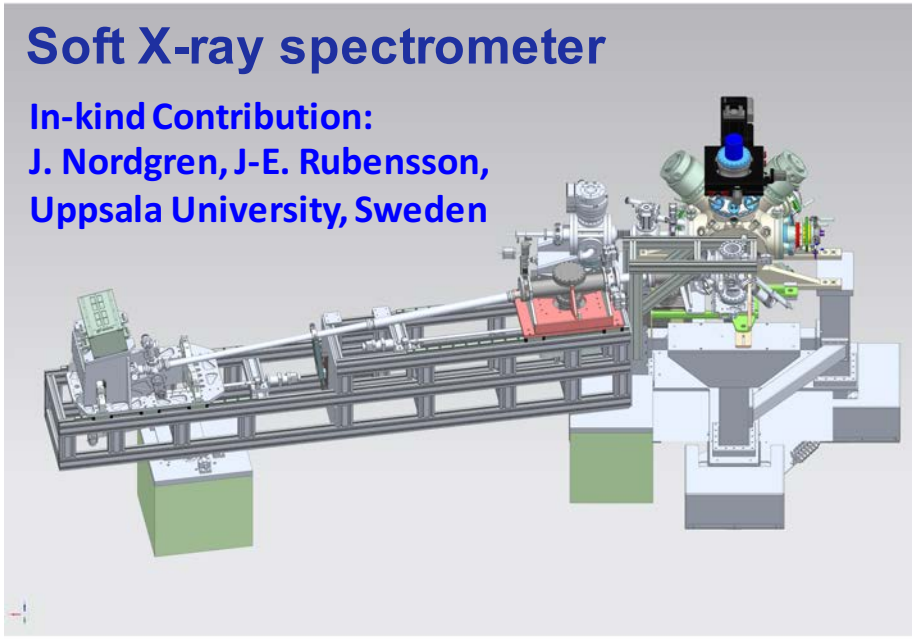
Workshop on 1D imaging soft X-ray spectroscopy at the SQS instrument of the EuXFEL

October 21-22, 2021
European XFEL, Schenefeld, Germany

Marcus Agaker, Thomas Baumann, Michael Meyer,
Joseph Nordgren, Jan-Erik Rubensson, Johan Söderström

Local organization: Maria Peter



Workshop Agenda

Thursday, October 21

09.00-09.05: Serguei Molodtsov (EuXFEL)
Welcome

09.05-09.25: Michael Meyer (EuXFEL, SQS)
A short introduction to SQS scientific instrument

09.25-09.55: Joseph Nordgren/Marcus Agåker (Univ. of Uppsala, Sweden)
A 1-D Imaging Soft X-ray Spectrometer for XFEL Experiments

09.55-10.10 Open discussions and questions

10.10-10.40 COFFEE BREAK

10.40-10.55: Monica Turcato (EuXFEL, DetOp)
The multi-delay-line detector

10.55-11.10: Tommaso Mazza (EuXFEL, SQS)
Beam properties and status for SASE 3 FEL and optical laser

11.10-11.30: Thomas Baumann (EuXFEL, SQS)
SQS diagnostics and instrumentation

11.30-11.45: Joachim Schulz (EuXFEL, SE)
Sample environments: liquid jet

11.45-12.00: Johan Söderström (Univ. of Uppsala, Sweden)
Gaseous samples and molecular beams

12.00-12.30 Open discussions

13.30-14.00: Victor Kimberg (KTH, Stockholm, Sweden)
Stimulated X-ray emission in molecules: experience and perspectives

14.00-14.30: Christian Ott (MPIK Heidelberg, Germany)
Absorption response of resonant atomic electron transitions to intense XUV electric fields

14.30-15.00: Nina Rohringer (DESY, Hamburg, Germany)
Nonlinear x-ray pump probe experiments in optically dense targets

15.00-15.30: Thomas Fennel (Univ. of Rostock, Germany)
Tracking ultrafast nanoplasma dynamics:
time-resolved imaging vs. photoelectron spectroscopy

15.30-16.00: COFFEE BREAK

16.00-16.30: Linda Young (Argonne Nat. Lab., USA)
Towards understanding x-ray propagation through optically thick media

16.30-17.00: James Cryan (PULSE, Stanford, USA)
Correlation Approaches to Nonlinear Spectroscopy at XFELs

17.00-17.30: Shaul Mukamel (Univ. of California, Irvine, USA)
Probing Elementary Molecular Events by Ultrafast Multidimensional X-ray Spectroscopy and Diffraction

17.30-19.00: Open discussion

Workshop Agenda

Friday, October 22

09.00-09.30: Benjamin van Kuiken (EuXFEL, SCS)
Resonant Inelastic X-ray Scattering Experiments in the Solid and Liquid State at the SCS Instrument of European XFEL

09.30-10.00: Jan-Erik Rubensson (Univ. of Uppsala, Sweden)
Time-resolved XES for beginners:
What do the Small Quantum Systems want to tell us?

10.00-10.30: COFFEE BREAK

10.30-11.00: Hans Jakob Wörner (ETH Zürich, Switzerland)
Time-resolved soft-X-ray spectroscopy in the gas and liquid phases

11.00-11.30: Marc Simon (LCPMR, Sorbonne University, France)
Perspectives in X-ray emission of Double Core Hole states

11.30-12.00: Riccardo Mincigrucci (Elettra Sincrotrone Trieste, Italy)
Recent Non-Linear optics results at the EIS instruments

12.00-13.30: LUNCH BREAK

13.30-17.00: Discussion on Community Proposals

17.00-17.15: Summary of discussion rounds

17.15: End of Workshop

Deadline for the next call at European XFEL (2nd semester 2022):

December 3rd, 2021

The SQS "Small Quantum Systems" Scientific Instrument of the European X-ray Free-Electron Laser

M. Meyer, European XFEL

Workshop on 1D-Imaging Soft X-Ray Spectroscopy at SQS

October 21, 2021

The SQS "Small Quantum Systems" Scientific Instrument of the European X-ray Free-Electron Laser

M. Meyer, European XFEL

Workshop on 1D-Imaging Soft X-Ray Spectroscopy at SQS
October 21-22, 2021

Outline

- General layout of SQS instrument
- SASE3 parameters
- Science examples

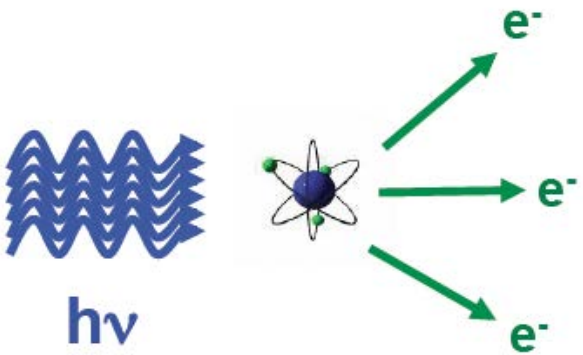
Scientific scope of SQS

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

AQS
Atomic-like Quantum Systems

10^{18} W/cm^2

Non-linear phenomena



Extremely high photon density

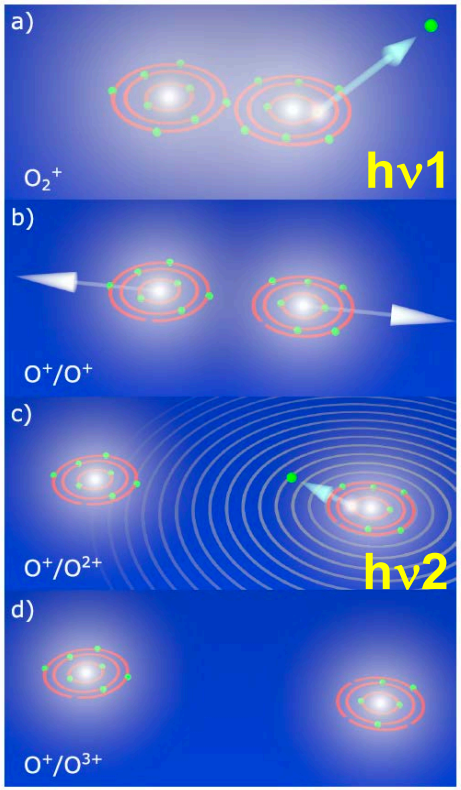
How atoms survive in intense fields?

