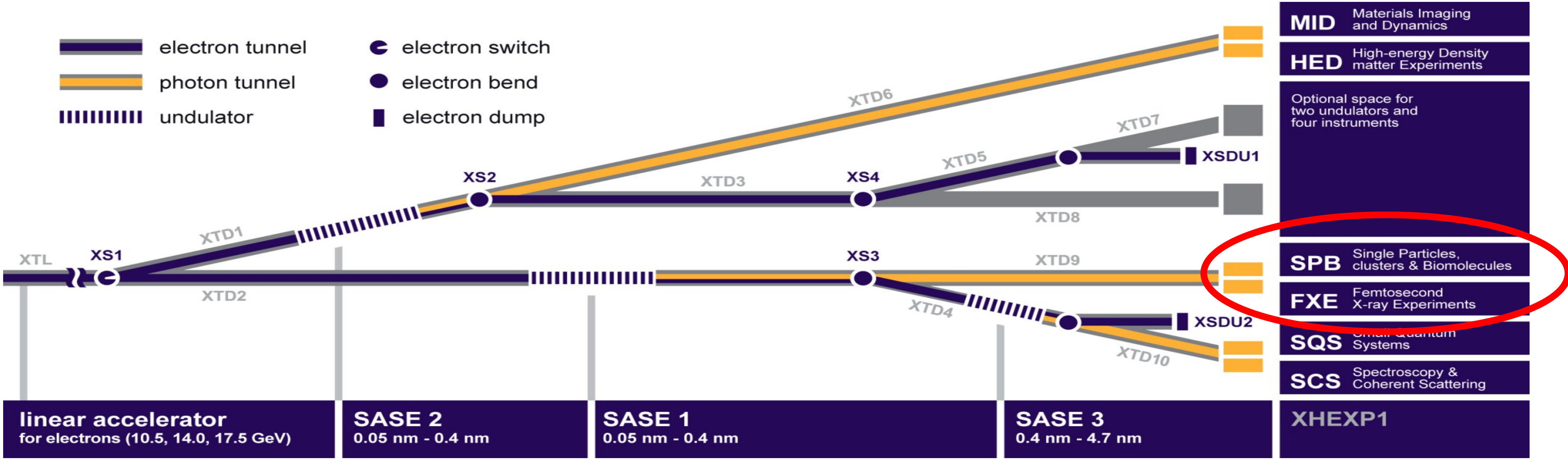
Wissenschaftler Prof. Christian Bressler erklärt Bürgermeister Olaf Scholz, Forschungsministerin Johanna Wanka und der Kieler Wissenschaftsministerin Karin Prien den Aufbau eines Experimentes Roland Magunia

Hamburg feiert seinen Superlaser

„Basis für die **Innovationen von morgen**": 800 Gäste nehmen in Schenefeld die 1,5 Milliarden Euro teure Forschungsanlage in Betrieb

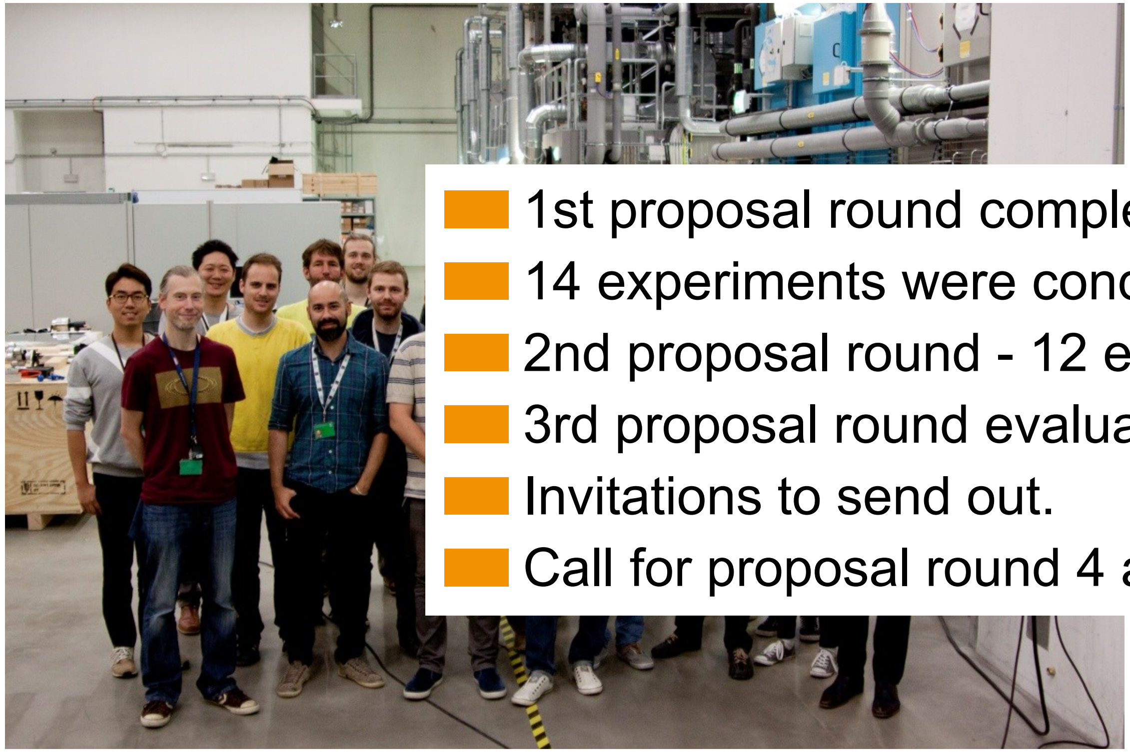
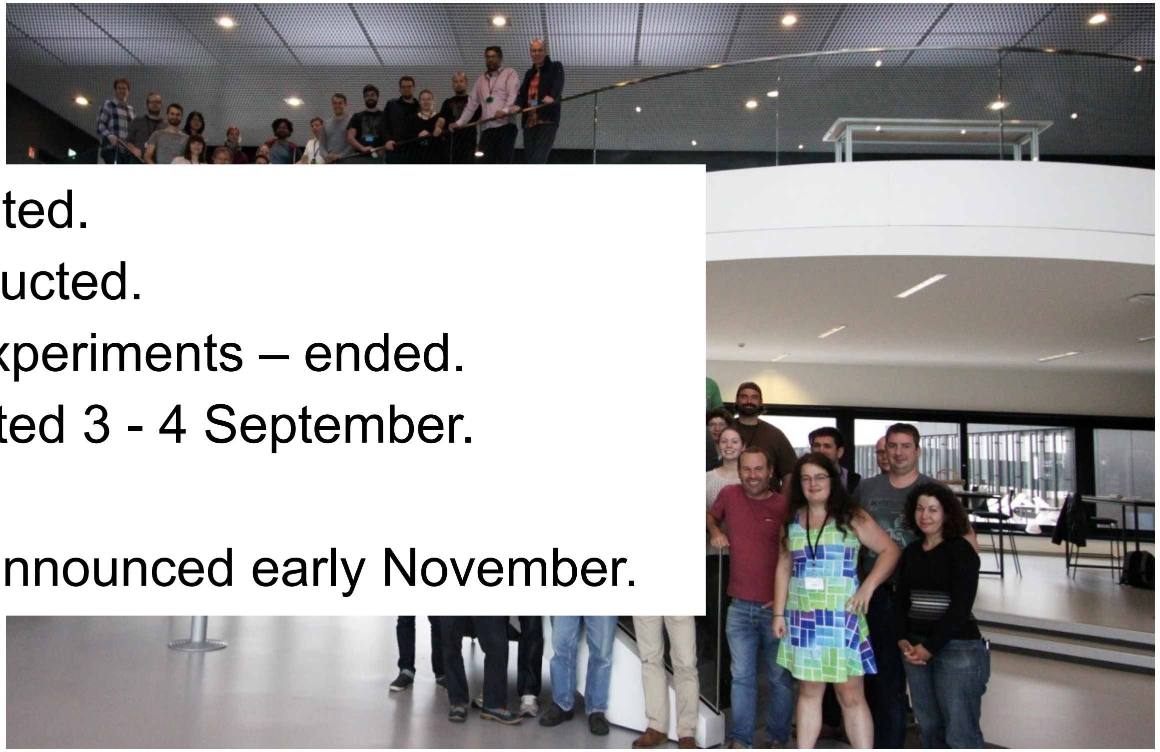
SASE1, SASE2 & SASE3 tunnels

Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24 (Hard XR)	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 – 3 (Soft XR)	4.6 – 0.4



