Collaboration between ELI Beamlines and Solaris

Action: ELI ERIC Polish information day (8.3.2023)

Author: Jakob Andreasson

Outline;

Mix of presenting people and projects, history and science related to “ELI BL/Solaris” and presentation of ELI BL presnet readiness and capabilities

"*building research infrastructures in Visegrad countries within the European research area*"

Collaboration between ELI Beamlines and Solaris; people, science and technology

- Under development since 2016, mainly supported by Visegrad funding (with some satellites).
- Technology development: X-ray sopectroscopy at ELI Beamlines.
- Science: Photochemistry using complementary X-ray and optical techniques

User operations at ELI BL

- User readiness; some statistics from first years of user operations

Complementarity between big facilities; Outlook

- Synchrotrons, FELs, Laser labs
- Plans and wishes at ELI BL
- Solaris-ELI BL “joint laboratory”, PhD/young researcher programmes

ELI BL/"Solaris" core joint projects

Three rounds of Visegrad projects

Years	Applicant (Institution)	Coordinator	Project title
01/01/2017 - 31/12/2017	Institute of Physical Chemistry Polish Academy of Sciences, Seat: Warsaw, Poland	Prof. Jakub Szlachetko	Development of time-resolved X-ray spectroscopy methodologies at Extreme Light Infrastructure (ELI)
2018-2019	MTA Wigner Fizikai Kutatóközpont/Wigner Research Centre for Physics, Hungarian Academy of Sciences Seat: Budapest, HU	Dr. Zoltán Németh	Pioneering experiments with ultrafast X-ray techniques at the Extreme Light Infrastructure
2020-2022	Fyzikální ústav AV ČR, v. v. i. (FZÚ)/Institute of Physics of the Czech Academy of Sciences (IoP CAS) Seat: ELI BL, CZ	Dr. Anna Zymaková	Association of complementary X-ray and optical spectroscopy methods and communities

Bilateral mobility project PAN-20-20

Period: 01.01.2020 - 31.12.2022

Project title: Development of multipurpose liquid sample delivery system for X-ray spectroscopy applications

Establishment of the "Consortium at ELI for X-ray spectroscopy (CELIXS)"

https://xrayspectroscopyeli.wixsite.com/celixs

Experiments and publications with Polish/V4 scientists

RnD

Instrument development and commissioning -> Molecular dynamics, Photo-chemistry, bio-physics, charge trasfer, plasmonics, …

Synchrotron beamtime 2023: *"Comparative study of liquid sample systems: towards a roadmap for optimizing user choice"*

Period: 05-May-2023 to 09-May-2023

PI: Anna Zymaková

Beamline: P64 (von Hamos X-ray spectroscopy station)

Anticipated participants: Maria Naumova (DESY, DE), Alessandra Picchiotti (Hamburg University, DE), **Wojciech Błachucki** (IFJ PAN, PL), **Rafał Fanselow** (IFJ PAN, PL), Martin Precek (ELI ERIC, CZ), Petr Kahan (CZ), Gaia Giovanetti (DESY, DE)

CELIXS Applications and experiments at ELI BL

TA and FSRS UPM-57 Fanselow

TA and FSRS UPM-57 Fanselow

TA and FSRS UPM-59 Imbir

Right now!

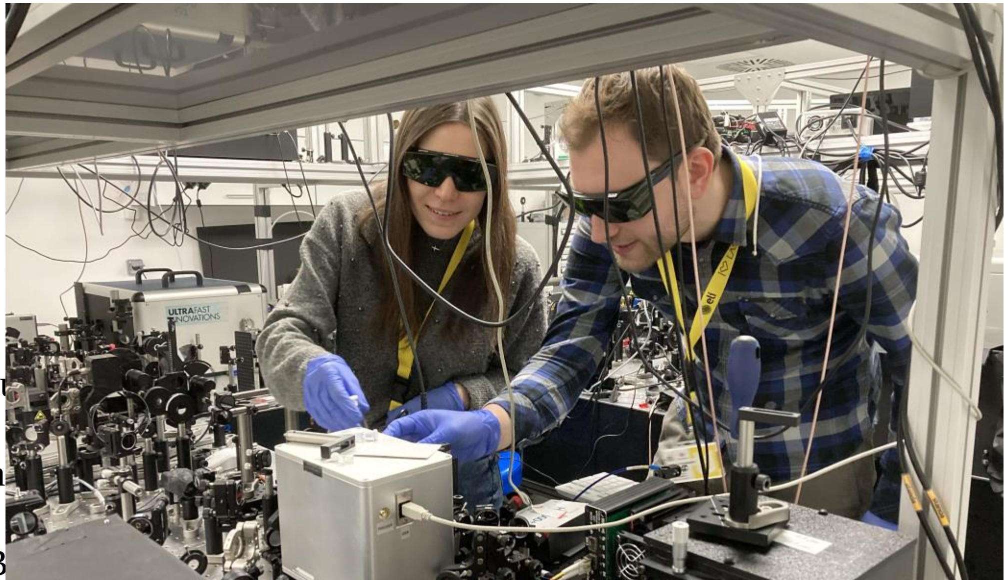
2021_E1C20006_Rafał Fanselow

2020E10021 Czapla-Masztafiak, Stanczyk

TA and FSRS UPM-56 Naumova

2021_E1C20020_Jens Uhlig

2021_E1C20022_György Vankó



UMP-59 Ultrafast measurements of the surface plasmon resonance dynamics of metal nanomaterials based on gold nanoparticles to investigate steady-state and time-resolved optical properties

Publications:

- First experiments with a water-jet plasma X-ray source driven by the in-ho

Journal of Synchrotron Radiation, Volume 28, Part 6, pages 1778-1785 (2021)

- Implementation of a crossed-slit system for fast alignment of sealed polyca

Journal of Synchrotron Radiation 27 (6), 1730-1733

- X-ray spectroscopy station for offline sample pre-characterization at ELI-B

Under review

- A fast-integrated X ray Emission spectrometer dedicated to the investigati

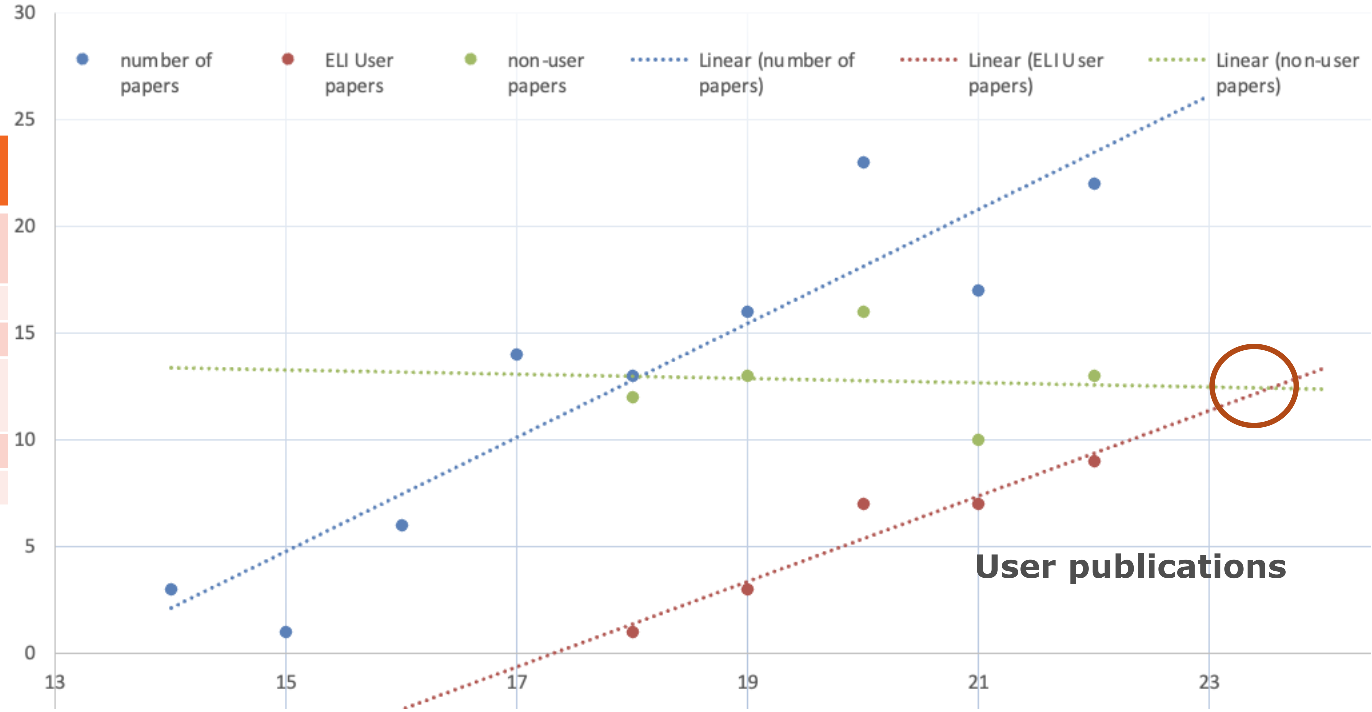
Under review (experiments in E4)

User experiments and publications:
ELI Beamlines E1 expriemntal hall and associated labs

ELI BL Summary for Open Call experiments (21.10.2022)

Call	Number of applications	No of experiments performed	Number of beamtime weeks
ERIC Call 1	17		
Call 2	29	24	58
Call 1	22	22	60.5
Covid Call	0	1	1,5
Call 0	22	19	24
Sum	90	66	144

Output: Peer reviewed scientific publications



User publications

2018	1		
2019	3		
2020	7		
2021	7		
2022	9		
2023	3	7under review	
	30		

Call 0

Benchmarking

User publications	E1 and associated labs (call 0 in 2019)	European XFEL (first call in 2017)
3 years or user access	23 (2020-2022)	21 (2018-2020)
4 years or user access		37 (2018-2021)
5 years or user access		55 (2018-2022)

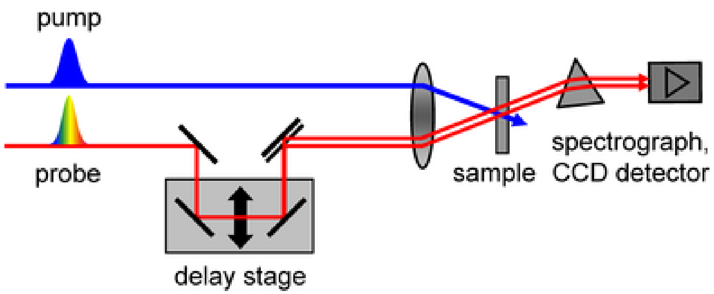
https://www.xfel.eu/science/publications/index_eng.html