Fast formation of high charges

REMI
REaction MIcroscope

20-30 fs

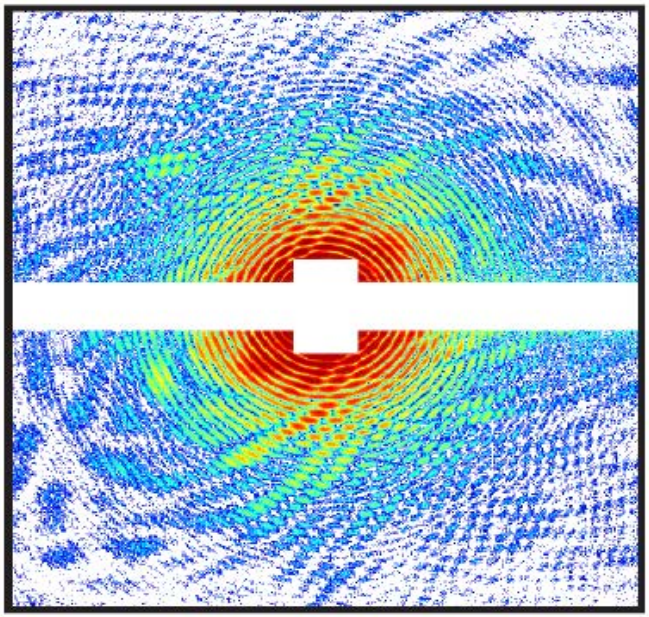
Time-resolved studies



NQS
Nano-size Quantum Systems

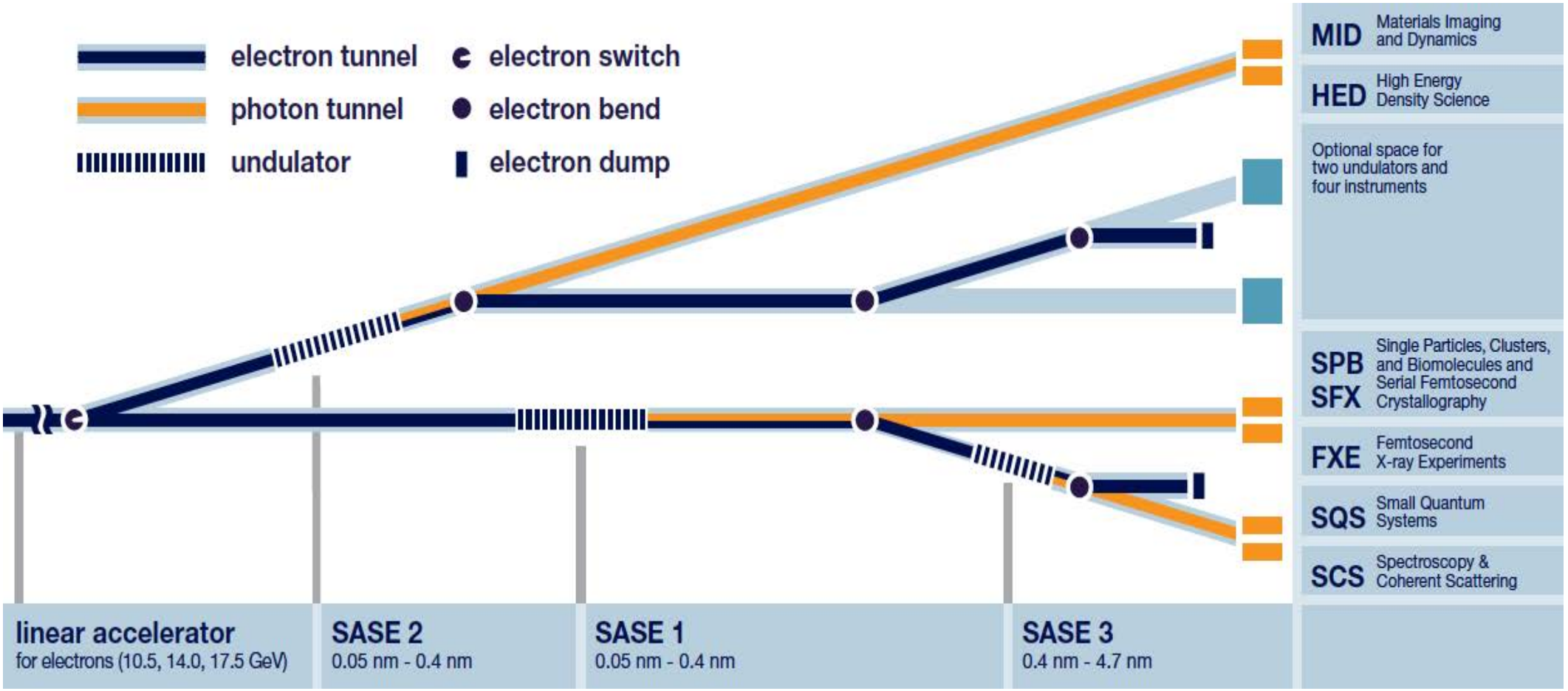
coherence

Imaging experiments

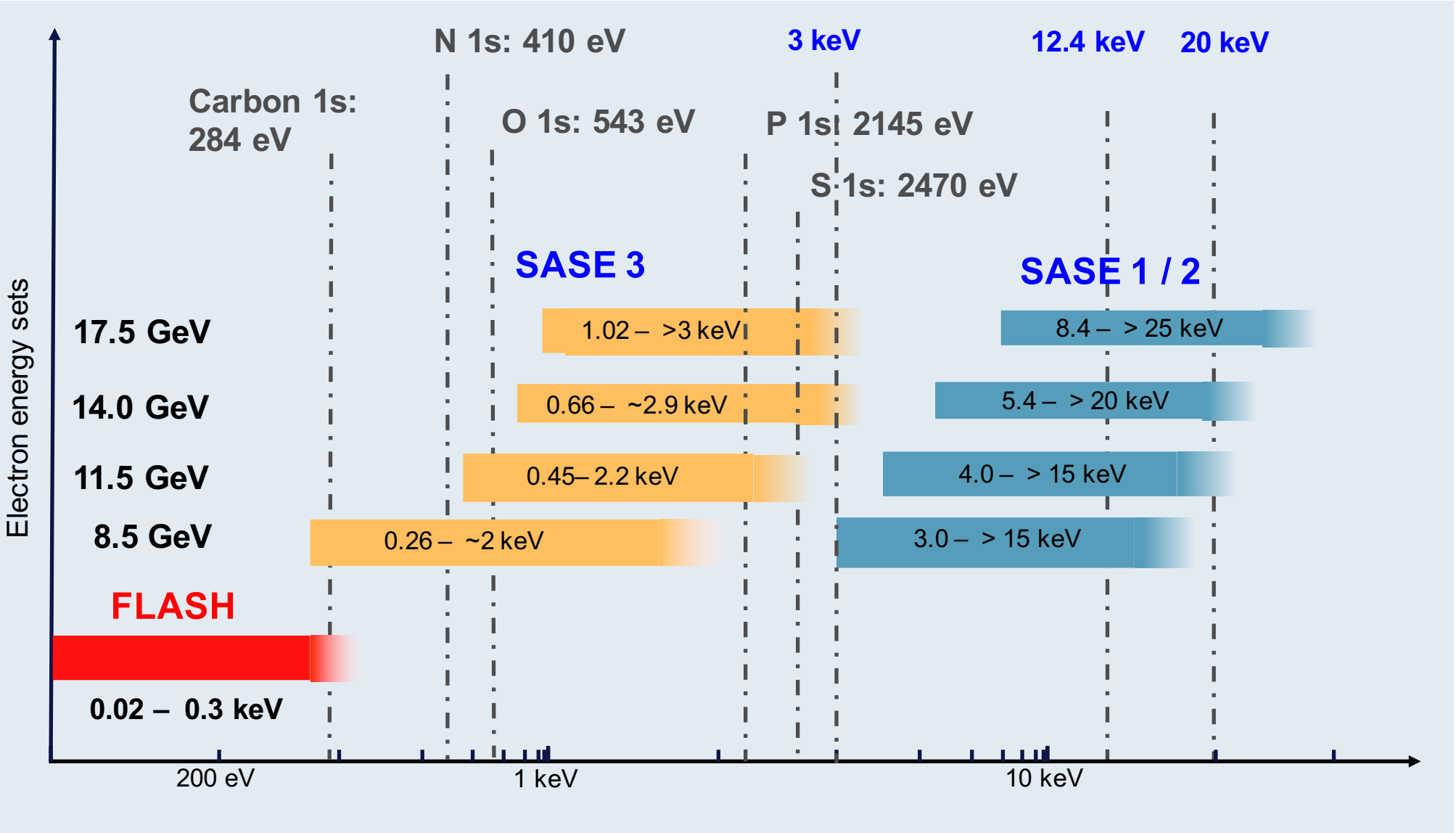


Doped He droplet

European beamline layout & experiment stations



Photon energy ranges



Soft X-Ray radiation parameters

Photon Beam Parameter	Unit	Operation 2021	Final Operation
Electron energy	GeV	11.5, 14, 16.5	8.5, 11.5, 16.5, 17
Photon energy	eV	500 – 1500 (@ 11.5 GeV) 660 – 2500 (@ 14 GeV) 920 – 3000 (@ 16.5 GeV) fully tunable !!	0.26 – 3
Spectral Bandwidth	%	~1% in SASE mode or monochromatized (resolution: 3000 @ 870 eV)	0.5 (SASE mode) 0.01 (monochromator)
Pulse duration (calc.)	fs	25 (FWHM)	2 - 100
Pulse energy	mJ	up to 8 (depending on photon energy)	Up to 10
Number of pulses		up to 400 per train (@ 1.1 MHZ)	2700 per train (@4.5 MHz)
Polarization		linear (horizontal)	Linear & circular
Focus size	µm	1 – 2 (@ F1 / F1') 2 – 3 (@ F2)	0.5 – 2

Two-color experiments

X-Ray - Optical Pump-Probe

Pump-Probe Laser (M. Lederer et al.)