Orange color: X-ray optics & Beam Transport

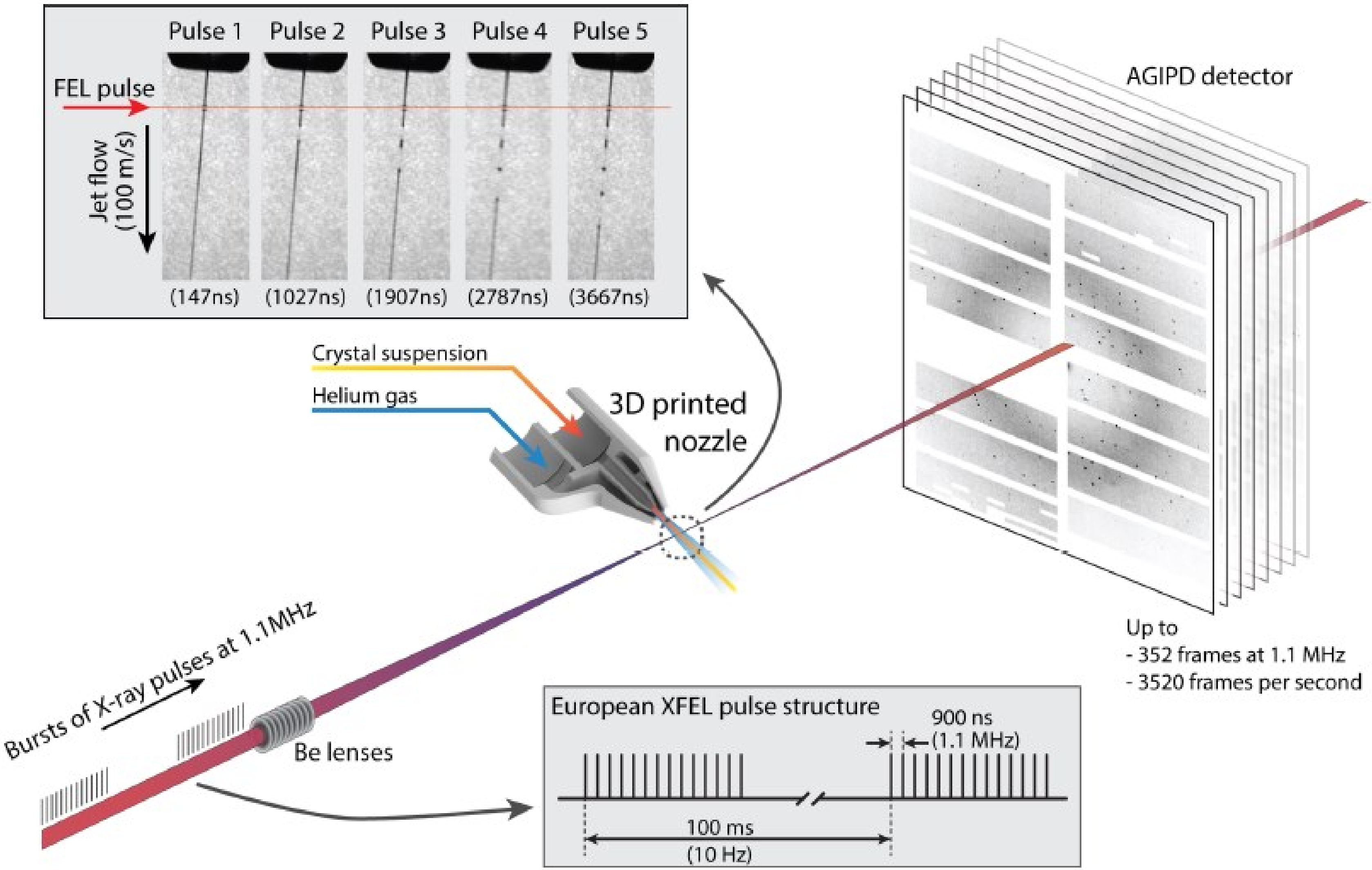
First users – 14 September 2017

- 1st proposal round completed.
- 14 experiments were conducted.
- 2nd proposal round - 12 experiments – ended.
- 3rd proposal round evaluated 3 - 4 September.
- Invitations to send out.
- Call for proposal round 4 announced early November.

Four months from first lasing to user operation !

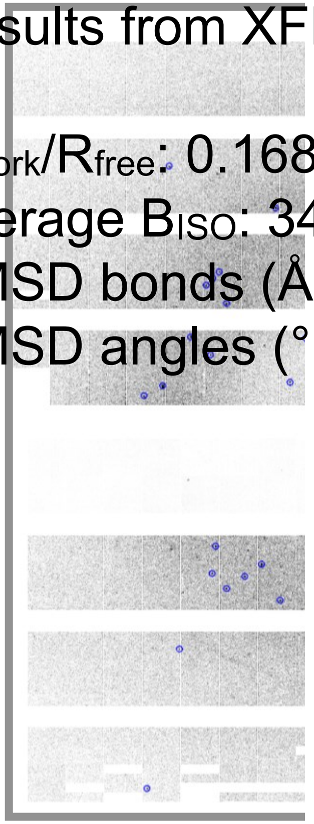
Serial Femtosecond X-ray Crystallography

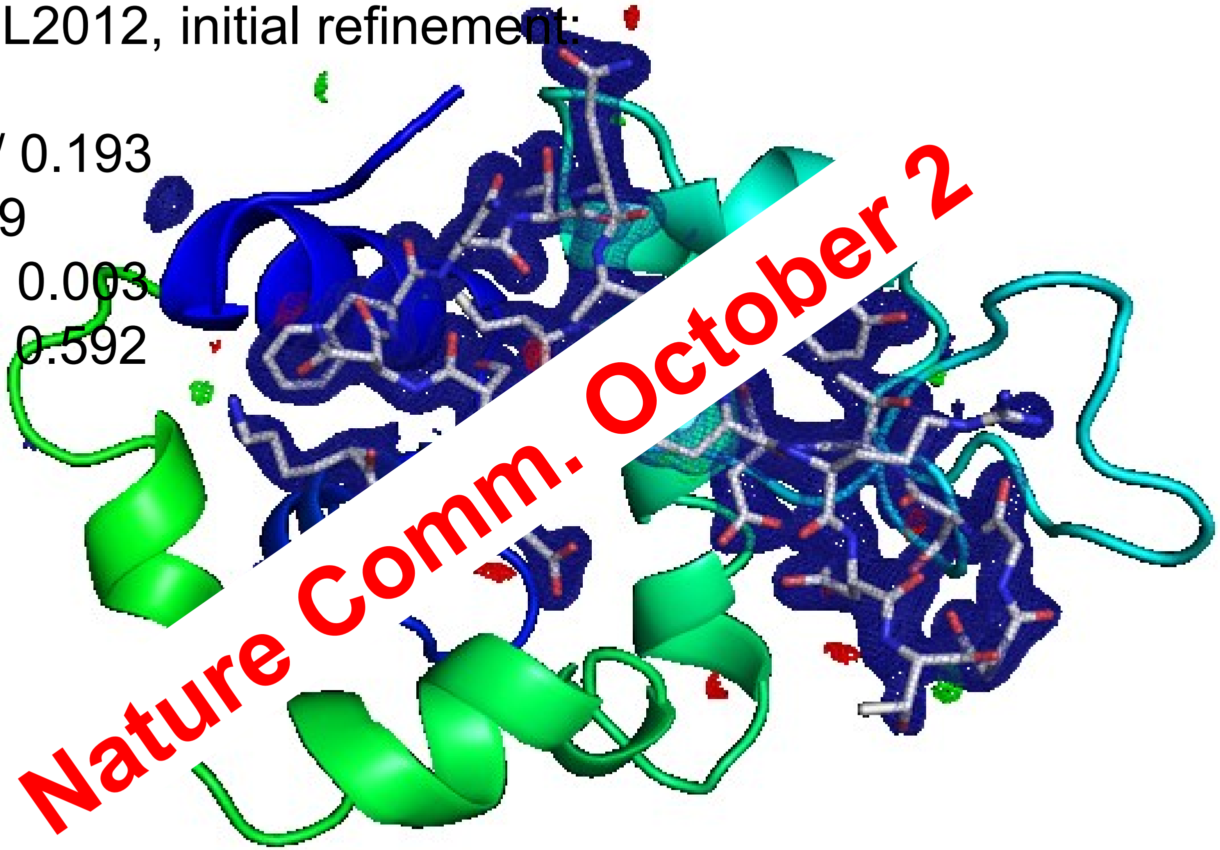


SPB/SFX experiment #2012: Many thousands of frames of diffraction data was collected and successfully analysed to give a structure!

Results from XFEL2012, initial refinement:

R_{work}/R_{free}: 0.168 / 0.193
Average B_{ISO}: 34.9
RMSD bonds (Å): 0.003
RMSD angles (°): 0.592