ELI Beamlines

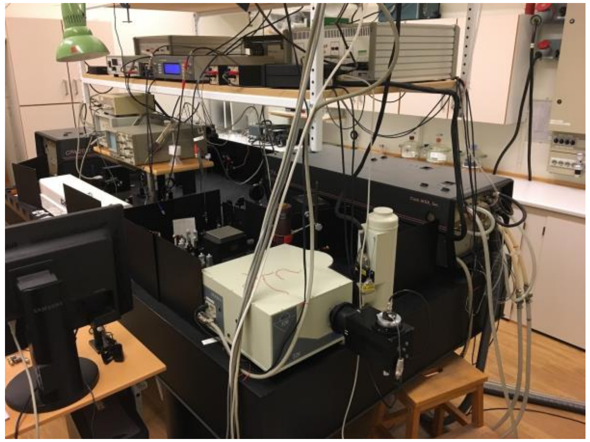
Complementarity to facilities and university labs

High complementarity:
Structure and dynamics

ELI Beamlines
- Flexible pump-probe experiments, THz to X-rays,
- Synchronization and temporal resolution
- Combination of complementary energy ranges and source parameters.
- Complementary ultrafast techniques (e.g. X-ray and IR)
- Photon probes in combination with electron and ion beams



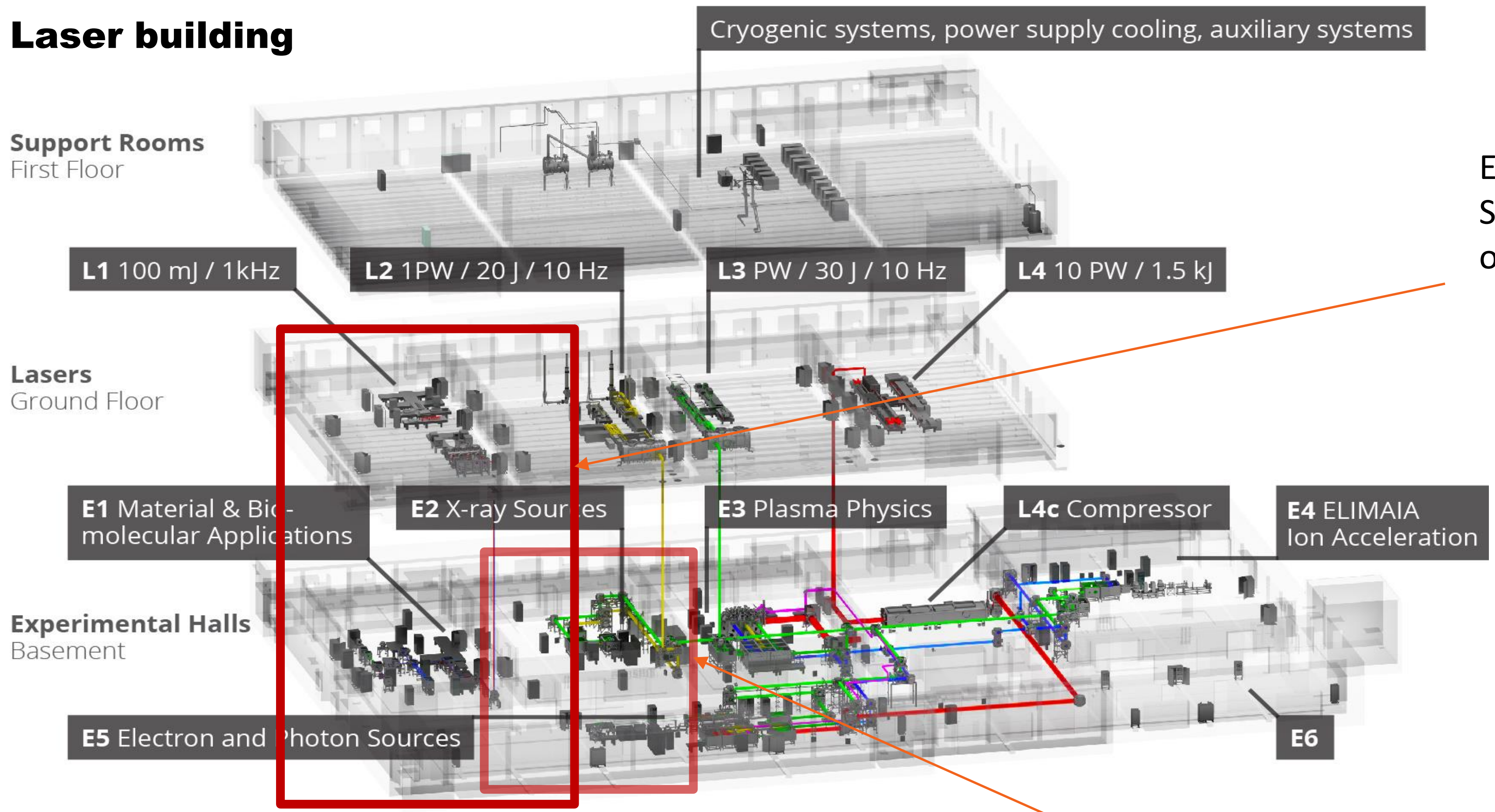
Synchrotrons:
- Availability, reliability, tuneability, beam control, flux.
- Limited temporal resolution, synchronization



University lab
- Availability (once you have it and it is working)
- Big effort to keep updated and maintained for an individual lab
- Often under-utilized

X-ray FELs
- Photons per pulse, fs pulses, tuneability
- Availability (cost of beamtime), synchronization

ELI BL Facility general layout



ELI Beamlines Systems in user operation so far

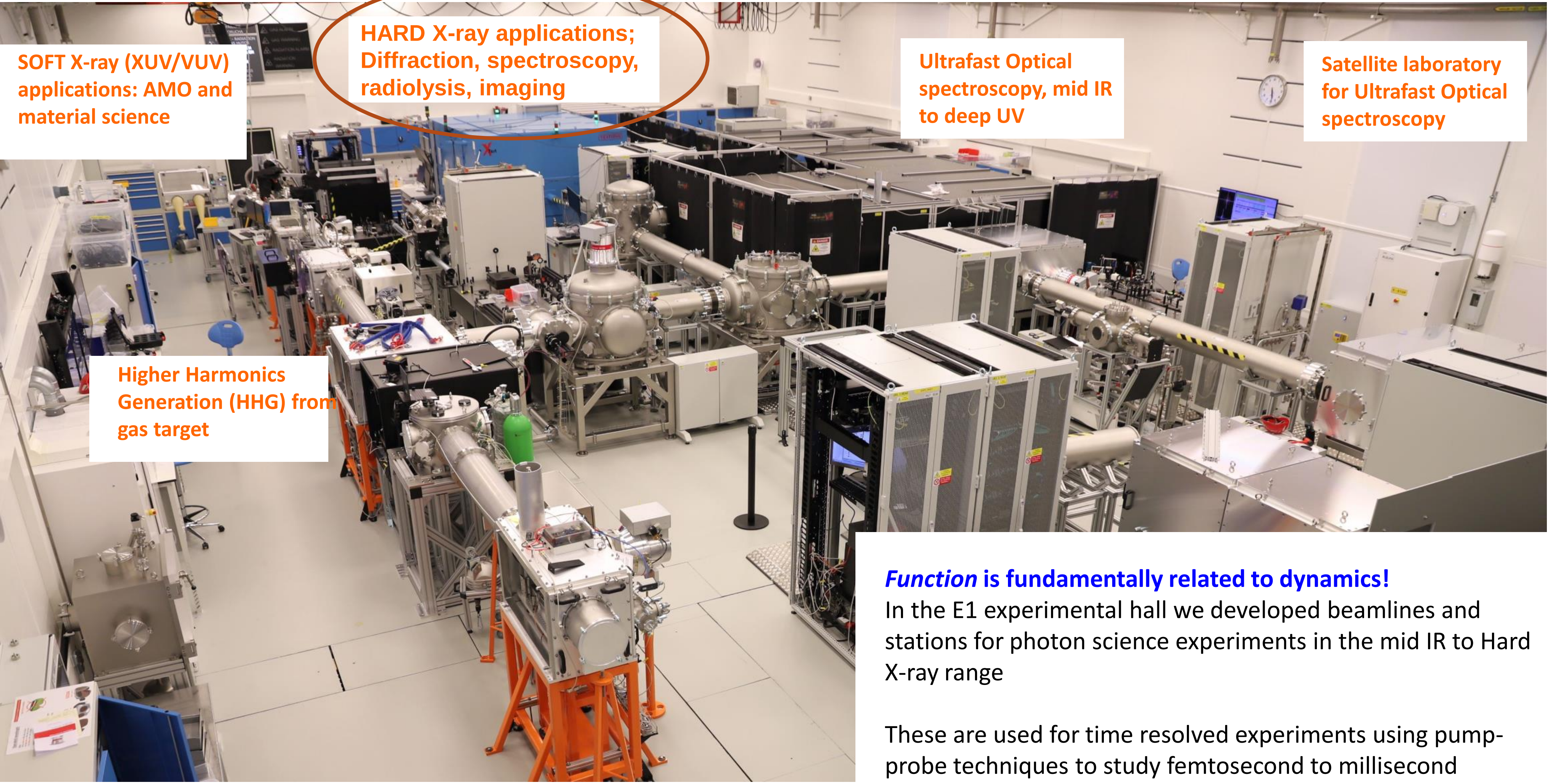
Outlook: Betatron in E2

E1 Experimental hall

Kilo-Hertz applications in Bio and Material science

Experimental Hall E1 – 3D “street view” tour

https://www.eli-beams.eu/facility/experimental-halls/e1-material-and-biomolecular-applications/



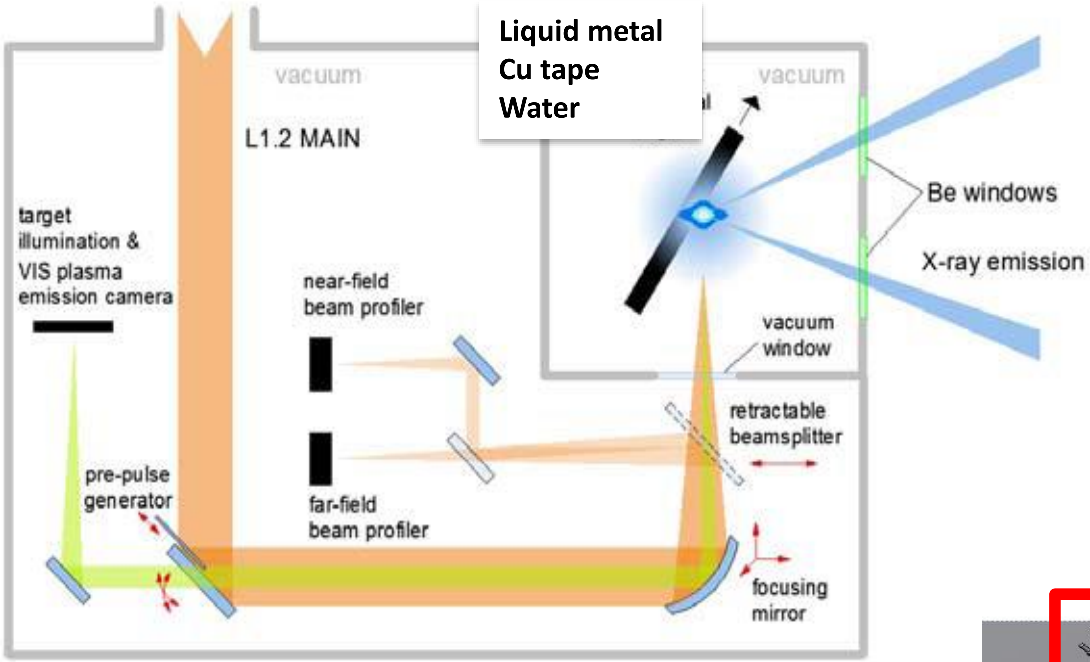
***Function* is fundamentally related to dynamics!**