< 20 fs, 800 nm, 0.2 mJ at 1.1MHz

< 20fs, 800 nm, 1 mJ at 188 kHz

SHG: 400 nm, 0.1 mJ, 30-50 fs

THG: 266 nm 0.06 mJ, <100 fs

Multi-pass cell (SQS & Laser Group)

< 50fs, 1030 nm, 2 mJ at MHz rep. rate

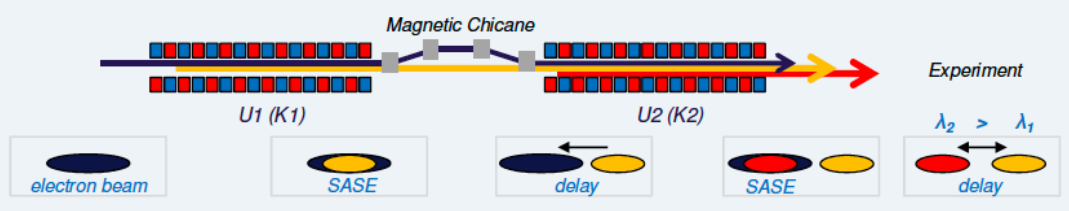
(under development)

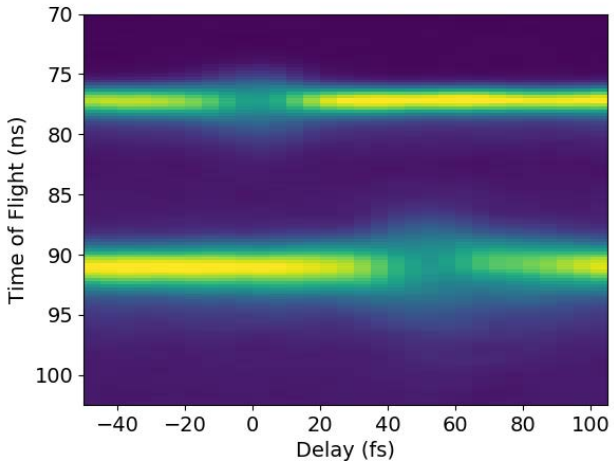
Pulse Arrival Time Monitor

Synchronization < 20 fs

X-ray – X-ray Pump-Probe

Magnetic chicane in SASE3 undulator





Electron spectra

C1s photolines

660eV and 688 eV

Delay 50 fs

(D. Rivas et al.)

Photon energy range: 500 – 1500 eV (→ 3000 eV)

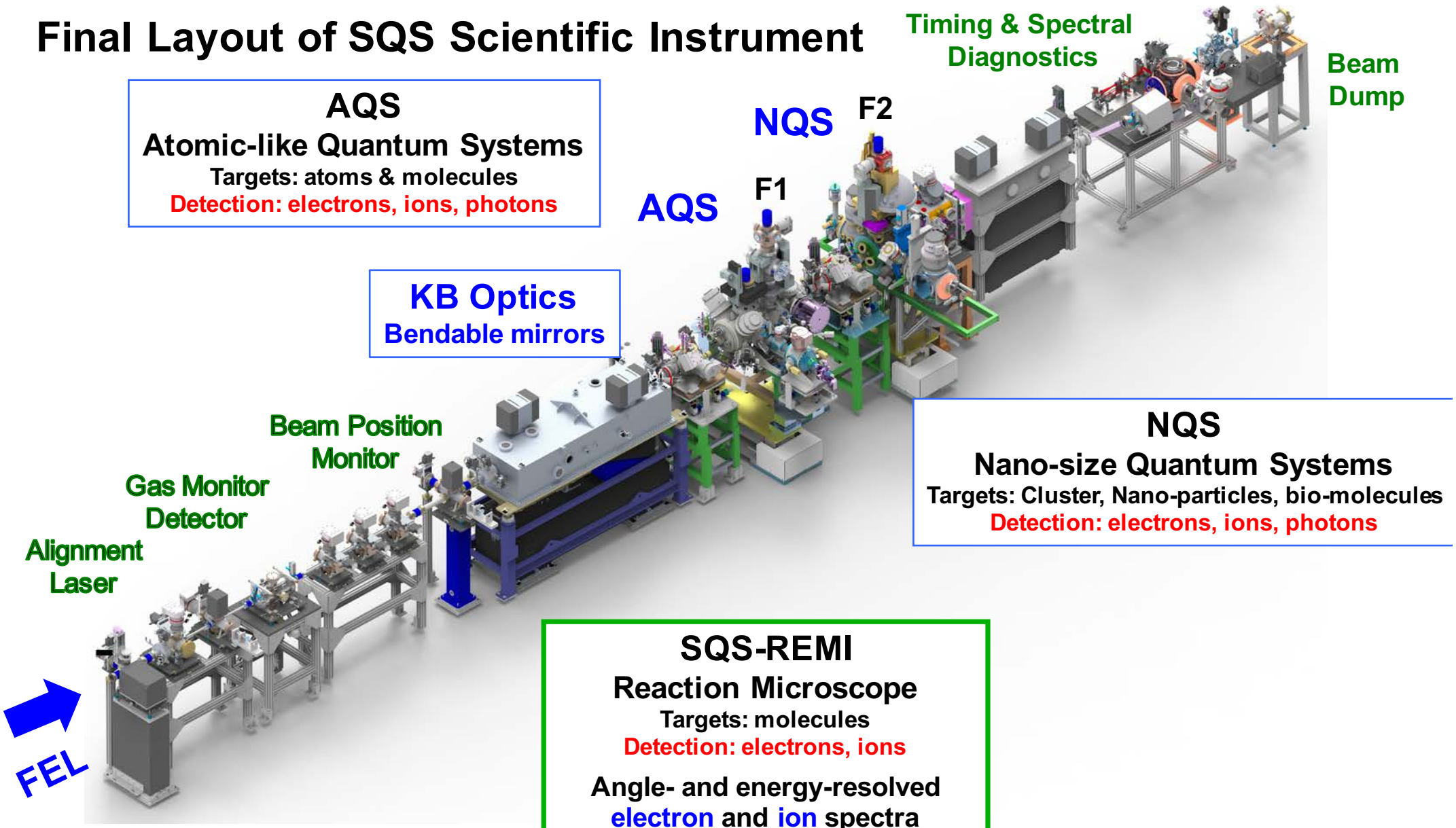
Pulse energy: up to 300 - 500 μJ

Pulse duration: < 30 fs

Temporal delay: up to 1 ps

Operation in close collaboration with S. Serkez & G. Geloni

Final Layout of SQS Scientific Instrument



AQS
Atomic-like Quantum Systems
Targets: atoms & molecules
Detection: electrons, ions, photons

NQS
Nano-size Quantum Systems
Targets: Cluster, Nano-particles, bio-molecules
Detection: electrons, ions, photons