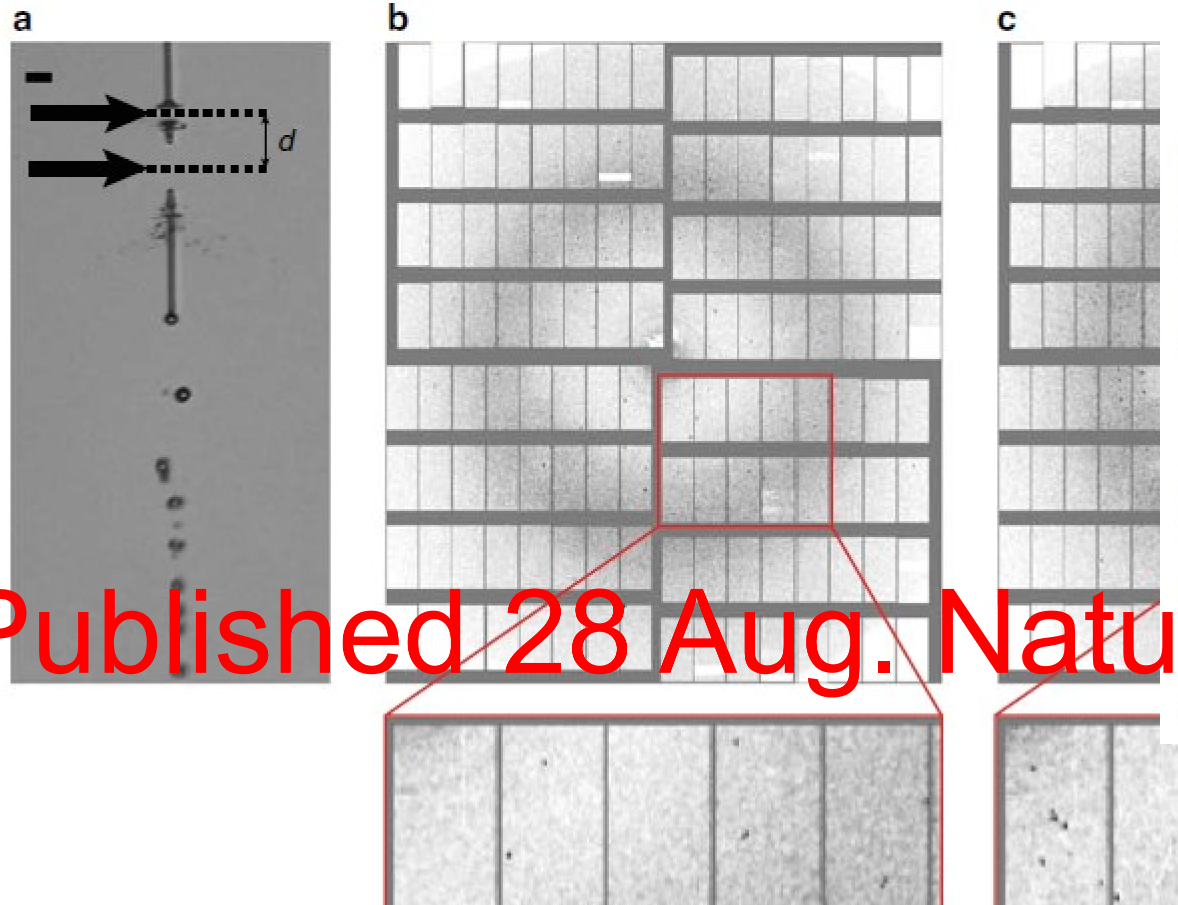


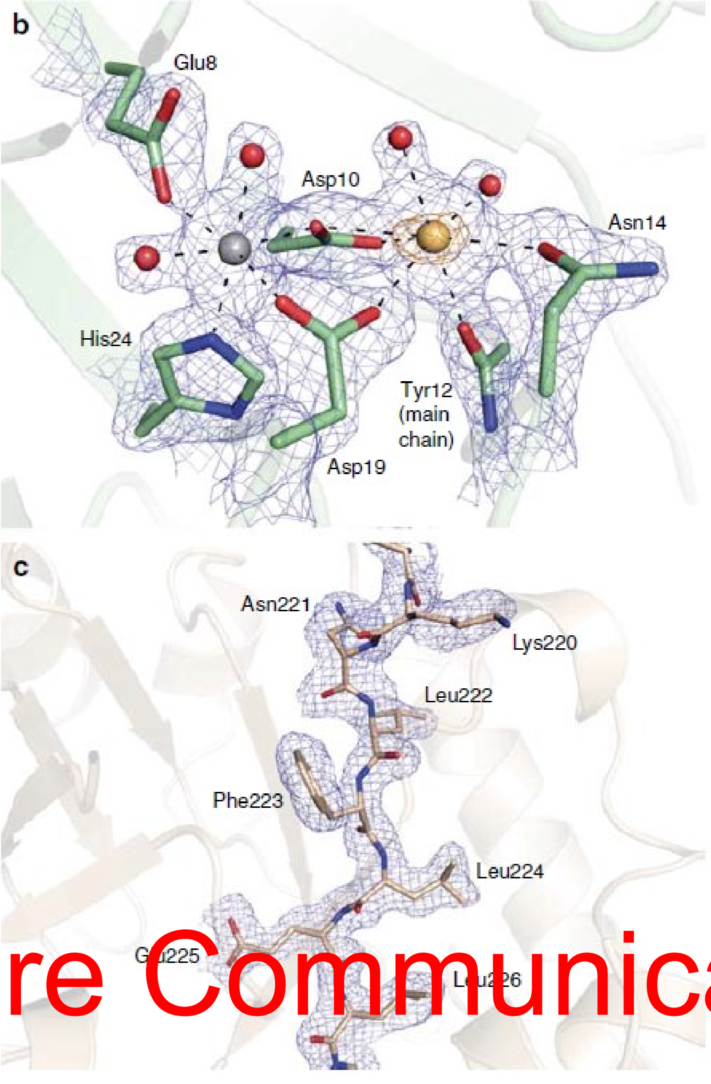
- This is the first realisation of the European XFEL purpose – a complete experiment from start-to-end demonstrated in the very first user experiment at the facility at the SPB/SFX instrument (Data September 2017, Analysis November 2017). That is, structural biology works at XFEL!

Courtesy Adrian Mancuso

Megahertz data collection from pro
microcrystals at an X-ray free-elec

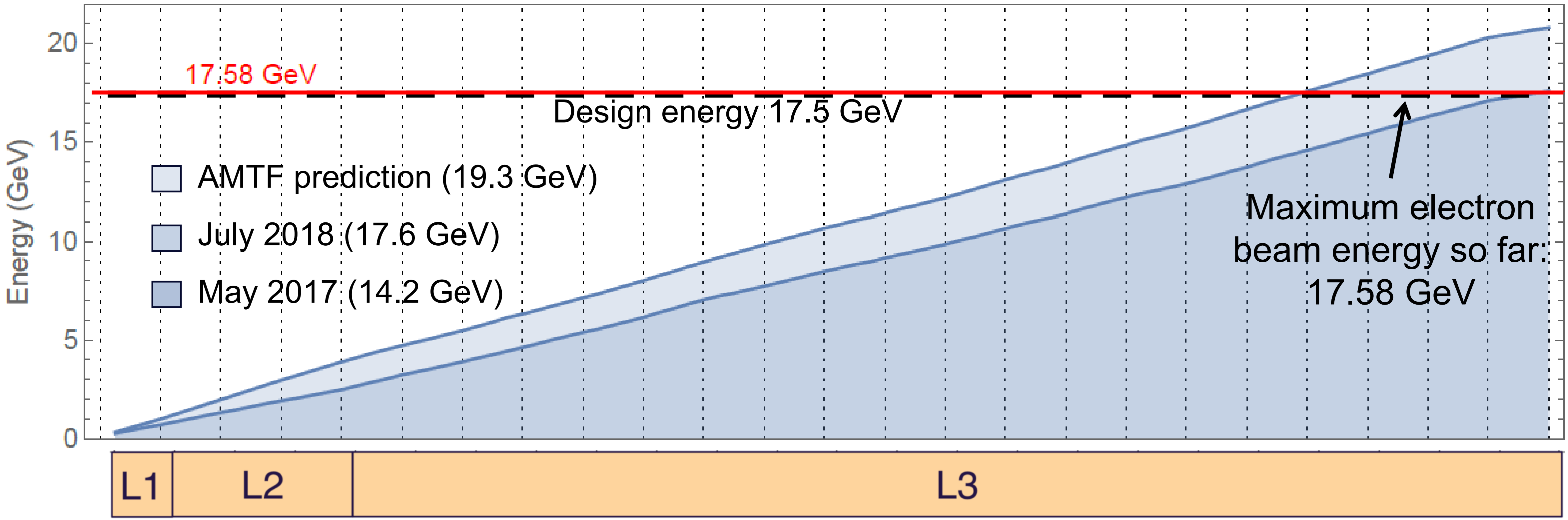
Marie Luise Grünbein[1], Johan Bielecki[2], Alexander Gorel[1], Miriam Stricker[1], R
Marco Cammarata[3], Katerina Dörner[2], Lars Fröhlich[4], Elisabeth Hartmann





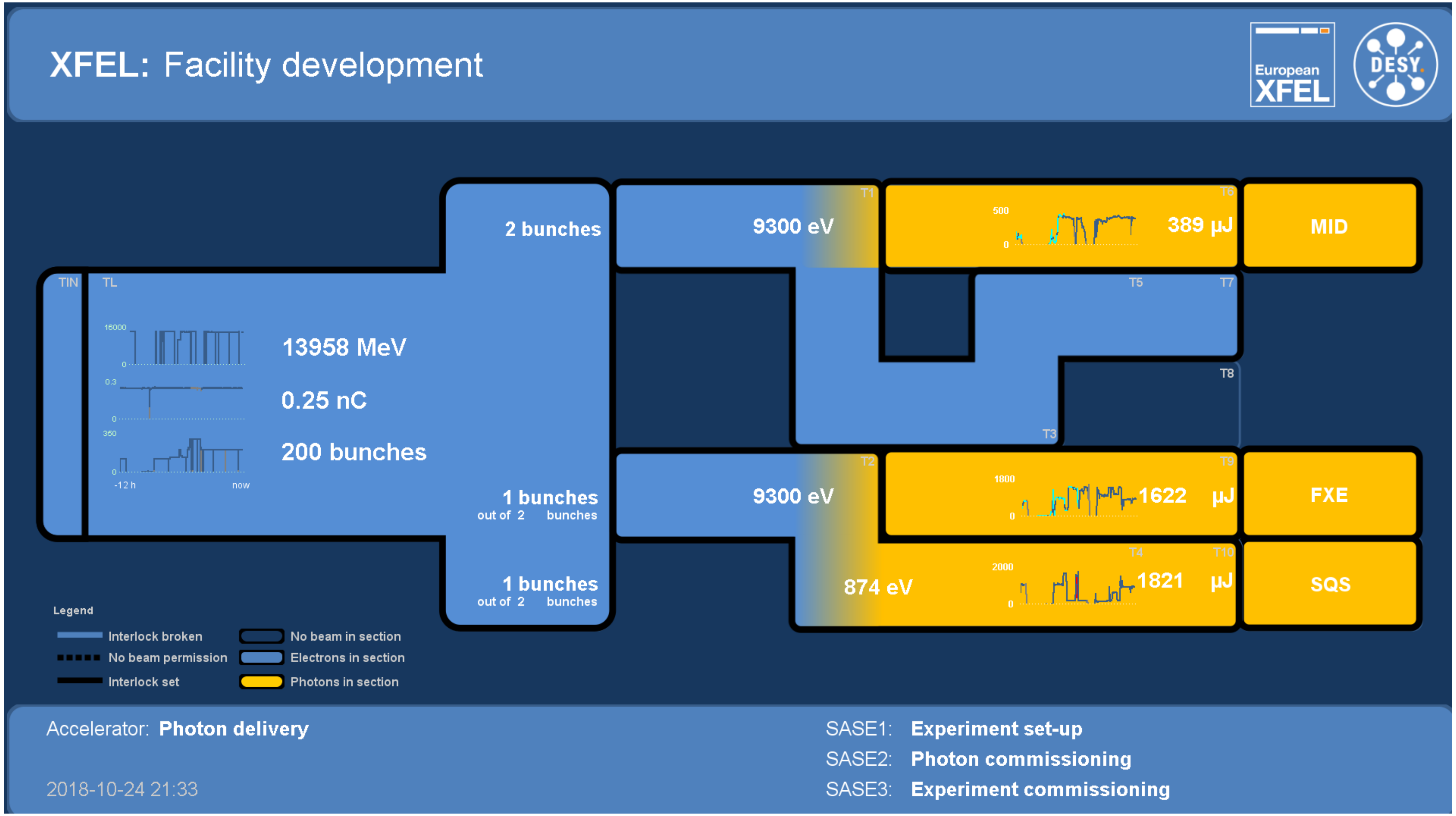
Published 28 Aug. Nature Communication

Energy reach of European XFEL: Design energy reached on 12 July 2018



- All 25 RF stations are in operation
- The maximum electron beam energy so far is **17.5 GeV**, user operation with **14.0 GeV.**
- There is still potential to increase the RF performance.