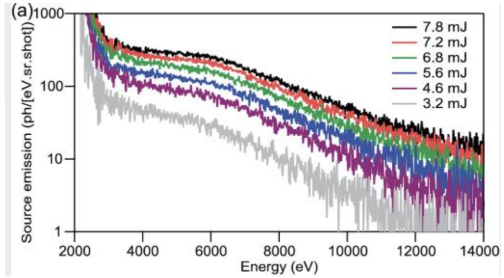
In the E1 experimental hall we developed beamlines and stations for photon science experiments in the mid IR to Hard X-ray range

These are used for time resolved experiments using pump-probe techniques to study femtosecond to millisecond dynamics

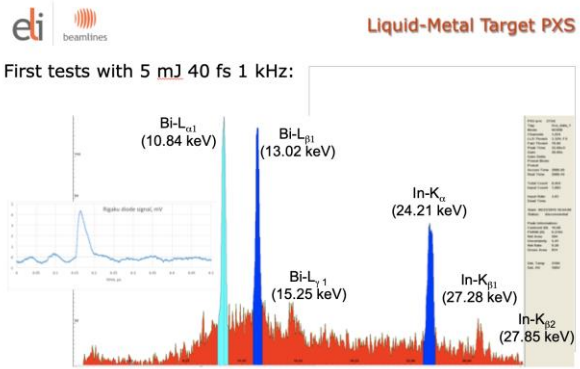
Hard X-ray science, diffraction and spectroscopy

Plasma X-ray sources: Energy range: 2 to 30 keV, 1 kHz

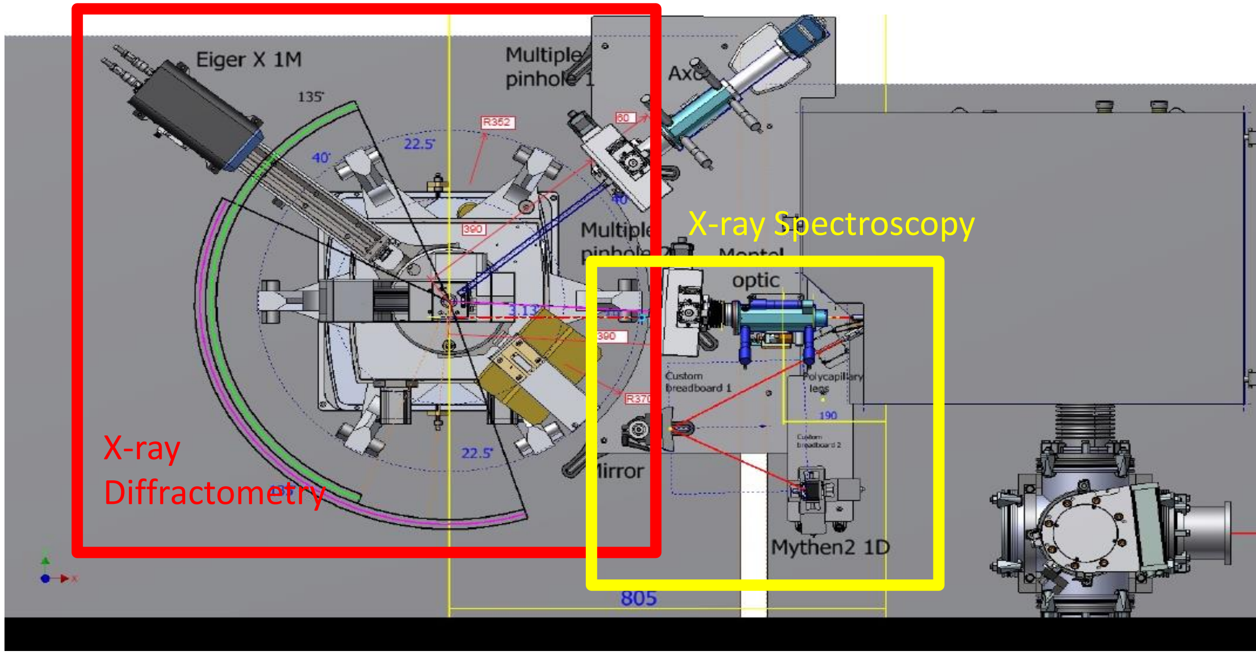




Station using the polychromatic emission for absorption and emission spectroscopy



Station using the monochromatized emission for diffraction and scattering



Liquid metal jet source
OPTICS LETTERS Vol. 27, No. 10, p 866, May 15, 2002
Cu tape source
F. Zamponi, et al., Applied Physics A volume 96, pages51–58 (2009)
Elsaesser et al. The Journal of Chemical Physics 140, 020901 (2014)
doi: 10.1063/1.4855115
Water jet source (Adaptation of source from Jens Uhlig, Lund University, Sweden)
L. Miaja-Avila et al. Structural Dynamics **2**, 024301 (2015)
doi: 10.1063/1.4913585

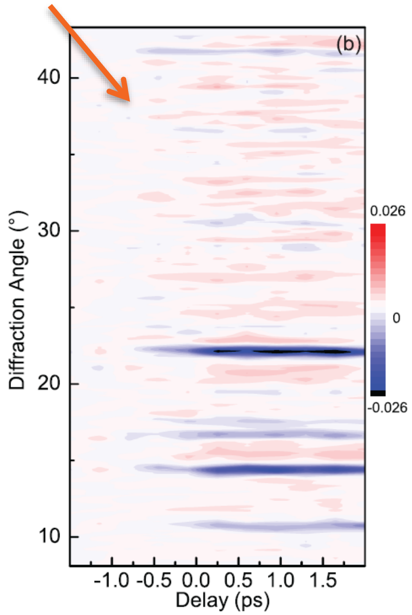
TREX: Time-Resolved Experiments with X-rays

Diffraction/scattering

Otical activation, see e.g,
Freyer et al. The Journal of Chemical Physics 138, 144504 (2013); doi: 10.1063/1.4800223

Structural Dynamics 7, 014301 (2020); https://doi.org/10.1063/1.5126316

Or work from Bargheer lab: http://udkm.physik.uni-potsdam.de/



THz activation

Structural biology:
Panel 9, Wed. 10:55 - 11:20
Presentation from G. Katona
University of Gothenburg, Sweden
Structural Response of a Protein Crystal to Strong Pulsed THz Fields

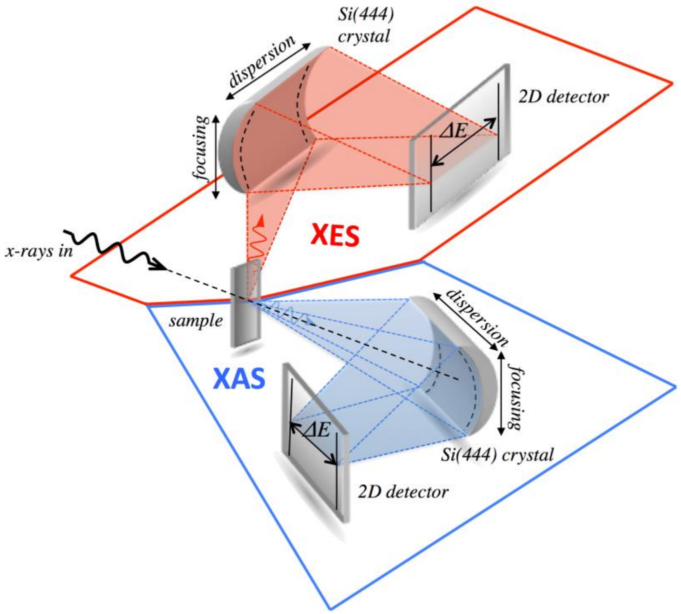
Condensed matter:
Terahertz-driven phonon upconversion in SrTiO3
M. Kozina, et al.
Nature Physics | VOL 15 | APRIL 2019 | 387–392

THz-activation->Optical pulse shaping

X-ray Absorption/Emission Spectroscopy XAS/XES

XAS: Give information on the local coordination of e.g. TM ions through an analysis of the features of the XAS spectrum

XES: Gives information on the charge state of the metal ion.