SQS-REMI
Reaction Microscope
Targets: molecules
Detection: electrons, ions

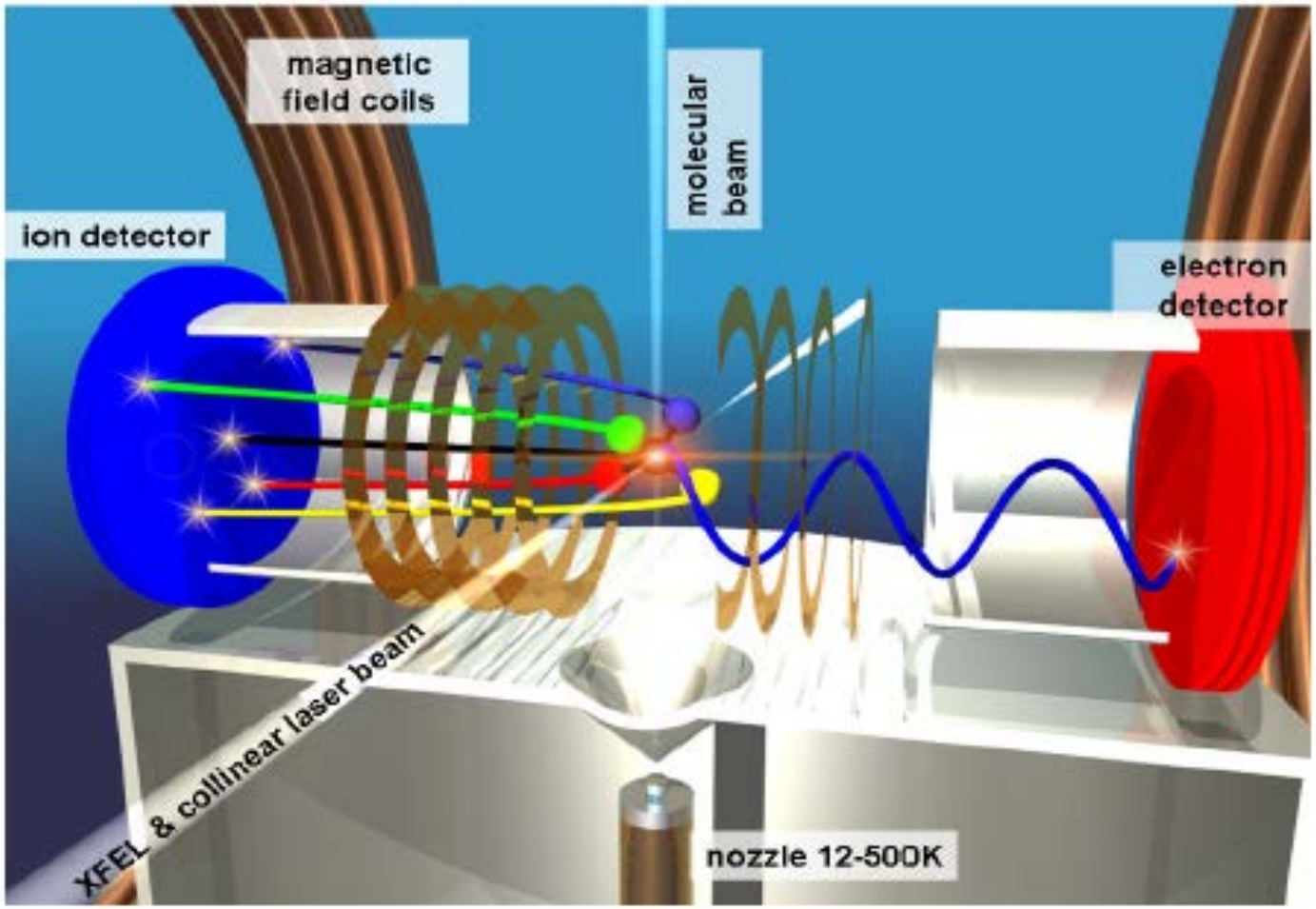
Angle- and energy-resolved
electron and ion spectra
in coincidence