Simultaneous SASE FELs operation

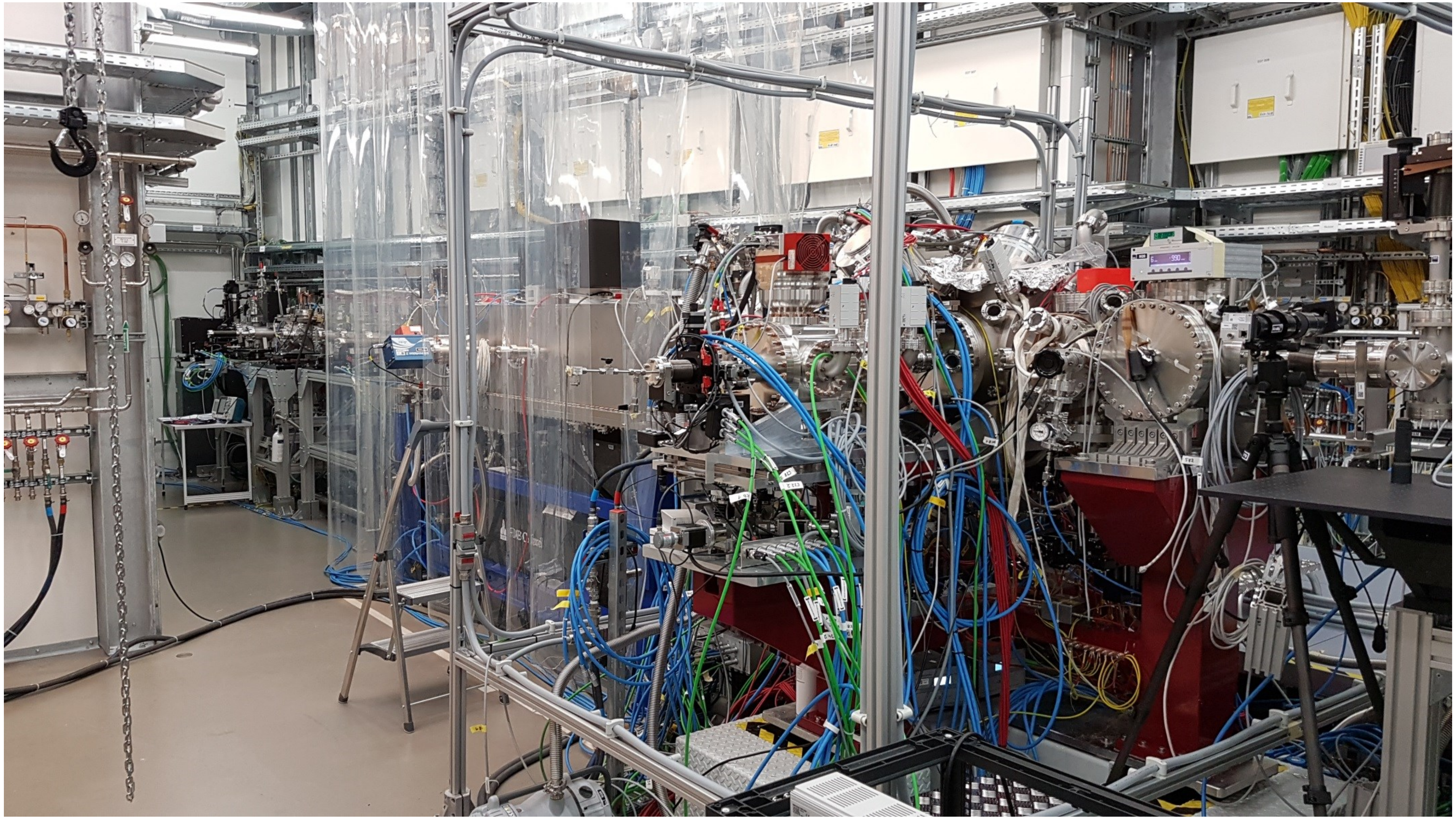


http://tesla.desy.de/status_PNGs/XFEL_StatusPublic.png

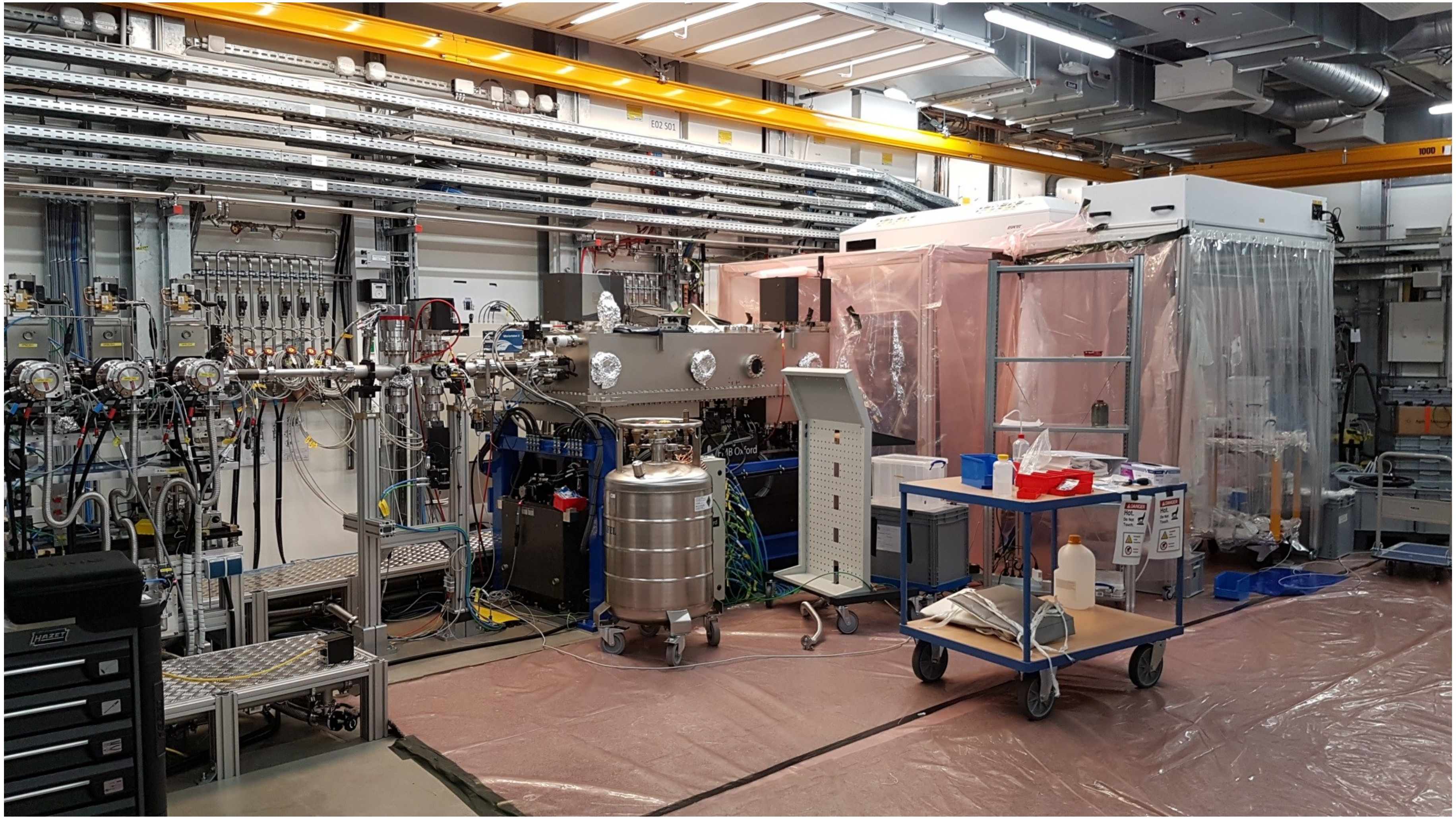
In operation:
- 3 SASE FELs
- 3 photon beamlines
- 4 experiments