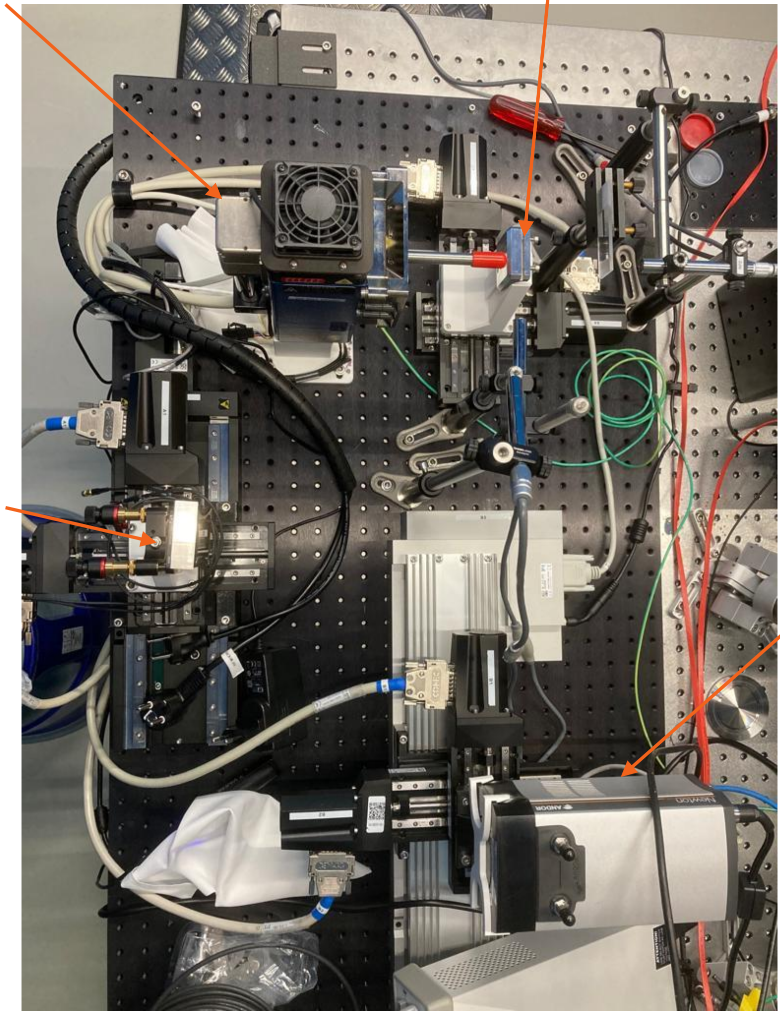


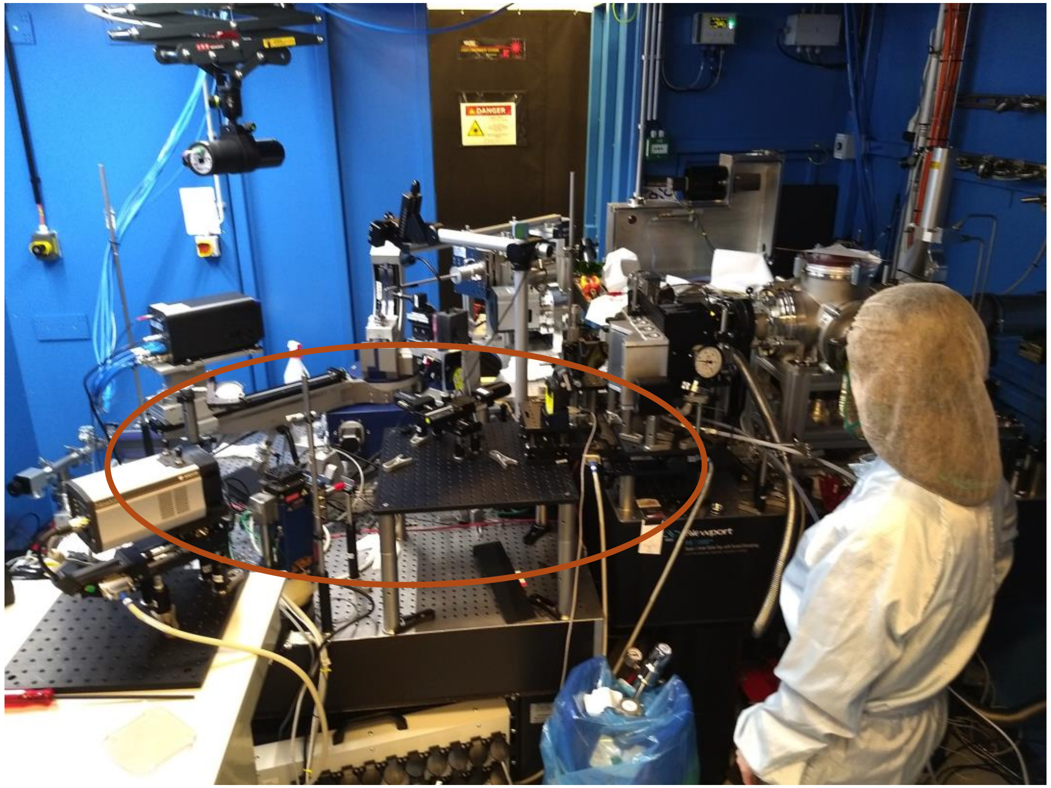
ELI Beamlines von Hamos XES/XAS spectrometer concept
Visegrad collab:
J. Sa
J, Szlachetko
G. Vanko
et al.

XAS/XES studies, ideally complemented by optical/IR spectroscopy is an ideal tool for studies on charge transfer dynamics. See e.g.
Phys. Chem. Chem. Phys., 20, 6274-6286 (2018) and
Nature Chemistry volume 10, pages 355–362 (2018)

Recently in the X-ray hutch…

Spectroscopy station, present status





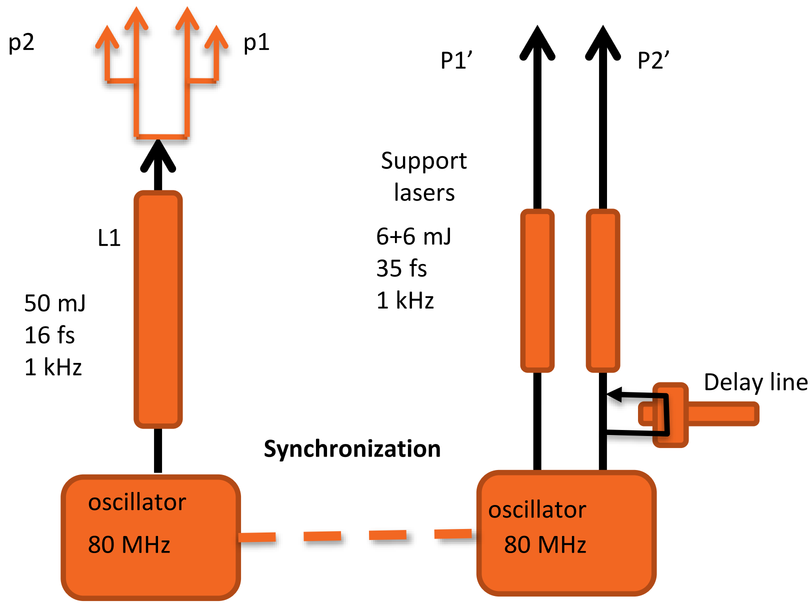
TREX area for X-ray experimetns
Diffraction and spectroscopy

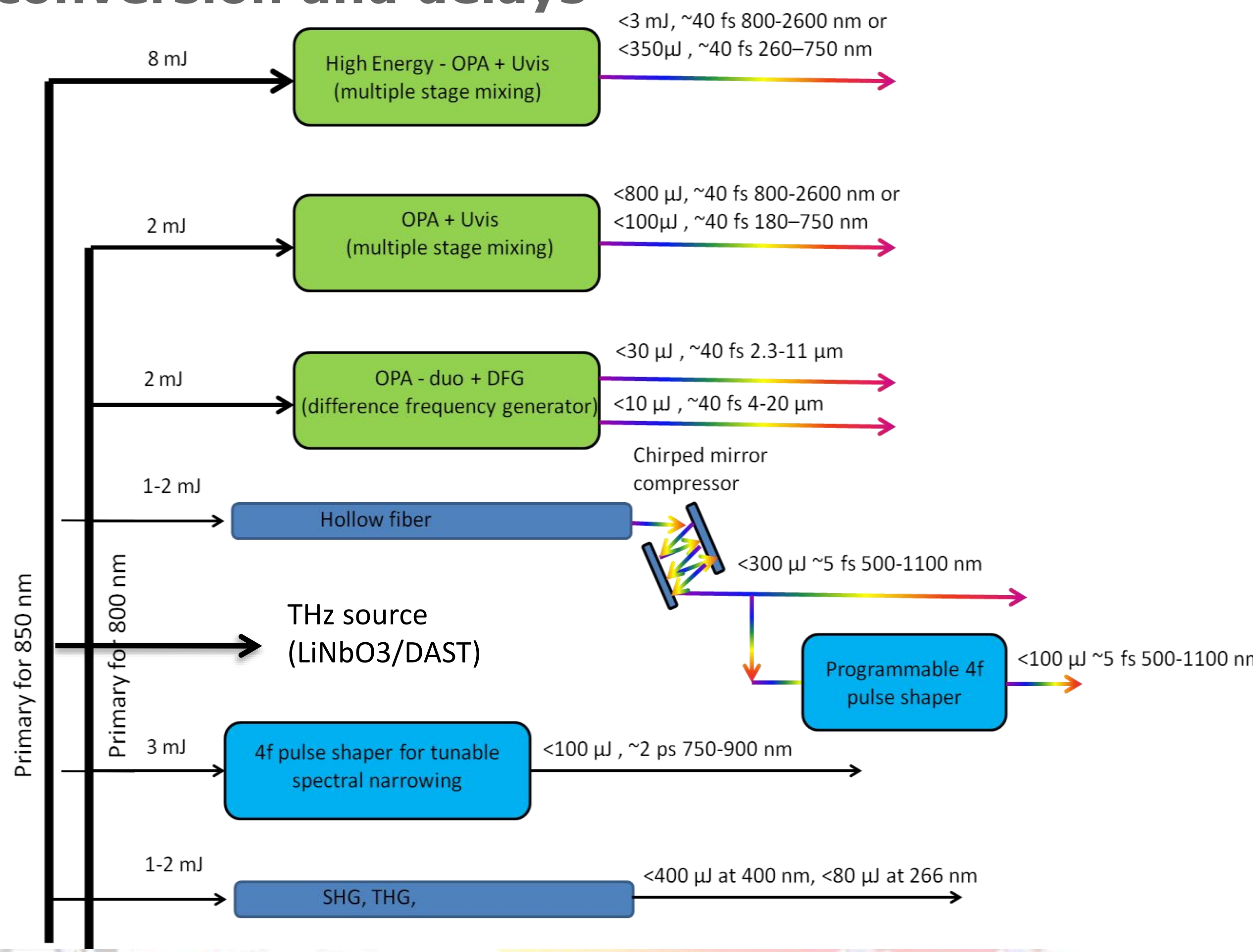
Modular station for X-ray spectroscopy

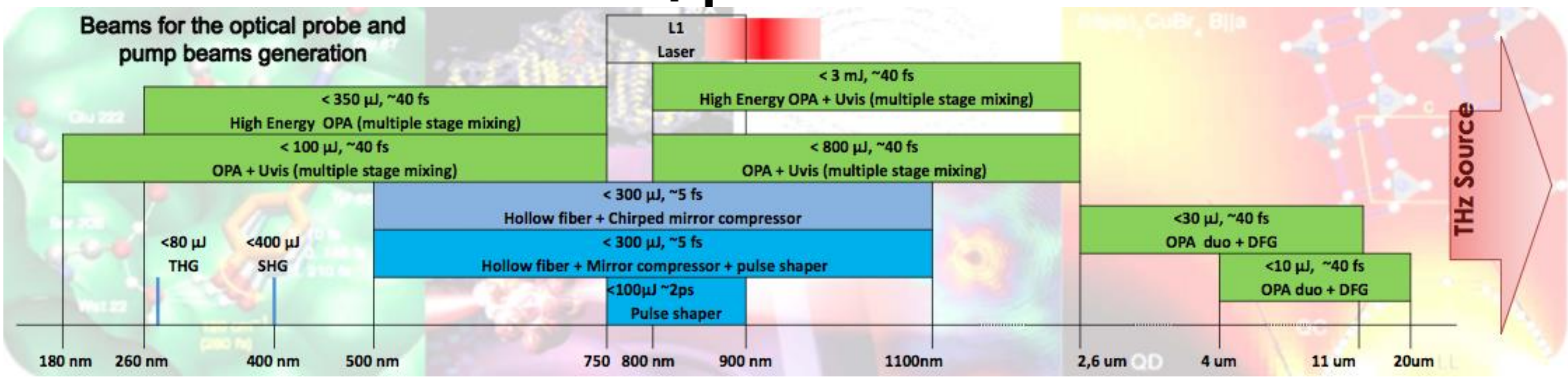
- Von Hamos Geometry
- Motorized and automated
- Modular and adaptable
- Configurations for absorption and emission spectroscopy
- Moveable between locations (PXS, E1, E4, Betatron in E2. ….)