SQS-REMI

REMI: Reaction Microscope

U. Frankfurt (R. Dörner et al.)

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



Ultra-high vacuum
< 10^{-11} mbar

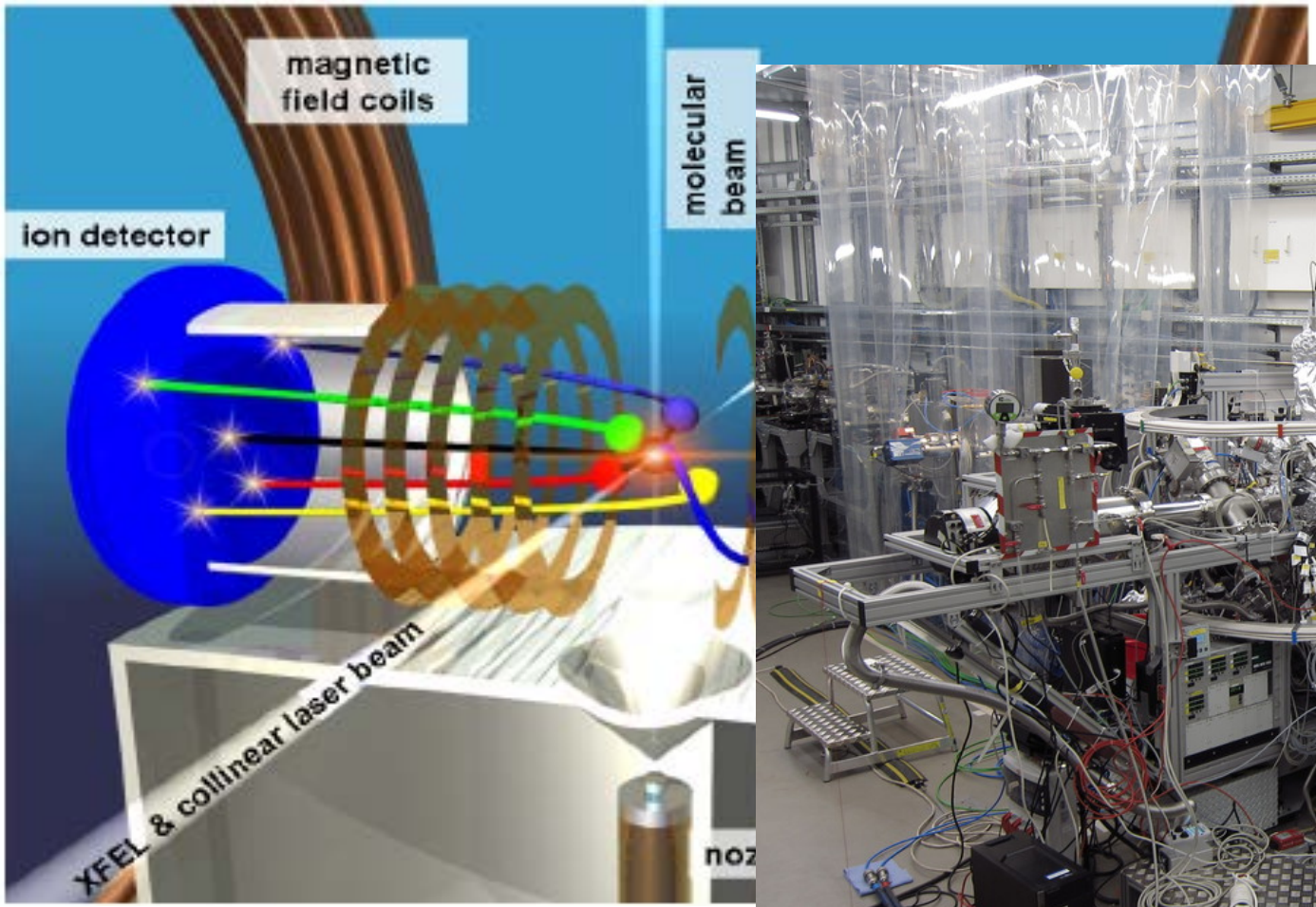
1 molecule / pulse

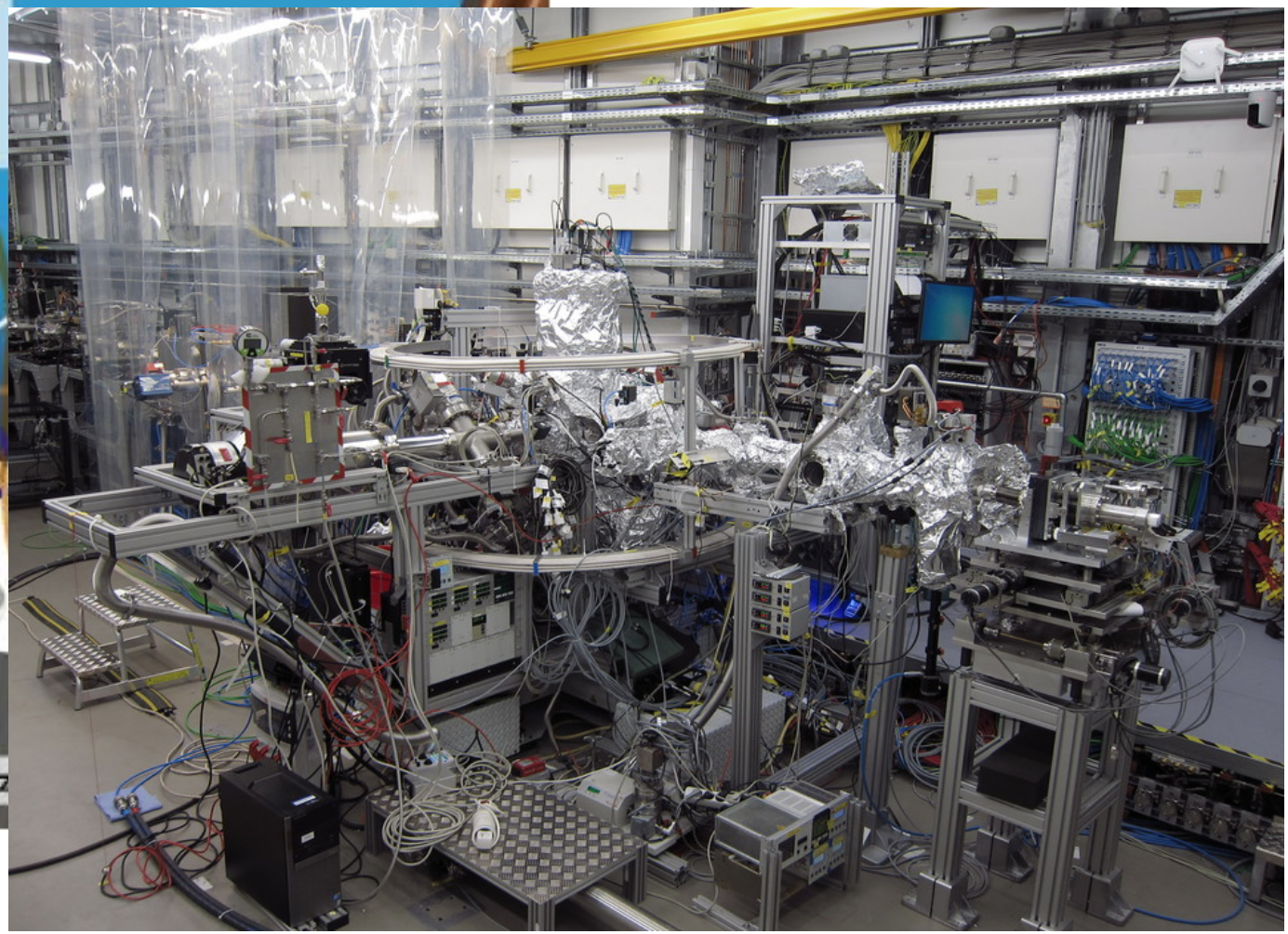
SQS-REMI

REMI: Reaction Microscope

U. Frankfurt (R. Dörner et al.)

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





Scientific results

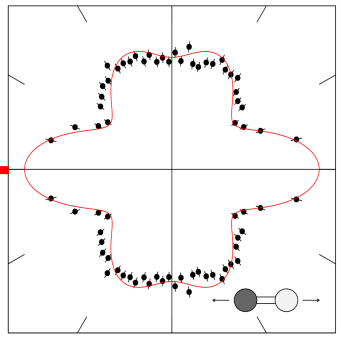
Photoelectron diffraction imaging of a molecular breakup (O2)

PI: Till Jahnke (U. Frankfurt)

G. Kastirke et al., PRX 10, 021052 (2020)

Molecular break-up visualized by non-linear processes

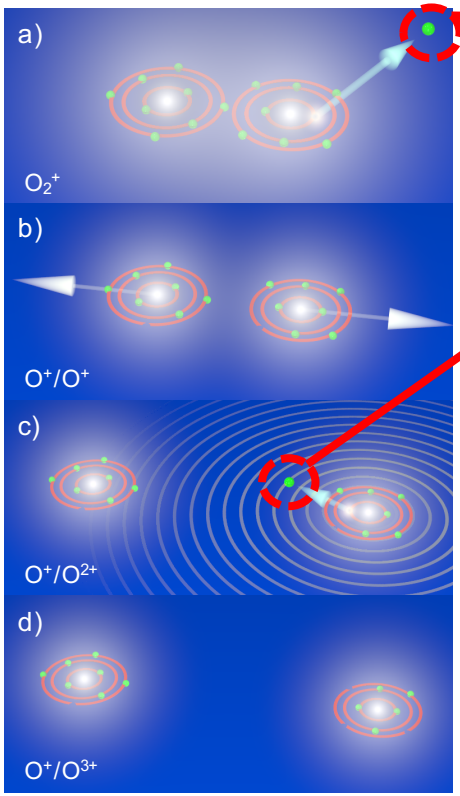
E(kin): 125 eV

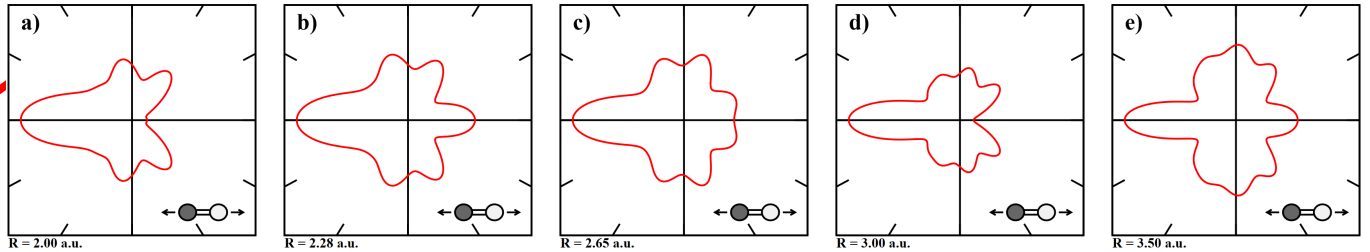


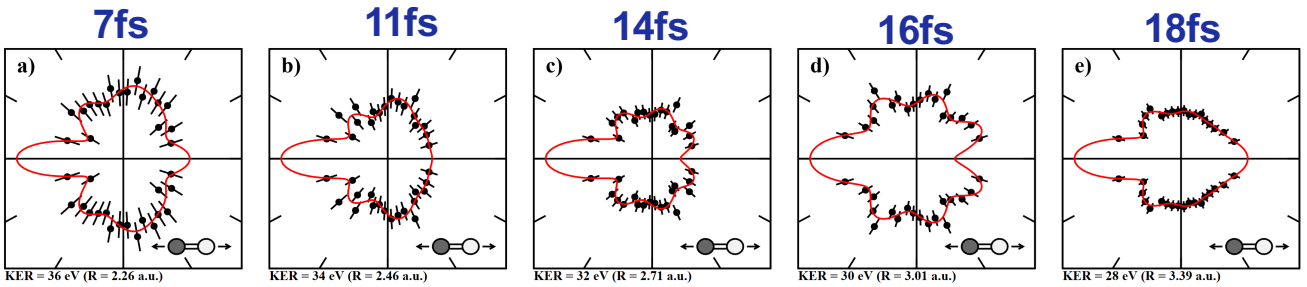
Electron angular distributions monitor the fragmentation process

SASE3: 665 eV, 300 pulses/s

Theory:
Relaxed core Hartree/Fock
Ph. Demekhin, Uni Kassel



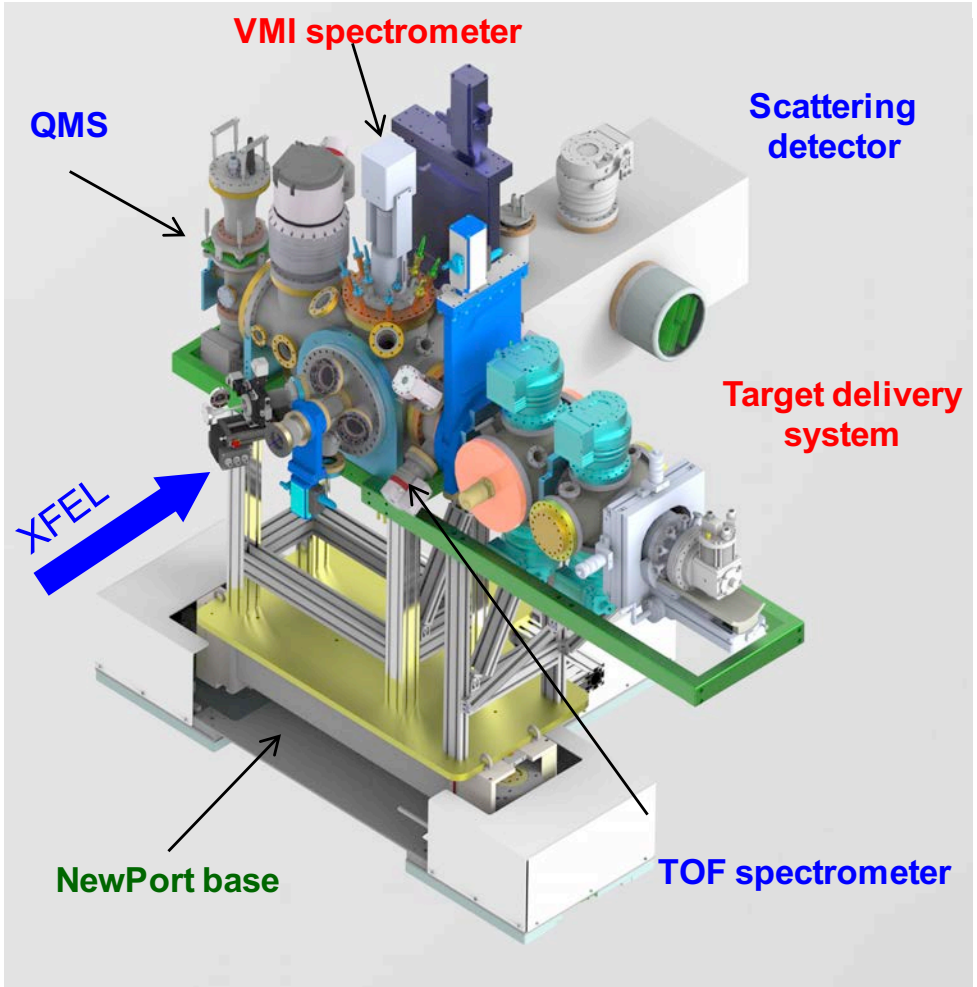




E(kin): 93 eV

Second electron „sees“ the repelled ion

NQS experimental chamber



NQS: Nano-size Quantum Systems

Targets: Cluster, Nano-particles, bio-molecules

Detection: electrons, ions, photons

Baseline equipment:

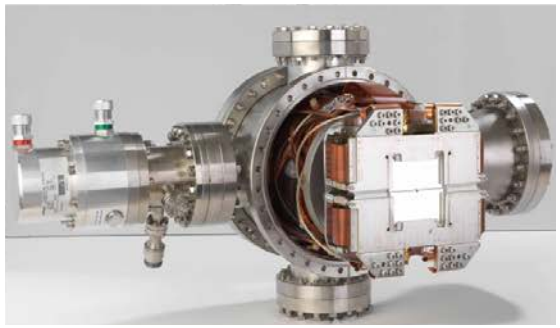
VMI & Ion Time-of-Flight

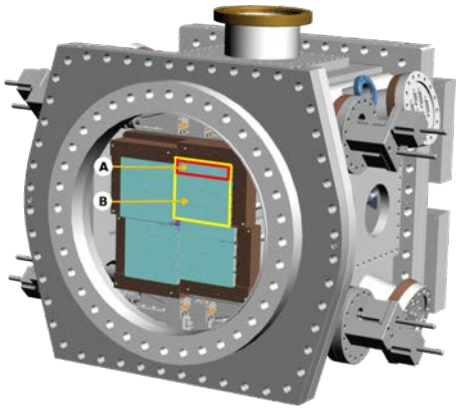
MCP-based scattering detector

Rare gas aggregation cluster source

pnCCD imaging detector (10 Hz)

DSSC imaging detector (4.5 MHz)



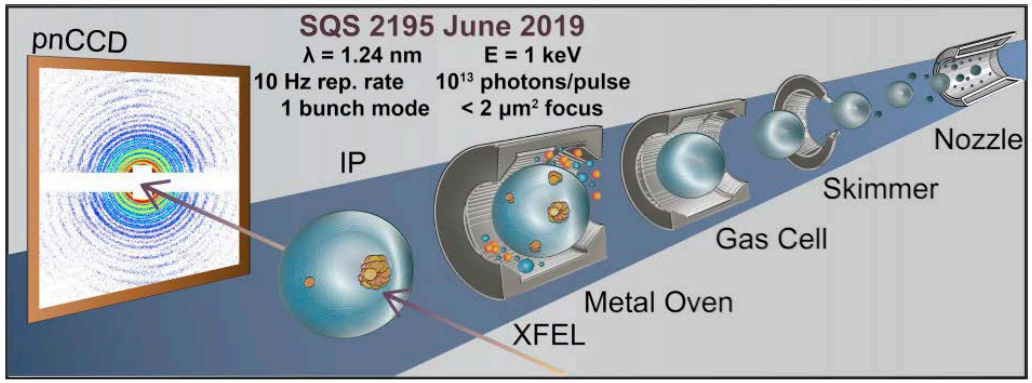


XCDI of pure and doped superfluid He droplets

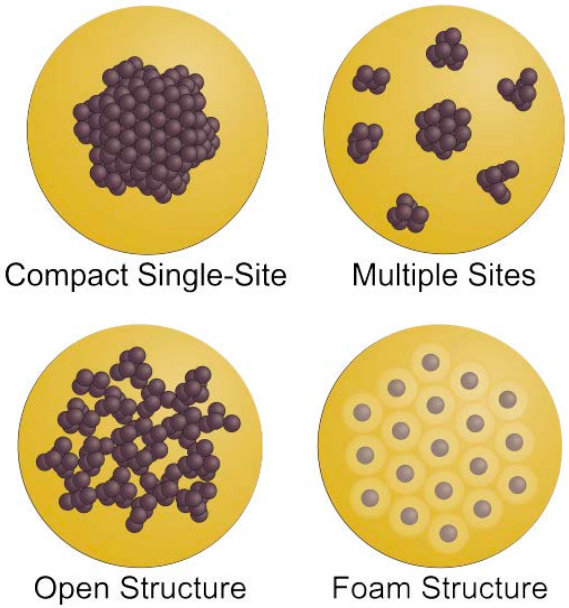
T = 4 - 10 K

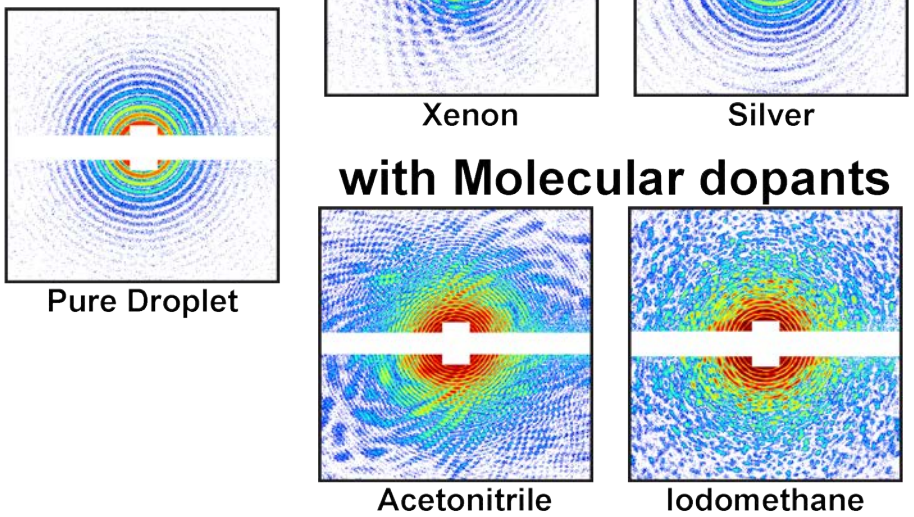
Imaging nanostructures in superfluid helium droplets

PI: R. Tanyag / D. Rupp (TU / MBI Berlin)
TU Berlin, MBI, SQS, U Aarhus,
DESY, U Rostock, USC, PnSensor, ETH