In commissioning:
- 2 experiments

SQS experiment, first users in 2018



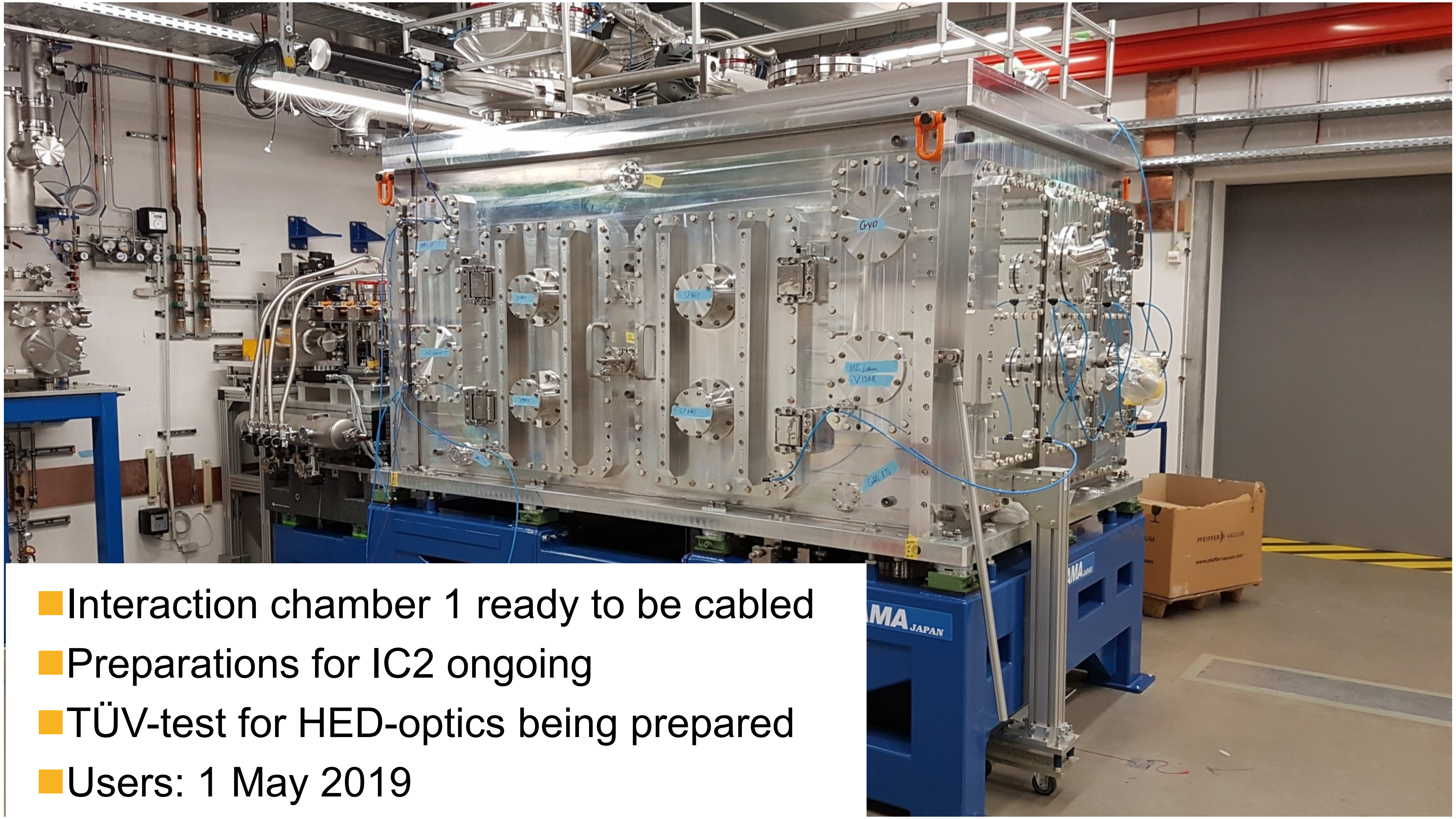
SCS experiment, first users in 2018



MID experiment: Installation and commissioning

- Beam is in the optics hutch! Commissioning since 25 October 2018!
- Exp.: Remaining cabling is ongoing; AGIPD to come in KW 45
- Users: 20 March 2019

HED experiment: Installation and commissioning



- Interaction chamber 1 ready to be cabled
- Preparations for IC2 ongoing
- TÜV-test for HED-optics being prepared
- Users: 1 May 2019

SASE4 & SASE5 tunnels

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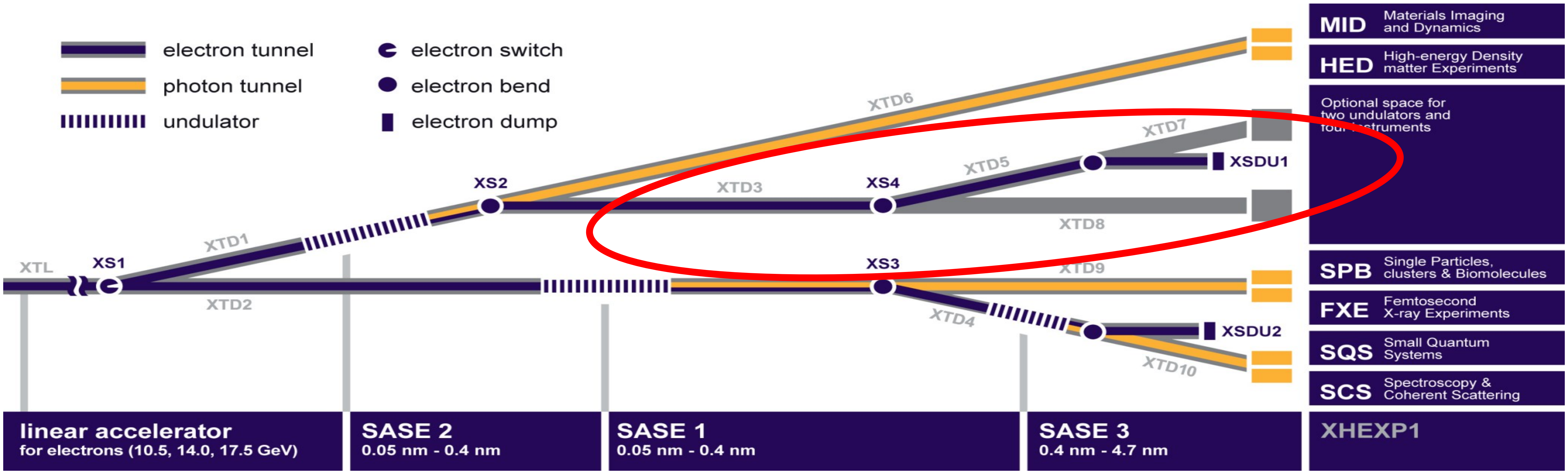


Orange color: X-ray optics & Beam Transport

Time scale and milestones for SASE 4 & SASE 5 implementation

- **2018**
  - Technical committee was formed.
  - Technical Workshop on possible solution for Photon Sources and related systems.
  - Technical committee will evaluate proposals for possible solutions.

- **2019**
  - A “library” of technically possible solutions will be communicated to the scientific community.
  - Science committee will be formed.
  - Workshops on scientific opportunities (*hard X-rays, soft X-rays, attoseconds, THz …*).
  - Working group on preparation of CDR and TDR will be formed.
  - Preliminary investigations of funding possibilities.

Time scale and milestones for SASE 4 & SASE 5 implementation

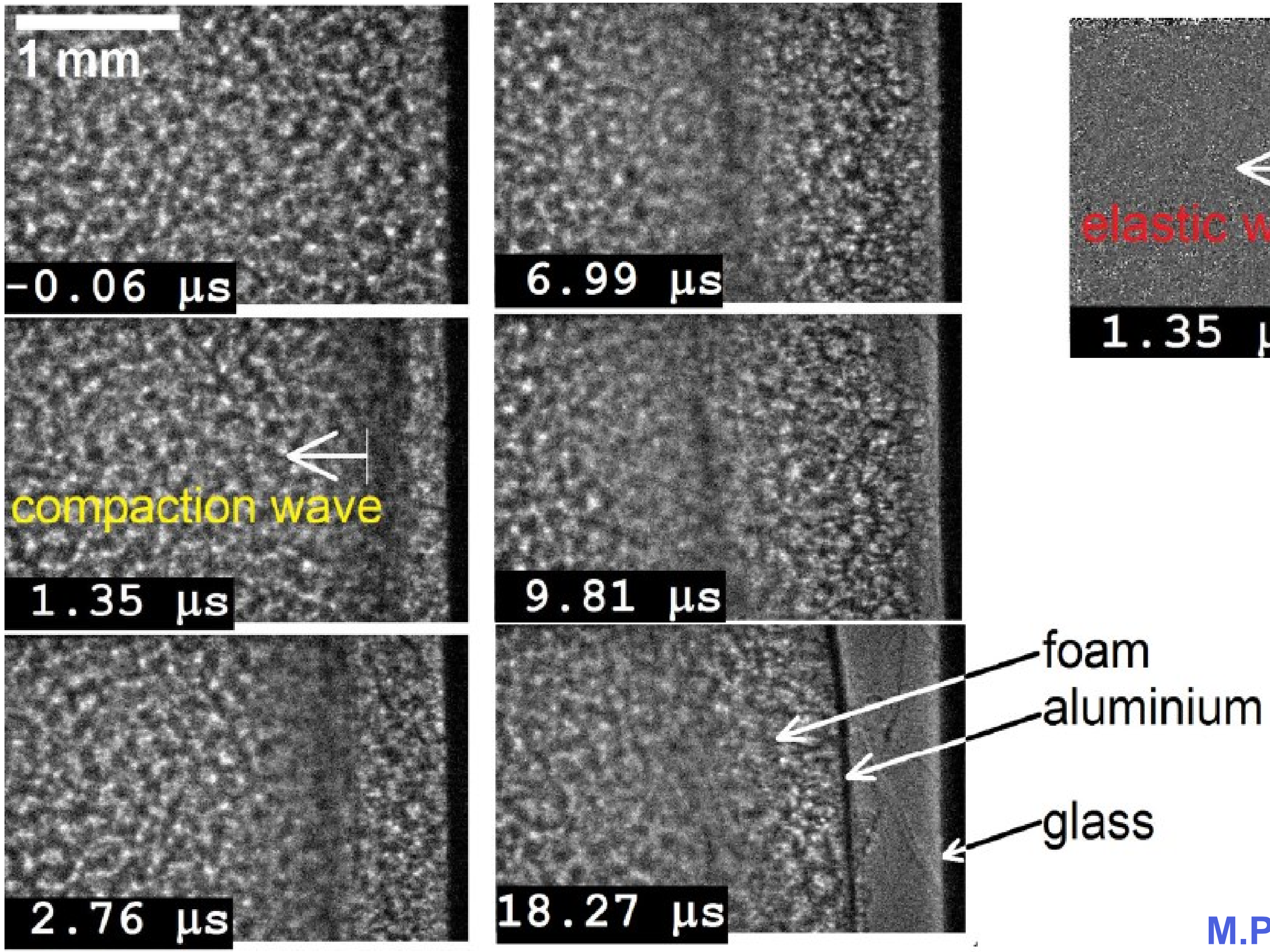
- **2020**
  - Presentation to SAC and European XFEL Council.
  - Start development of CDR for new Photon Sources, photon beam transport systems and 2-6 new experimental stations.
- **2021**
  - Start development of TDR based on CDR as described above.
  - Securing funding and initiate Council decision on implementation.
- **2022**
  - Starting construction of hardware in the tunnels and instruments.
- **2024**
  - Start of commissioning of instruments.
  - Beginning of early user program.