RP4 Optical pulse conversion and delays

0 fs to 1 ms delay with fs precision







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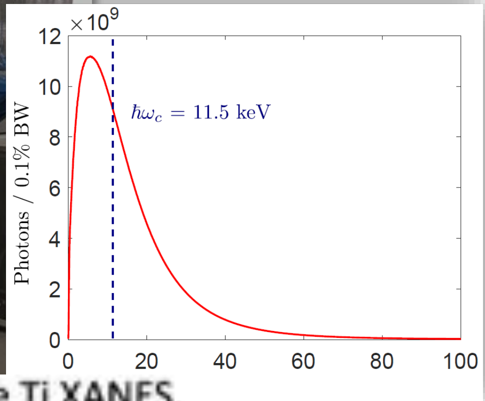
Outlook 1: New and upgrades X-ray sources

eli

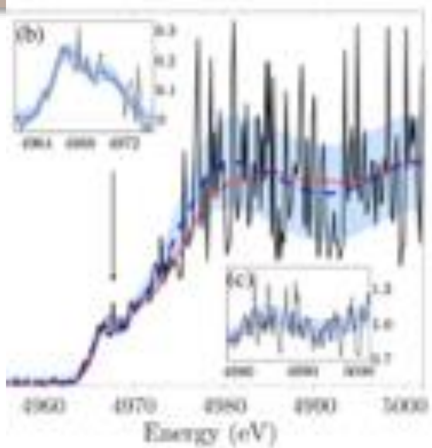
X-rays: MIR drive of PXS for diffraction and utilization of LPA sources for X-ray spectroscopy



Betatron spectrum

- E2 ideal for Transition Metal k-edge spectroscopy.
- In L1 (L1/ALFA) promising for TM L-edge spectroscopy

K-edge Ti XANES,
Gemini, CLF (200 TW)



Single shot

Kettle et al.
PRL **123**, 254801 (2019)

NATURE PHOTONICS DOI: 10.1038/NPHOTON.2014.256

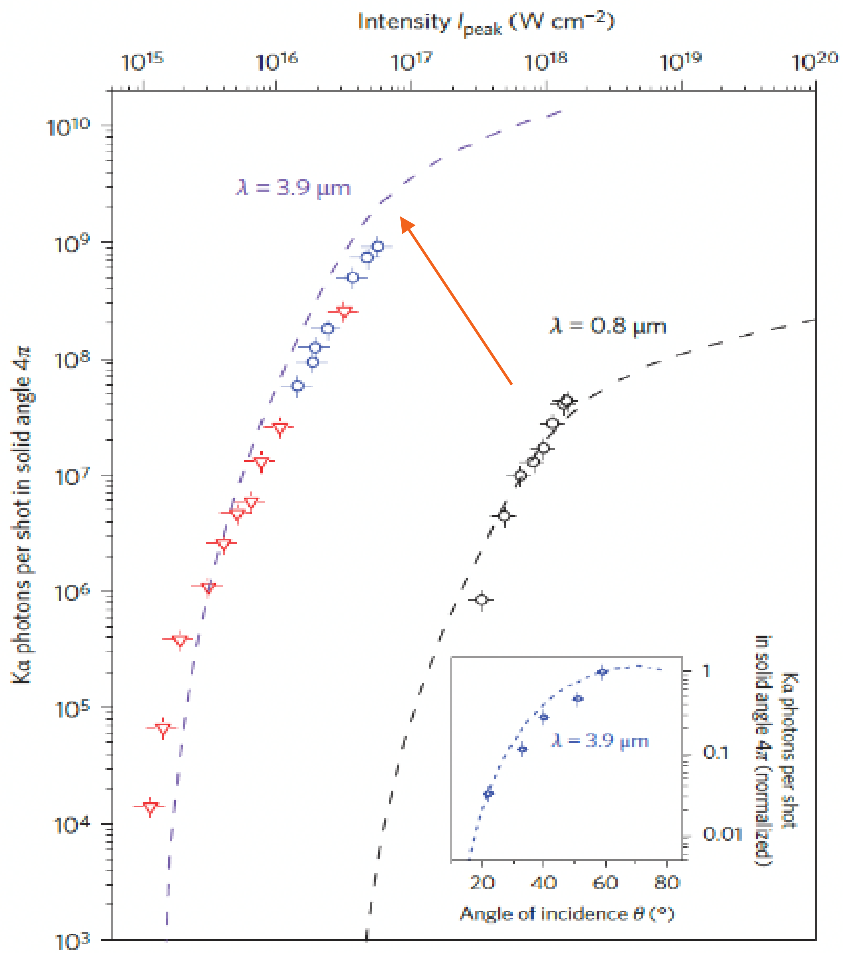
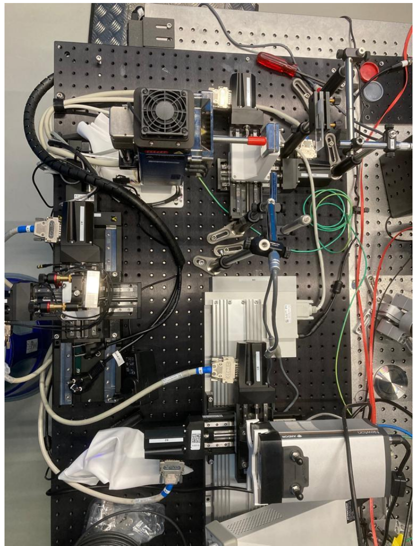


Figure 2 | Generated X-ray Kα flux as a function of the laser-peak intensity. Comparison of experiment (symbols) with theory (dashed lines)

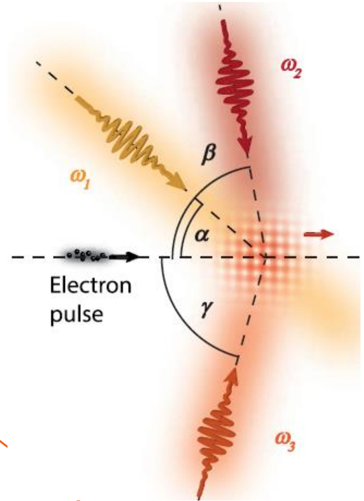


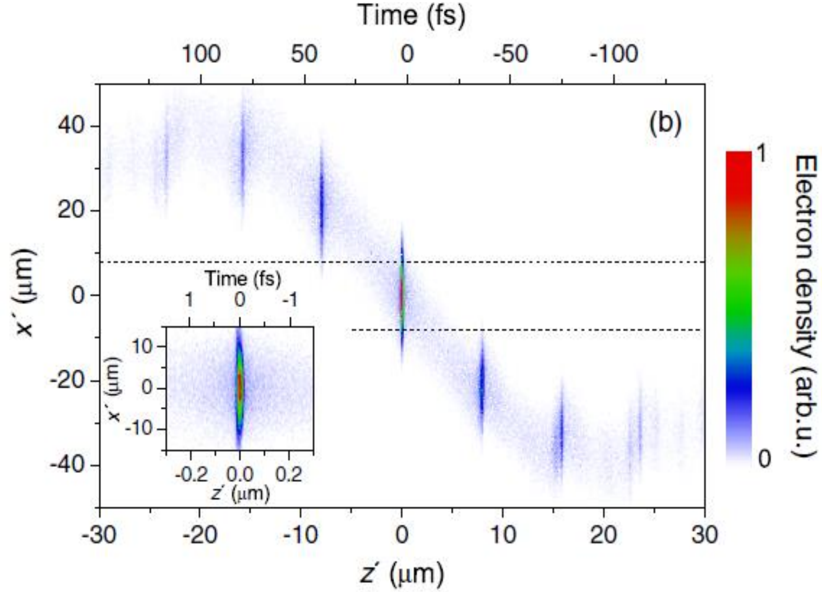
2 orders of magnitude increase by going to MIR drive and 3 kHz

Outlook 2: Ultrafast electron diffraction/microscopy

Interfering laser generate isolated electron pulses for time resolved electron diffraction (ED) and microscopy

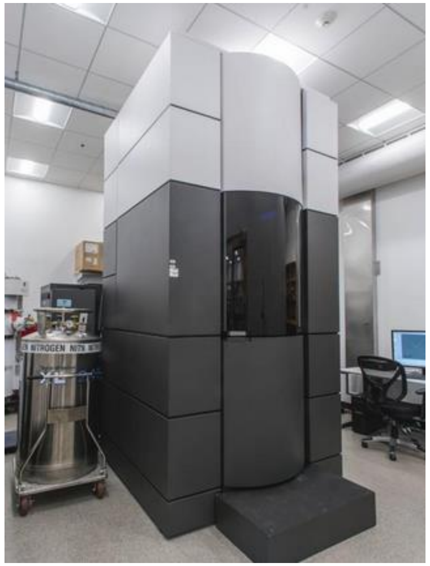
Future



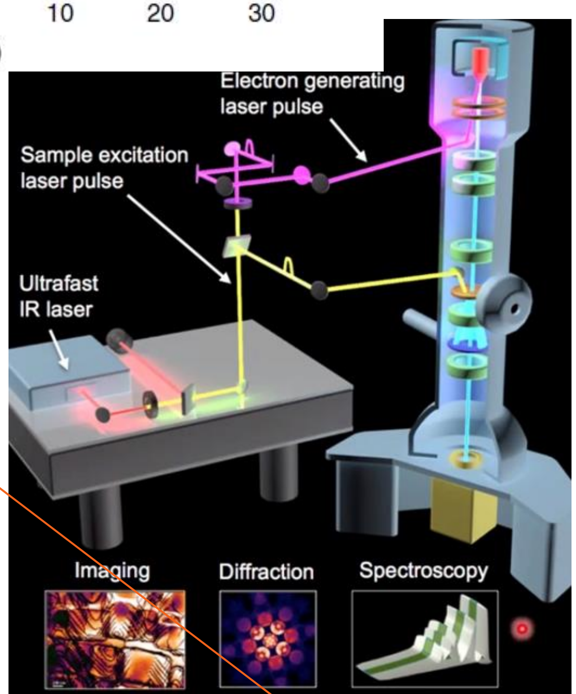


M. Kozak. PHYSICAL REVIEW LETTERS 123, 203202 (2019)

Past and Present



Synchrotrons and EMs for structure. Ultrafast lasers for dynamics



Outlook 3

Formalizing collaborations:
Solaris/ELI (BL) joint laboratory for research into structure and dynamics (function)

To get to function you need to understand both structure and dynamics!

Synchrotrons:
- Strong expertise in X-rays; methods and instruments. Established user community in this area. Structural methods, including cryo EM. Emerging capabilities in ultrafast techniques.

ELI Beamlines
- Strong expertise in ultrafast techniques, in particular optical and VUV range. Established user community in this are. Emerging capabilities in X-ray science and structural science, including EM.