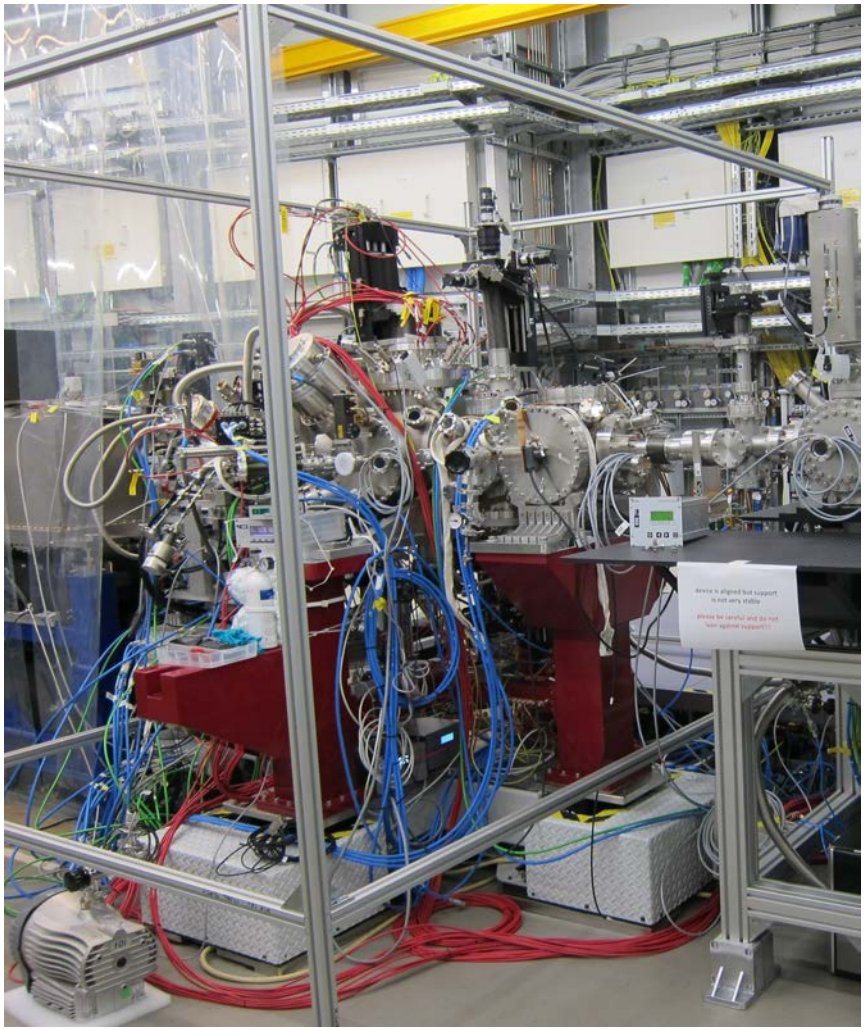


Out-of-equilibrium Nanostructures





AQS experimental chamber

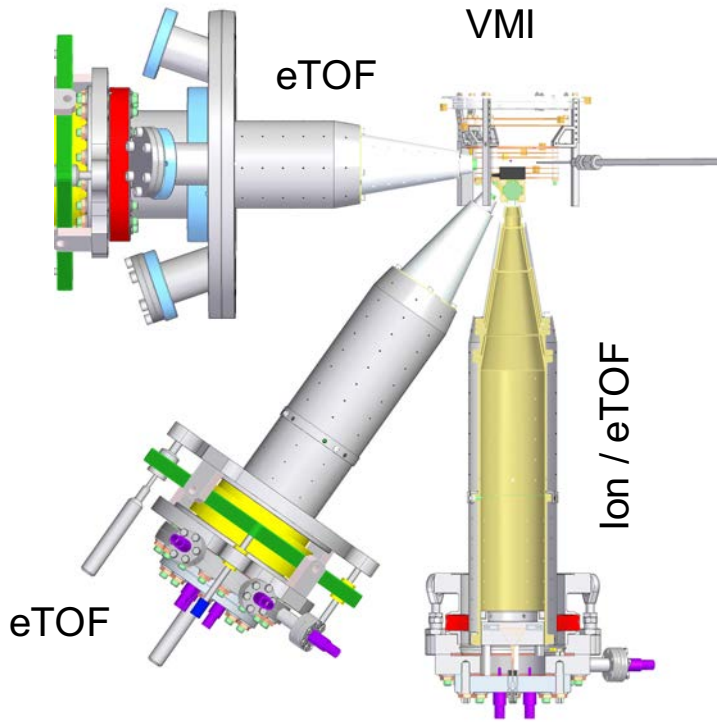


AQS: Atomic-like Quantum Systems

Targets: atoms & molecules

Detection: electrons, ions, photons

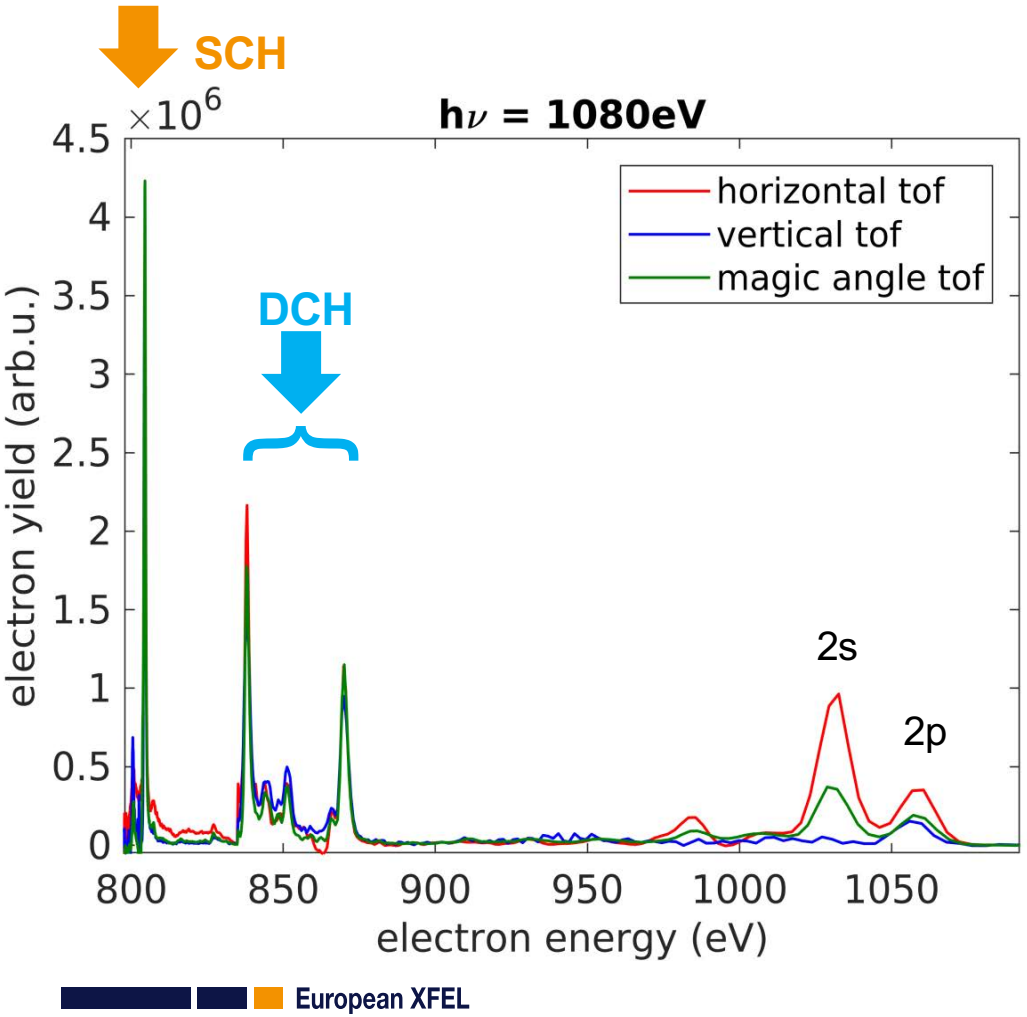
- **eTOFs** — **High energy resolution**, **Non-dipole studies**
- **VMI** — **Angular distribution**, **e / ion – coincidences**
- **MBES** — **high acceptance**, **e / ion - coincidences**



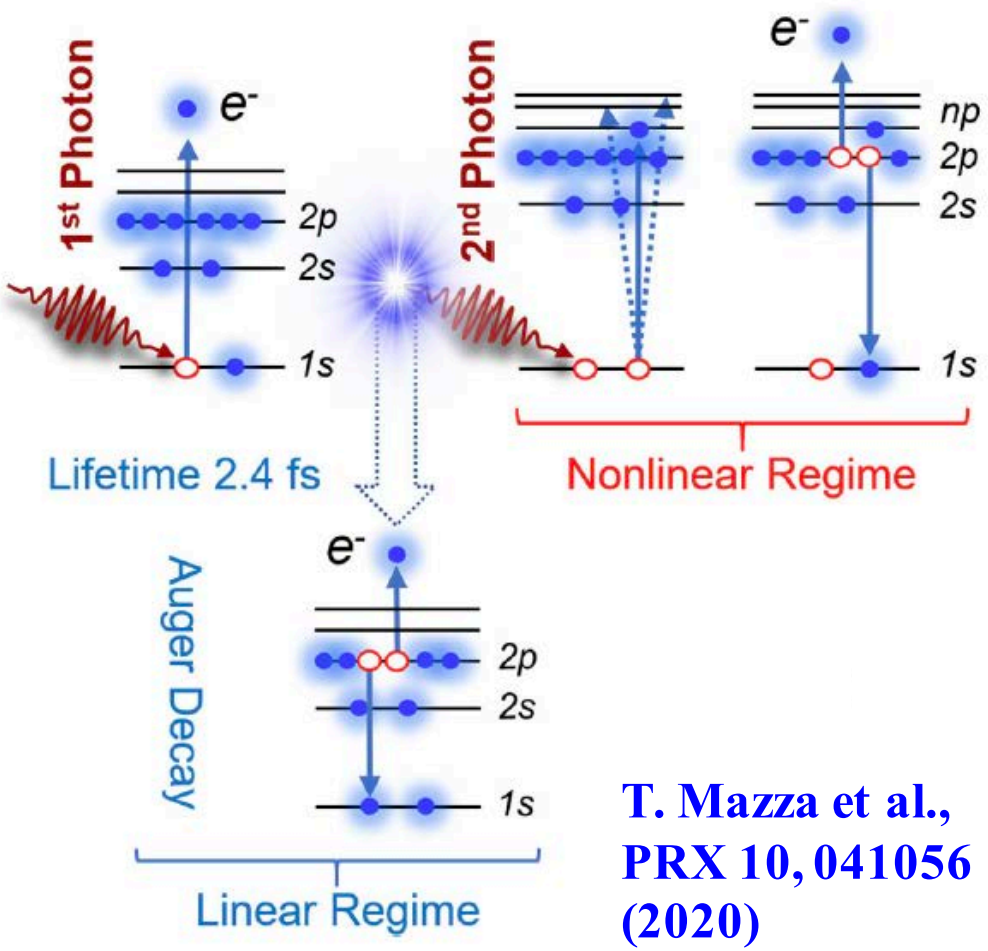
Double Core Hole spectroscopy

Single Core Hole: Ne $1s^2 2s^2 3p^6 + h\nu \rightarrow Ne^+ 1s^1 2s^2 3p^6 + e$

Double Core Hole: Ne $1s^2 2s^2 3p^6 + 2h\nu \rightarrow Ne^+ 1s^0 2s^2 3p^6 + e$