Hard X-ray XFEL science

- **Very high photon energies (up to 100 keV) will open up broad applications, especially in material research and including industrial opportunities**
  - Hard X-ray photon energies can reveal internal structure and dynamics of dense matter.
  - Ultra-short wavelengths will allow increase of sampled volume in the reciprocal space giving possibility of simultaneous multi-Bragg reflection spots observation.

- **MHz repetition rate + ultra-high pulse energy radiation**
  - New possibilities for X-ray microscopy allowing imaging of irreversible stochastic processes (cracking) with velocities reaching several km/s.
  - Study of processes that cannot be investigated with routine pump-probe experiments.

X-ray imaging of laser-driven shock compression



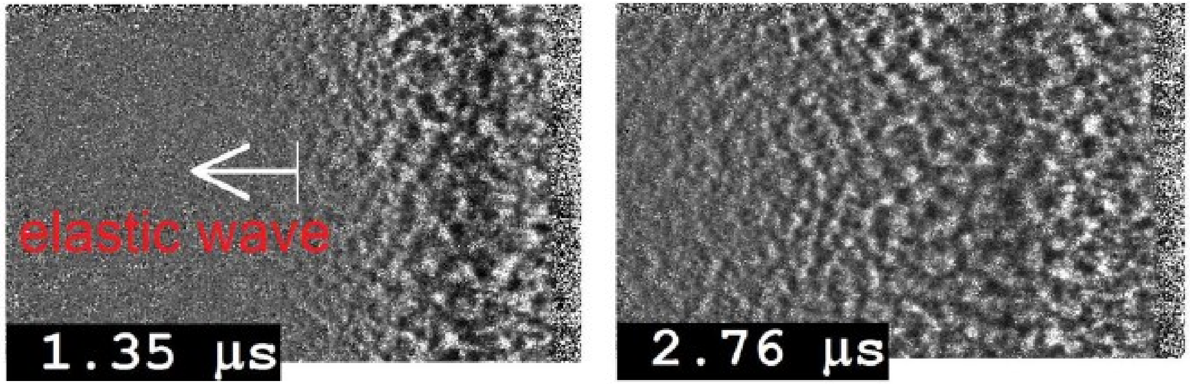


Fig. X-ray phase-contrast images of a polyurethane foam subjected to a laser shock applied on the right surface (the laser was directed through a glass plate onto an aluminium foil).

M.P. Olbinado, et al. *J. Phys. D* 51, 055601 (2018)

Hard x-ray multi-projection imaging for single-shot approaches

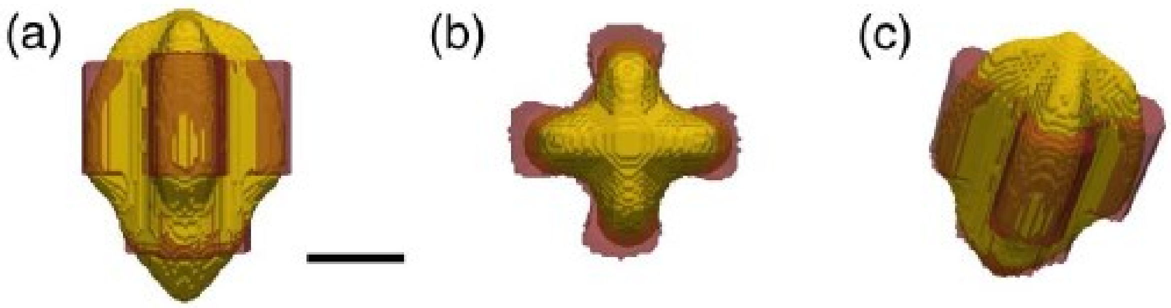


Fig. 3D reconstructions of a Si crystal projected along (a) direction perpendicular to direct beam, (b) direct beam, and (c) arbitrary direction.

P. Villanueva-Perez, et al. *Optica* 5, 1521 (2018)

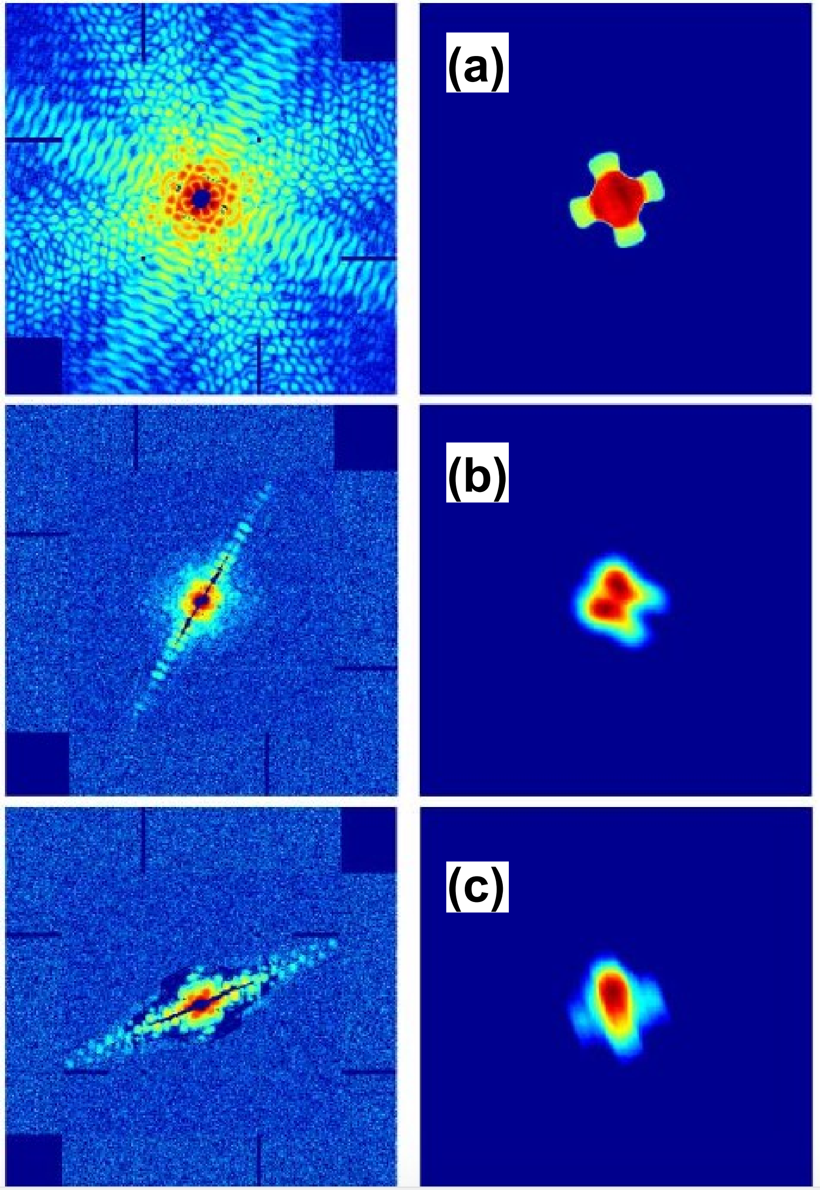


Fig. Far-field imaging experiment. (a) direct beam and (b), (c) two accessible projections. From left to right, columns show the experimental diffraction pattern, and corresponding CDI reconstruction.

Compressional seismic wave

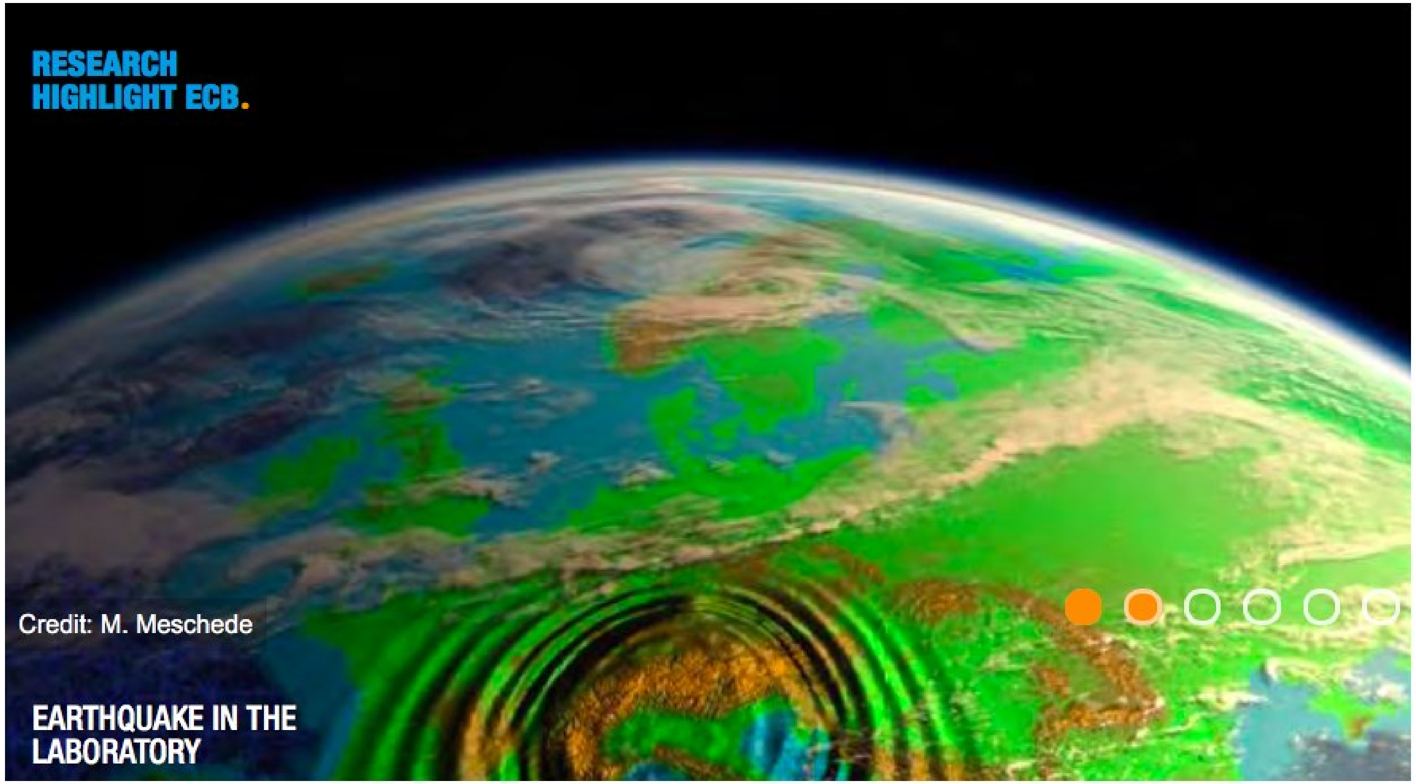


Fig. Propagation of a compressional seismic wave through $(Mg_{0.8}Fe_{0.2})O$ ferropericlase by employing a piezo-driven dynamic diamond anvil cell that allows to oscillate pressure at seismic frequencies was simulated.