Joint laboratory, benefits:
- Apply for joint funding
- Collaboration on instument development
- Exchange of staff, training
- Joint/shared equipment

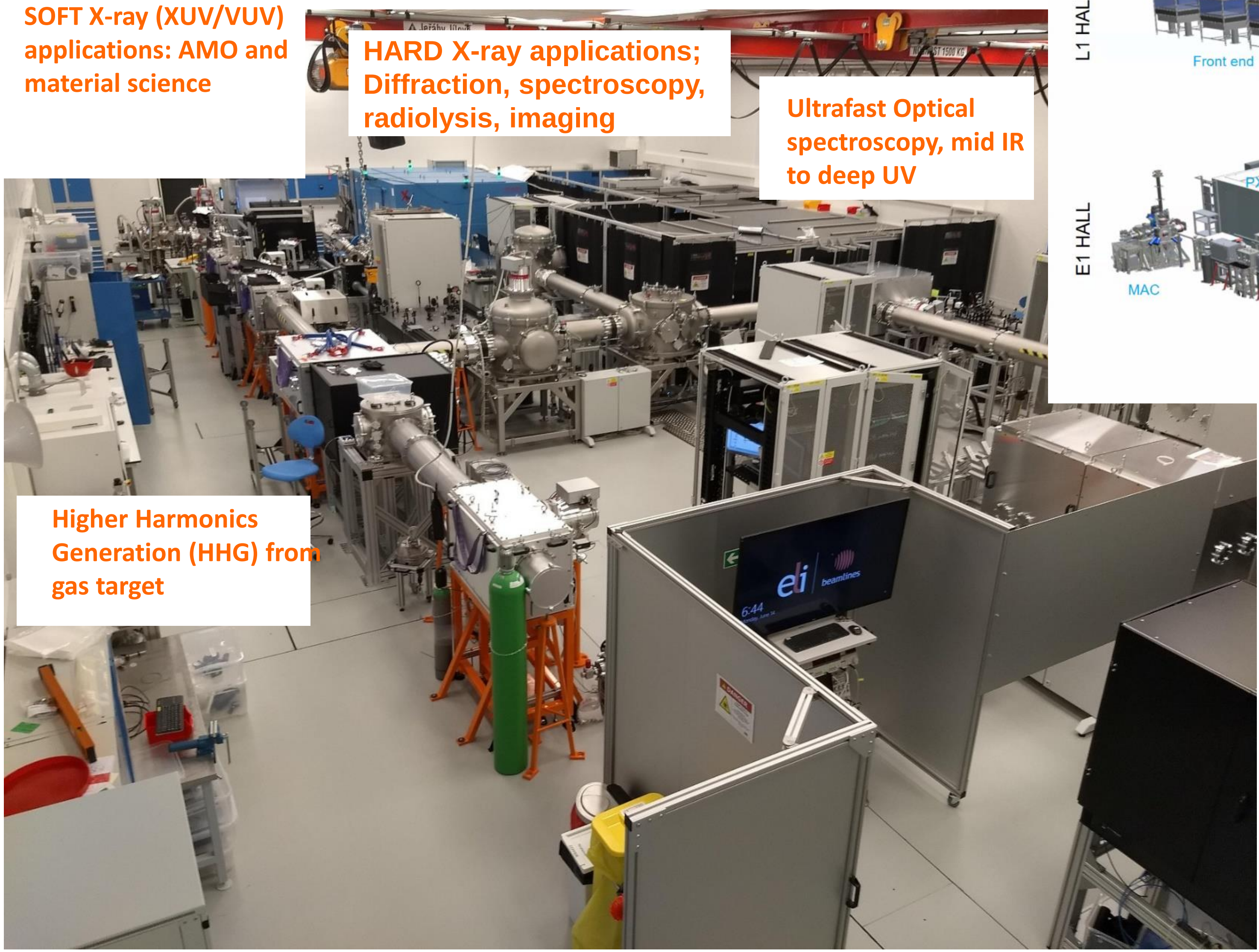
Thank you
for your attention!

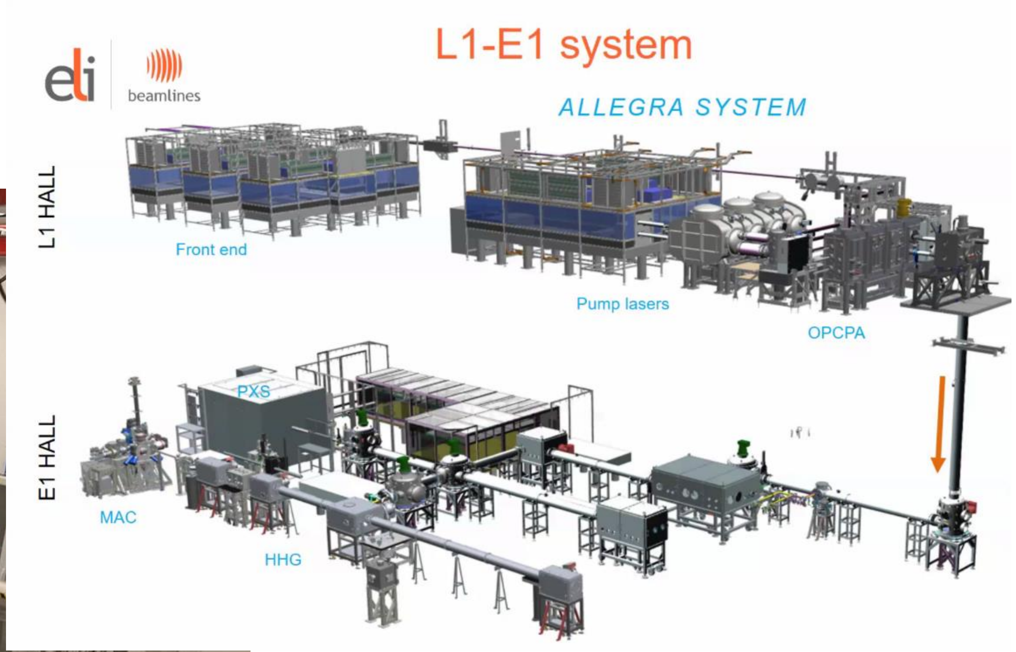
Action: ELI ERIC meeting in Krakow (8.3.2023)

Author: Jakob Andreasson

ELI Beamlins E1 experimental hall and the L1 Allegra kHz laser

Contact person: Jakob Andreasson,
Head of Department for Structural Dynamics





***Function* is fundamentally related to dynamics!**

In the E1 experimental hall we developed beamlines and stations for photon science experiments in the mid IR to Hard X-ray range

These are used for time resolved experiments using pump-probe techniques to study femtosecond to millisecond dynamics

Applications:
XAS recent results using Betatron source

Ultrafast XAS measurements

Now coupling **femtosecond resolution…**

Allows investigation of:
- Femtochemistry, photobiology, …
- Industrial research. E.g., batteries
- Rapid material phase changes
- **Snapshot probing of extreme states**

Techniques
- <u>XANES & EXAFS</u>
- Absorption edge shifts
- Excited state absorption lines

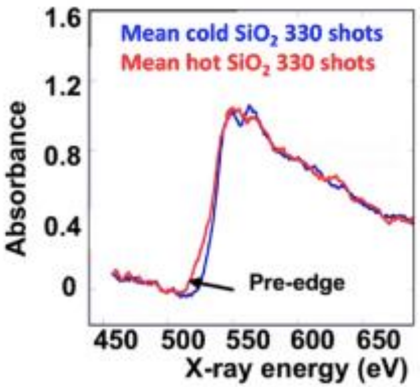
Etc.

Provide
- Temperature
- Electronic and local atomic structure
- Ionisation energies/rates
- Electron-Ion equilibration rates

Etc.

Laser Wakefield Acceleration XAS: Examples

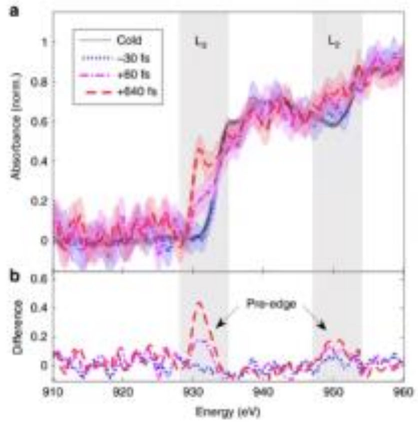
L-edge SiO2 XANES
MEC, LCLS (<100 TW)



≈ 300 shots

F. Albert, IPAC 2018

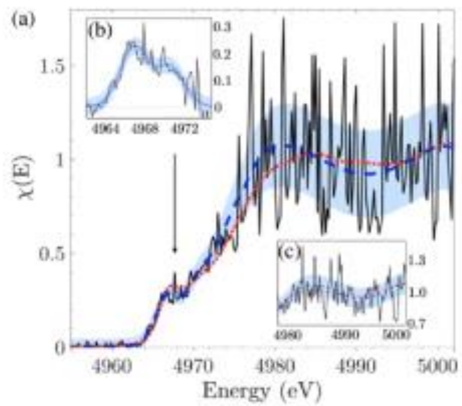
L-edge Cu XANES
LOA (<100 TW)



≈ 50 shots

Mahieu *et al.*
Nat. Comms. **9**, 3276 (2018)

K-edge Ti XANES,
Gemini, CLF (200 TW)



Single shot

Kettle et al.
PRL **123**, 254801 (2019)

E1 experimental Hall: Operation and development of user end stations for:

Science with Coherent XUV radiation

- Atomic, Molecular and Optical (AMO) science
- Coherent Diffractive Imaging (CDI)
- XUV Material science
- XUV source development

Hard X-ray science

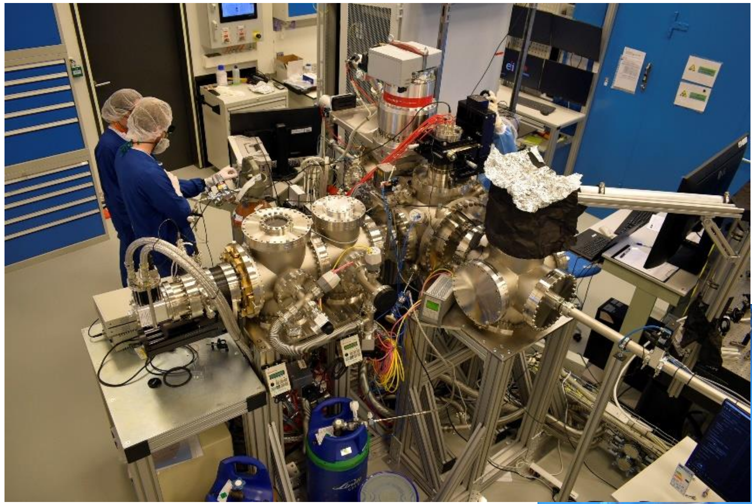
- X-ray diffraction and spectroscopy
- Pulse Radiolysis, X-ray imaging
- Plasma X-ray source development

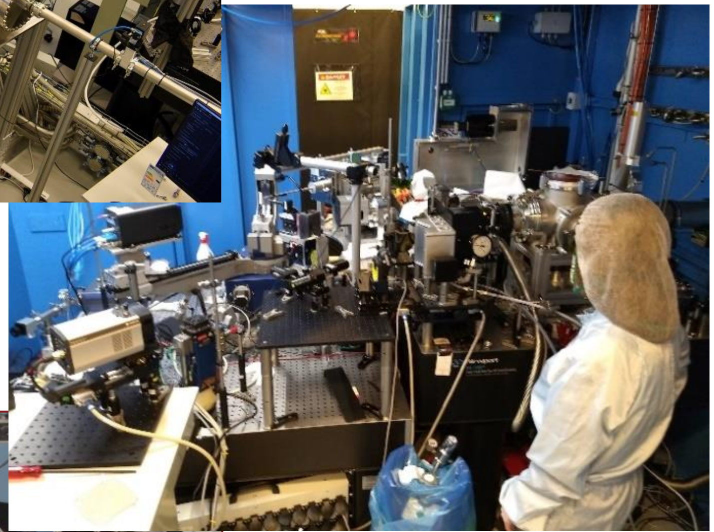
Ultrafast optical spectroscopy

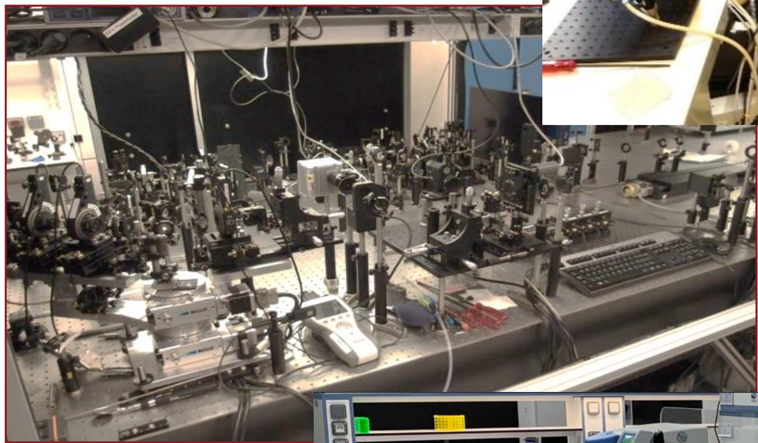
- Femtosecond Stimulated Raman Scattering and Transient Absorption
- Time resolved spectroscopic ellipsometry
- Transient Current Technique
- 2D IR spectroscopy

Sample preparations support lab

- Sample preparation, including Bio safety level 2
    - Wet processes, crystallization, cold room
- Laser spectroscopy
- Optical/light microscopy
- Electron microscopy

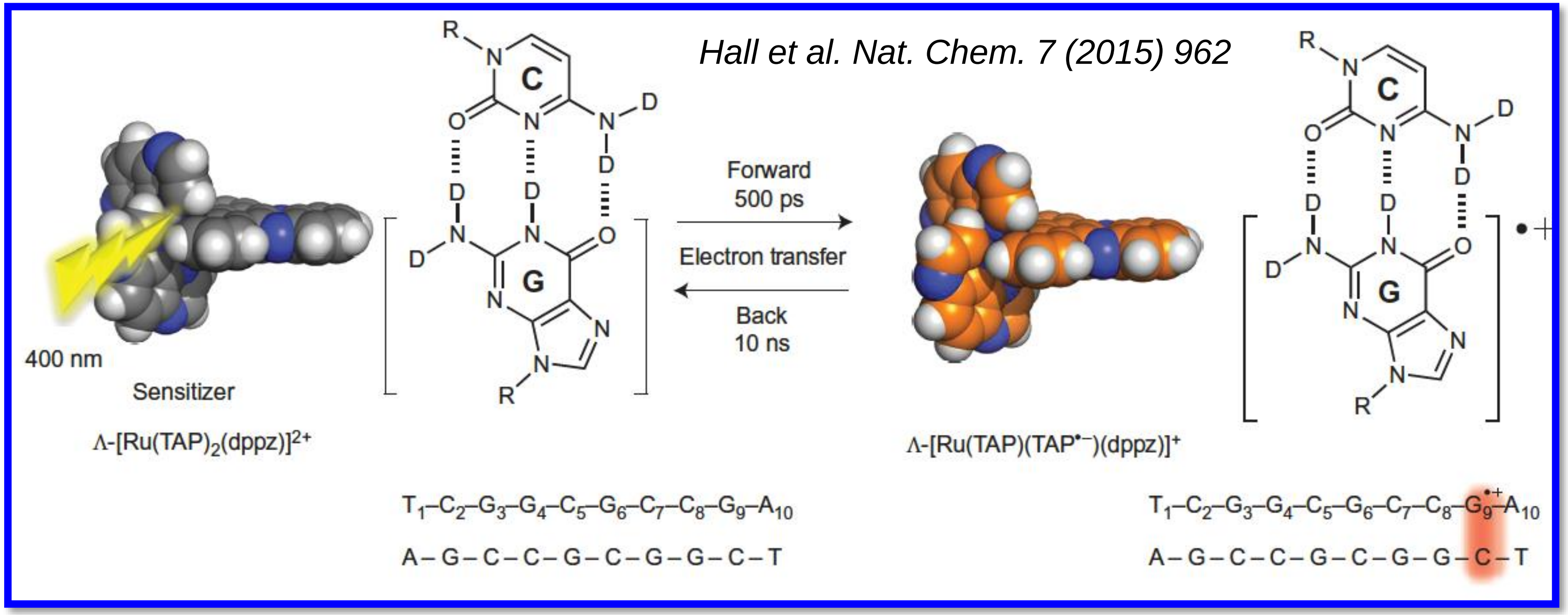






Slide from Jacinto Sa, Uppsala University

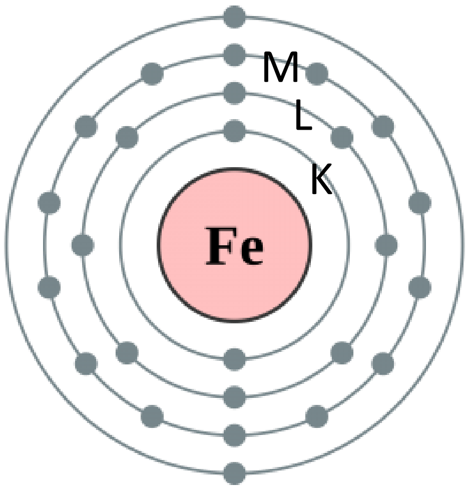
X-ray spectroscopy in Photo-activated therapy



Presently

- ✧ Mechanism followed by transient infrared absorption
- ✧ Little information on metal dynamics
- ✧ No quantification of metal complex participation

M-absorption edge of Fe (54eV)
L edge ~710 eV
K edge: ~7.1 keV



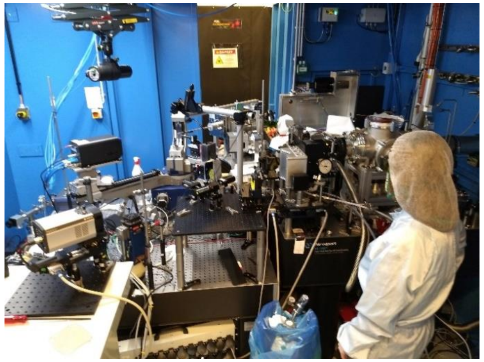
Suggestion at ELI Beams using time resolved X-ray spectroscopy

- ✧ Dynamics of copper sensitizer in physiologic solution
- ✧ Photo-oxidation dynamics with DNA
- ✧ Quantification of metal complex participation

Photopharmacology

X-ray applications

Plasma X-ray sources and experimental stations



Main type of pulsed X-ray sources:

- Copper tape
- water jet
- liquid metal jet (to come)

Main experimental techniques:

- Diffraction and scattering
- Absorption and emission spectroscopy
- Pulse radiolysis (to come)
- Phase contrast imaging (to come)

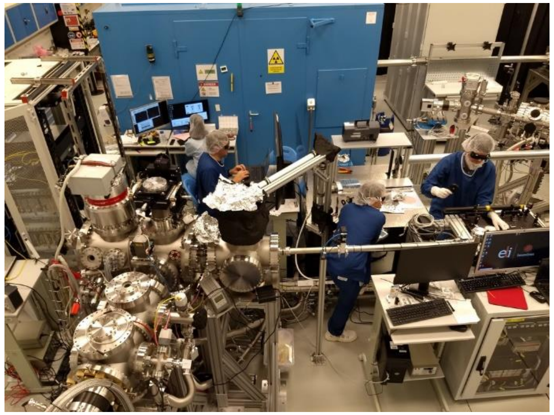
Core publications

A Zymaková, et al., Journal of Synchrotron Radiation Volume 28, Part 6, pages 1778-1785 (2021)
KP Khakurel, et al., Crystals 10 (12), 1146 (2019)
A Zymaková, et al., Journal of Synchrotron Radiation 27 (6), 1730-1733 (2020)

XUV science

AMO and material science (HHG source, MAC and ELIps stations)

Optical/XUV pump probe experiments using either XUV monochromator aor refocusing multilaty optics



Gas phase and fixed targets:

- Molecular beam, clusters, aerosols, 5 degrees of motion fixed target stage

Detectors:

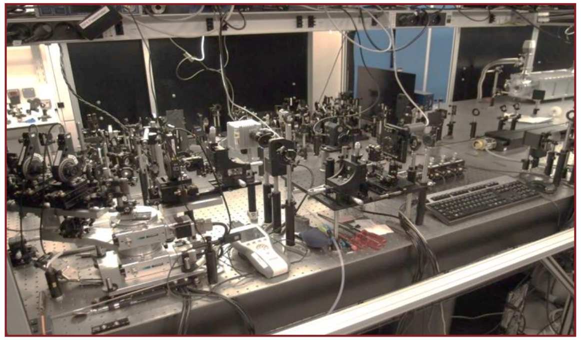
- Ion and electron Time of Flight
- Velocity Map Imaging (VMI)
- Magnetic Bottle Spectrometer (under development)
- XUV imaging detector

Core publications

E Klimešová, et al., The European Physical Journal Special Topics, 1-12 (2021)
O Hort, et al. Optics express 27 (6), 8871-8883 (2020)
Espinoza S. et al., J. Vac. Sci. Technol. B 38, 024005 (2020).
E Klimešová, et al.: Sci. Rep. 9, 8851 (2019)

Ultrafast optical spectroscopy

And pulse conversion for X-ray applications



Main experimental techniques:

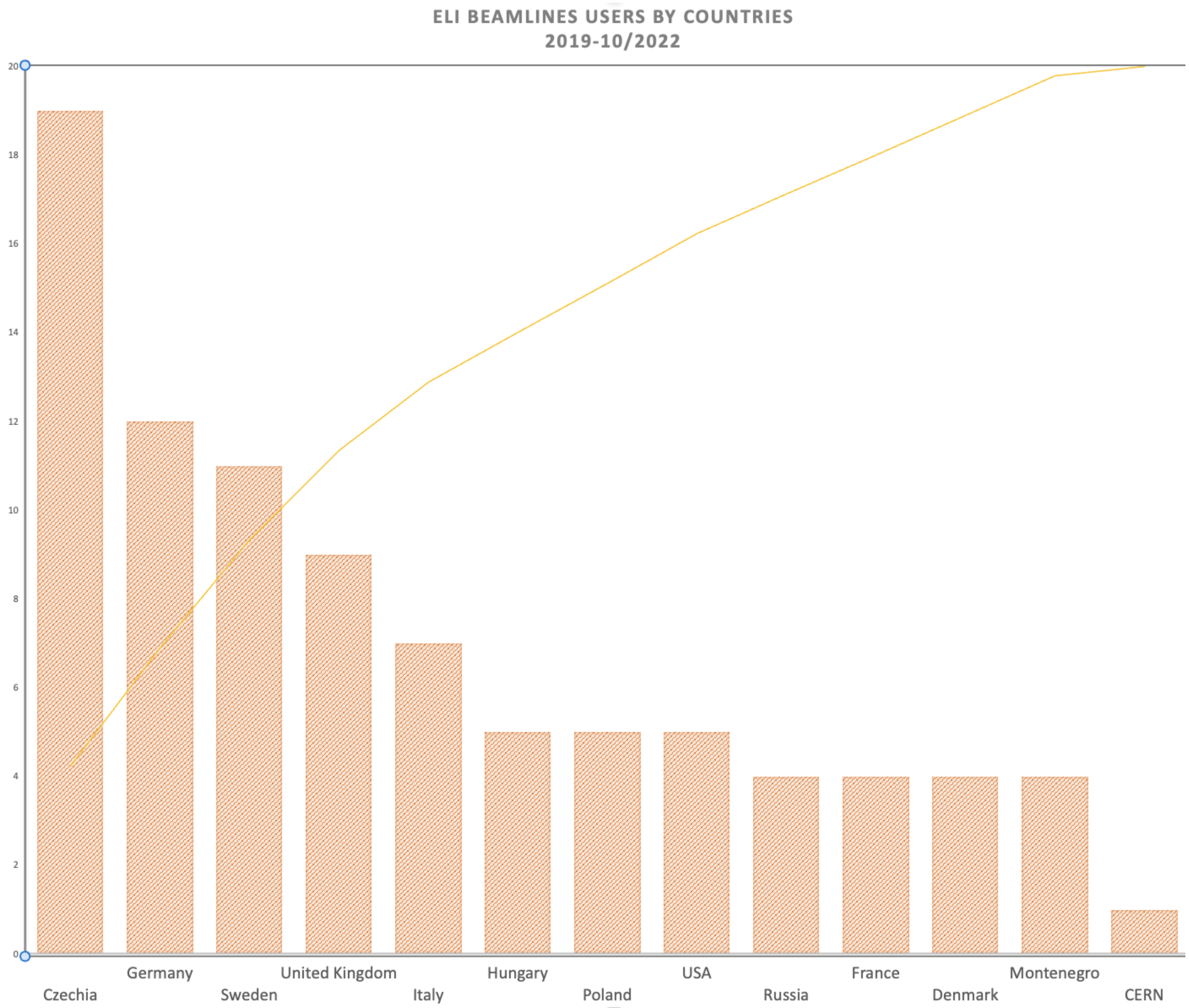
- Femtosecond Stimulated Raman, spectroscopic ellipsometry, transient optical absorption, Coherent control, transient current.

Main conversion capabilities:

- OPAs and DFGs
- 2^{nd} + 3^{rd} harm. Generation
- Fiber compression
- Optical pulse shaping
- THz generation (to come)
- White light generation

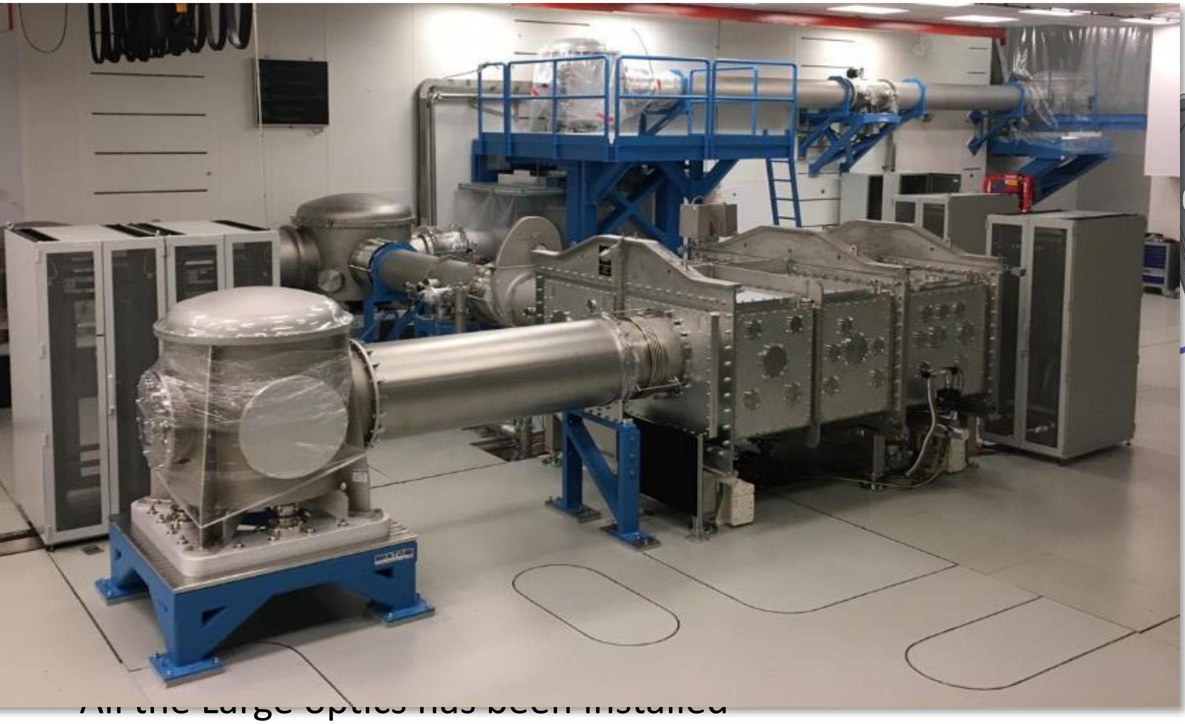
Core publications

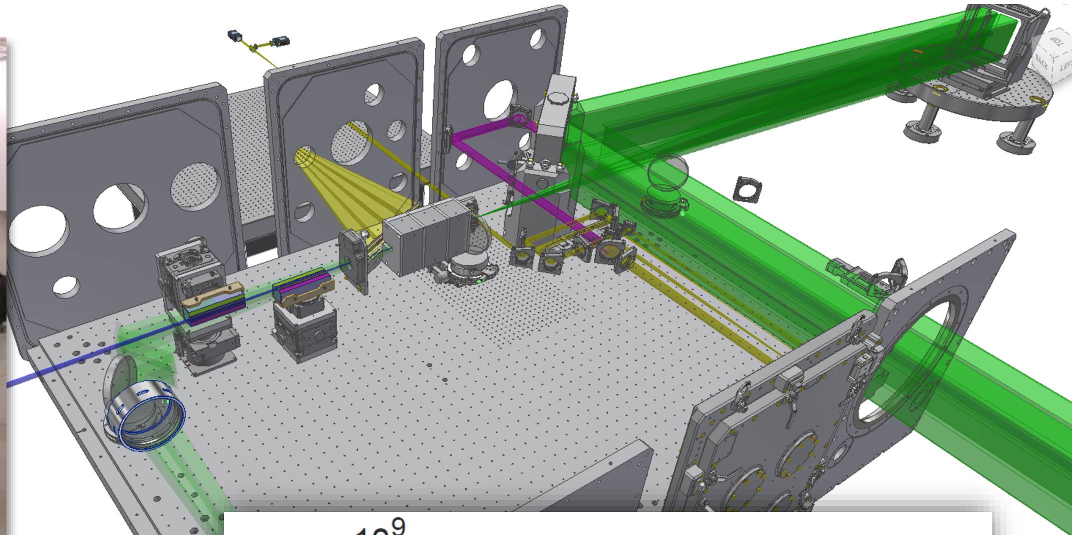
S Richter, et al., Review of Scientific Instruments 92 (3), 033104 (2021)
S Richter, et al., New Journal of Physics 22 (8), 083066 (2020)
PC Andrikopoulos, et al., Physical Chemistry Chemical Physics 22 (12), 6538-6552 (2020)
S Espinoza, et al., Applied Physics Letters 115 (5), 052105 (2019)
M Naumova, et al., Chemical Physics 20 (9), 6274-6286 (2018)

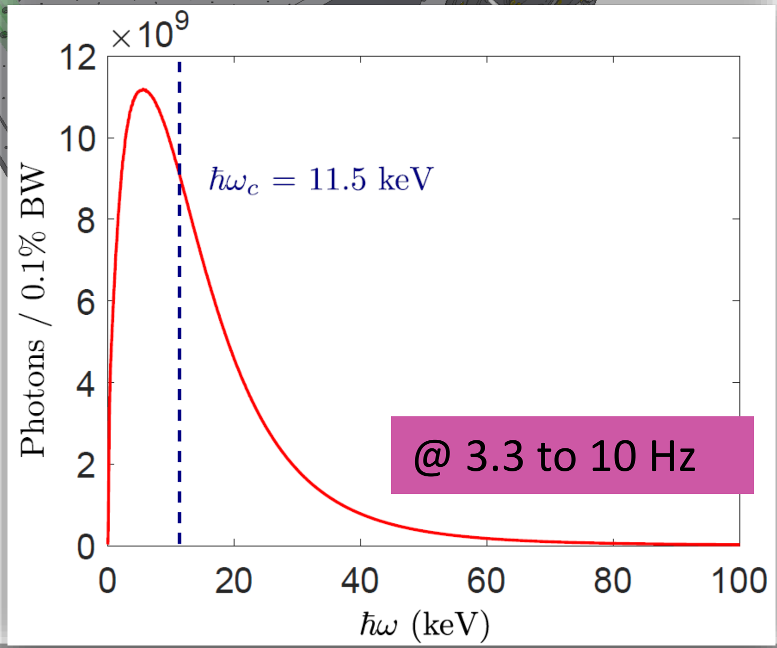

ELI BEAMLINES USERS BY COUNTRIES
2019-10/2022
20
18
16
14
12
10
8
6
4
2
0
Czechia
Germany
Sweden
United Kingdom
Italy
Hungary
Poland
USA
Russia
France
Denmark
Montenegro
CERN

Hard X-rays in E2

Gammatron Beamline – Betatron / Compton







- All the Large optics has been installed
- Local BT is currently being installed.
- The deformable mirror will be integrated in Jan 2023
- All laser, plasma electron & X-ray Diagnostics are ready
- User station is planned to installed in Dec 2022
- X-ray Optics (KB mirror) has been tendered (del May 2023)

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