H. Marquardt *et al.*
***Geophysical Research Letters* (2018)**

During pressure oscillations, X-ray diffraction images were continuously collected every 5–50 ms. The bulk modulus is directly calculated from these data at different pressures. Experiments show a pronounced softening of the bulk modulus throughout the spin crossover.

Soft X-ray XFEL science

Ultra-high pulse energy radiation

- Non-linear phenomena in photon-electron and electron-electron interactions.
- Stimulated processes in photon absorption/emission and electron relaxation.
- Imaging experiments with sub-μ focus in the optimum photon-energy range of 1-4 keV.
- Catalysis including dilute systems.

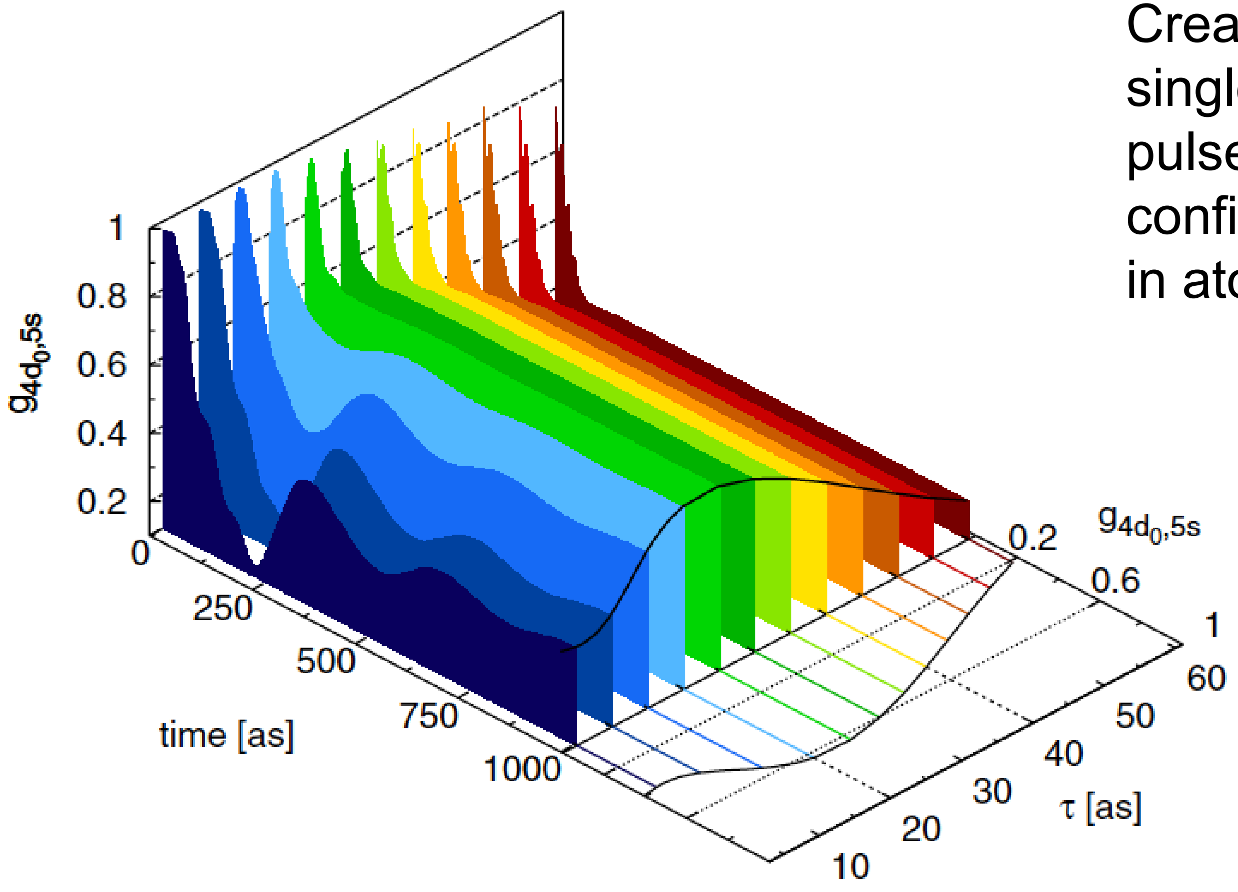
Attosecond pulses

- Follow ultra-fast electron transitions.
- Discover quantum coherence at the inter channel excitation crossover.
- Phase retrieval of electron waves in atoms and molecules.

Dedicated CircPol and 14/17.5 GeV compartible radiators

- CircPol stability better than 1% is required for studies of advanced magnetic materials (CMXD).
- Compatibility to hard X-ray operation below C edge.

Decoherence in attosecond photoionization

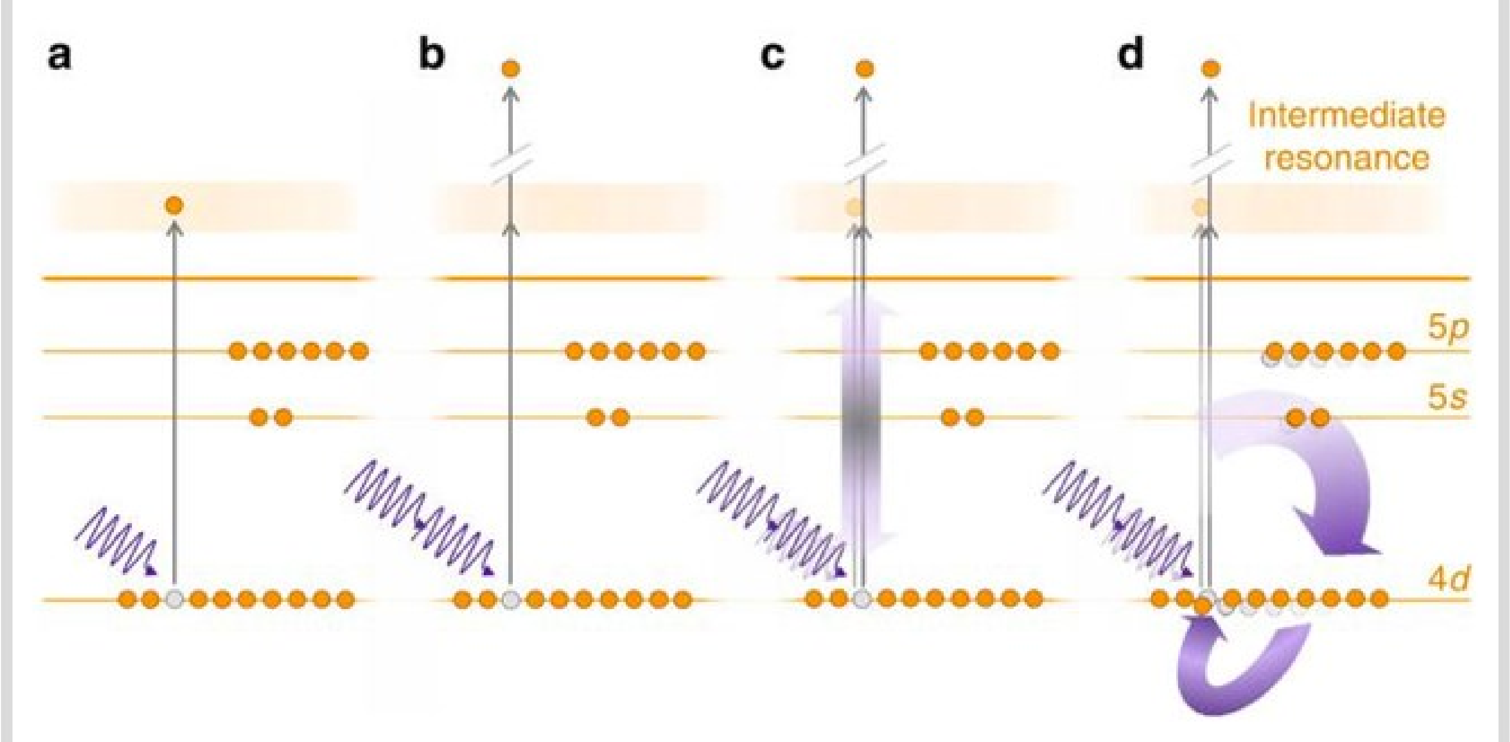


Creation of superpositions of hole states via single-photon ionization using attosecond EUV pulses is studied with the time-dependent configuration-interaction singles method in atomic Xe.

Fig. Time evolution of the coherence between the $4d^0$ and 5s hole states in xenon is shown for the full Coulomb interaction model. The photon energy is 136 eV and the pulse duration varies from 5–60 as.

S. Pabst, et al. *Phys. Rev. Lett.* 106, 053003 (2011)

Nonlinear photoionization in resonances of collective excitations in Xe

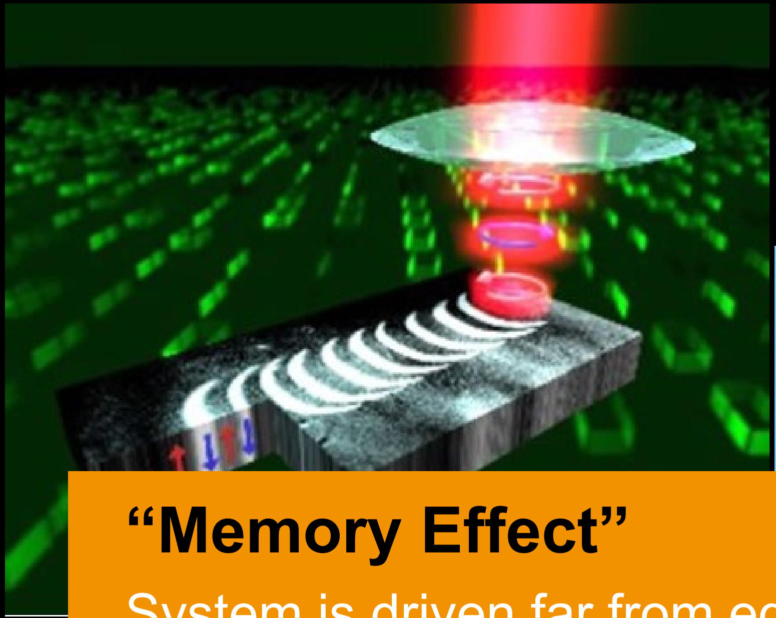


Collective behavior is a fingerprint feature in many-body systems, important for developments in fields such as magnetism, super-conductivity, etc. Nonlinear interaction of a many-body system can be used as an effective probe for characterizing otherwise unresolved features of its collective response.

Fig. (**a**) 1-photon ionization; (**b**) 2-photon ionization; (**c**) 1- and 2-photon processes according to the reduced model; (**d**) 1- and 2-photon processes accounting for electron–hole interaction in all channels open to ionization

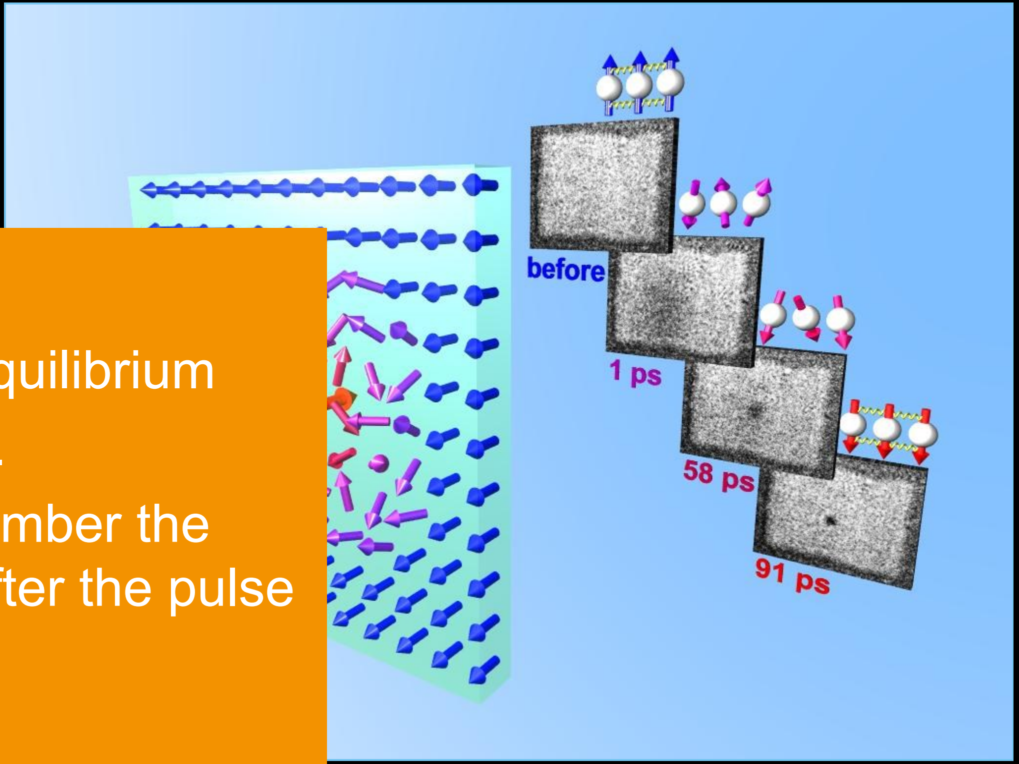
T. Mazza, et al. *Nature Communications* 6, 6799 (2015)

All-optical magnetization reversal



Stanciu, et al., PRL 2007

Deterministic switching
with circular polarized light pulses



"Memory Effect"

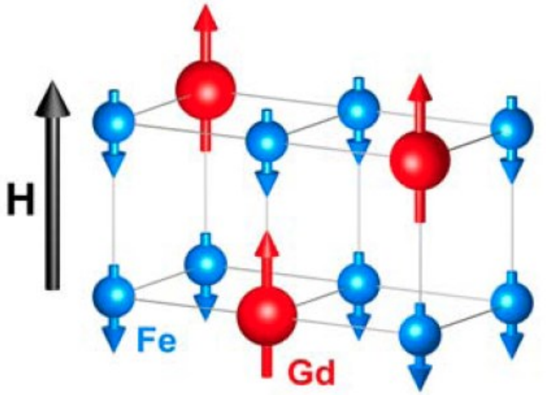
System is driven far from equilibrium leading to demagnetization.

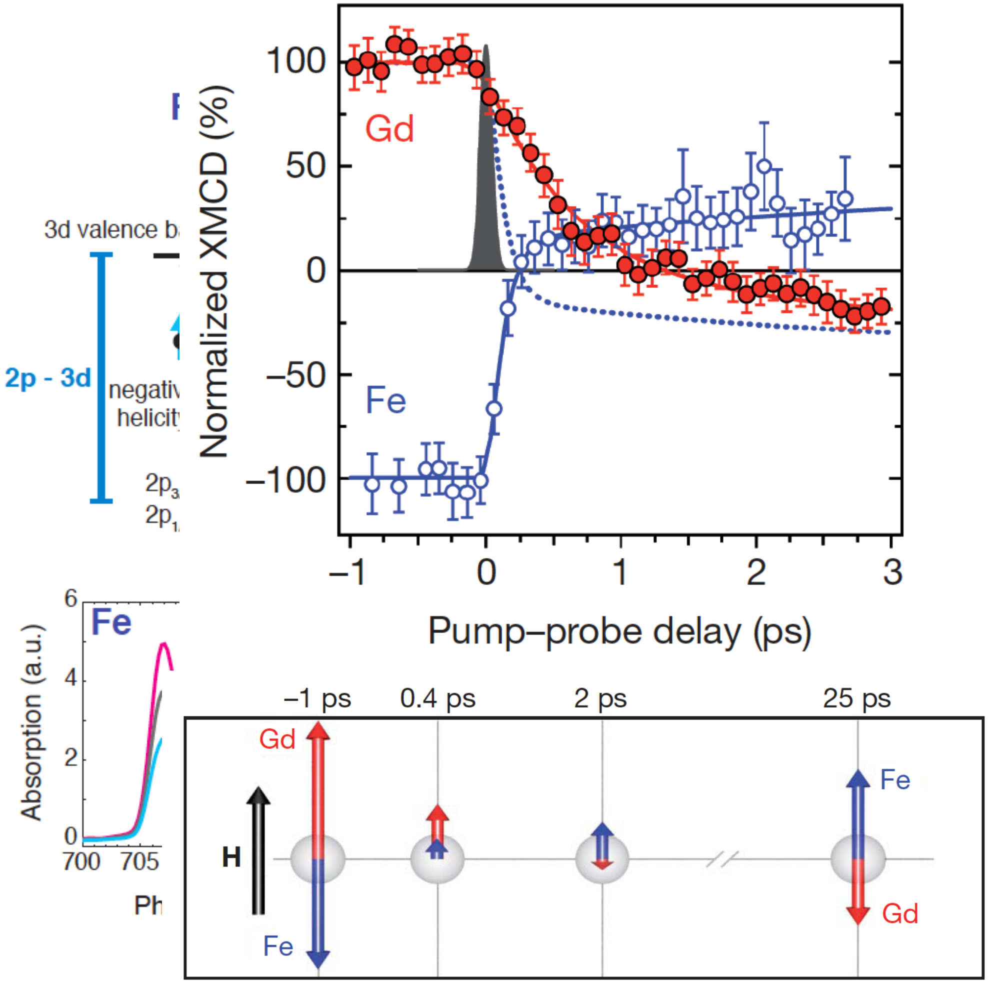
How does the system remember the photon spin a long time after the pulse passed the sample?

Courtesy from Nijmegen group

Elemental-resolved ultrafast magnetization reversal

Radu, et al., Nature 472, 205 (2011)





- Element-specific probe at Fe $L_{2,3}$ and Gd $M_{4,5}$ edge using XMCD contrast
- Gd and Fe sublattice show different magnetic response
- Transient Ferromagnetic-like state before both sublattices reversed

Workshop agenda

- Day 1, Session I: Introduction - Facility Description - Scientific trends
- Day 1, Session II: Hard X-rays
  - A hard (7 keV - 25 keV) and an ultra-hard X-ray source (25 keV -100 keV) for EuXFEL
  - Super-X: Simulations for super-hard X-ray generation with short period undulators for EuXFEL
  - Hard X-ray generation at SHINE
- Day 2, Session III: Soft X-rays
  - A soft X-ray line for generating pulses between 1nm and a few 10s nm for EuXFEL
  - External seeding possibilities at EuXFEL and THz addition
  - Superradiance for Soft X-ray production
- Day 2, Session IV: Other Concepts
- Day 2, Session V: Technological Aspects
- Day 2, Conclusions

Thank you for your attention !