Strong Competition between one- and two-photon processes

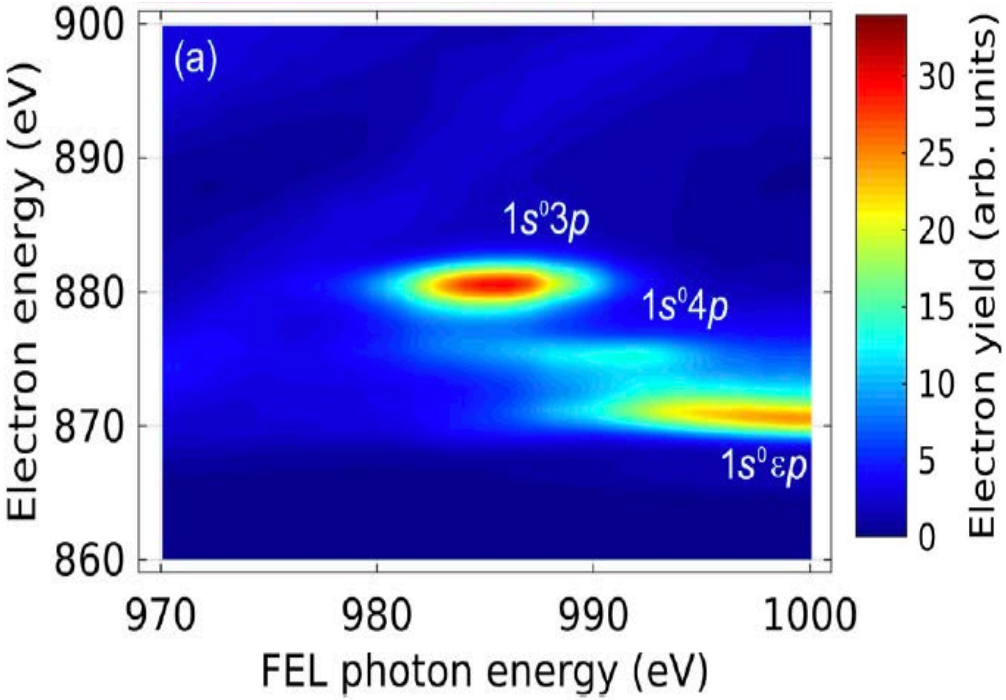


T. Mazza et al., PRX 10, 041056 (2020)

Double Core Hole spectroscopy

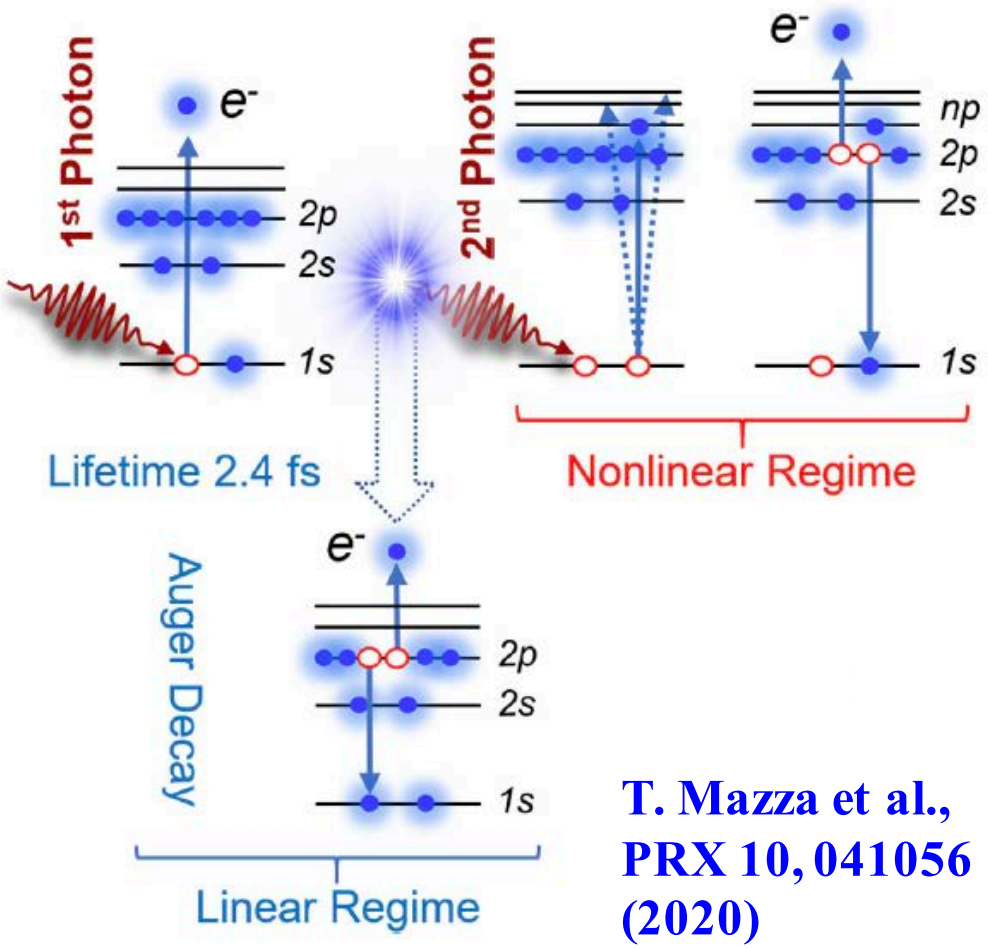
Spectroscopy
on short-lived transient states

Resonant Auger Maps
(XUV wavelength tuning)



$\Gamma(1s) = 2.4$ fs

Strong Competition between one- and two-photon processes



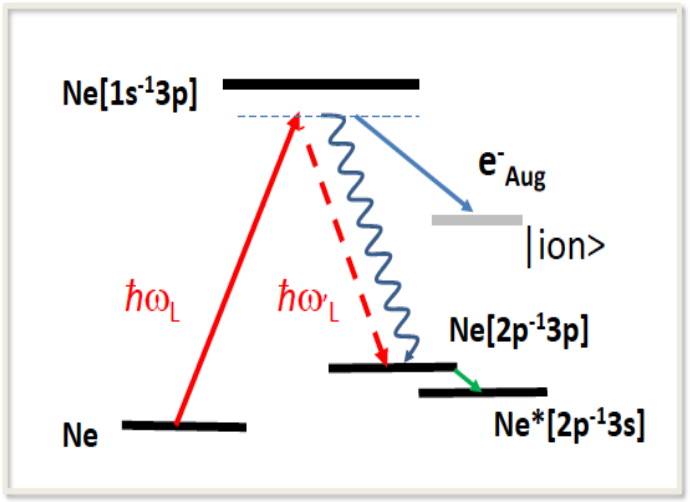
T. Mazza et al., PRX 10, 041056 (2020)

Stimulated X-Ray Raman Scattering

U. Eichmann et al., Science 369, 1630 (2020)

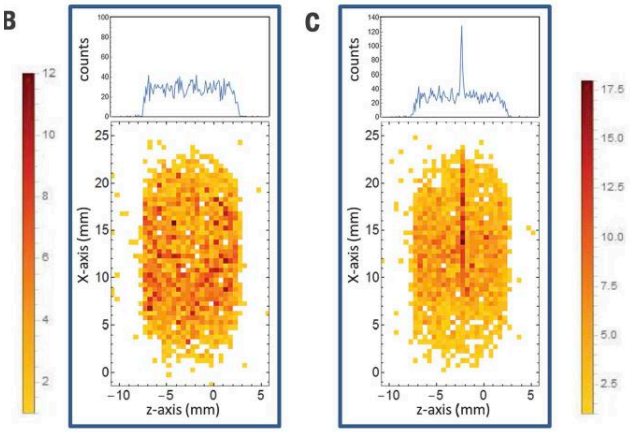
XFEL-induced stimulated emission in Ne atoms via atomic recoil measurement

SASE3: 1 mJ, 25 fs, 10^{17} W/cm²

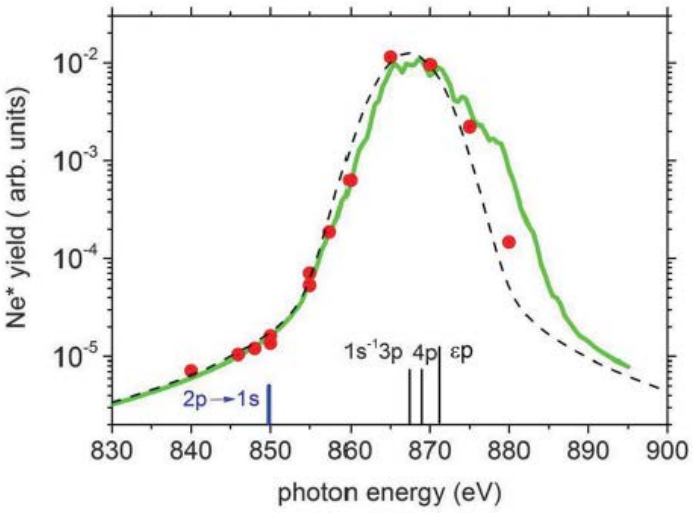


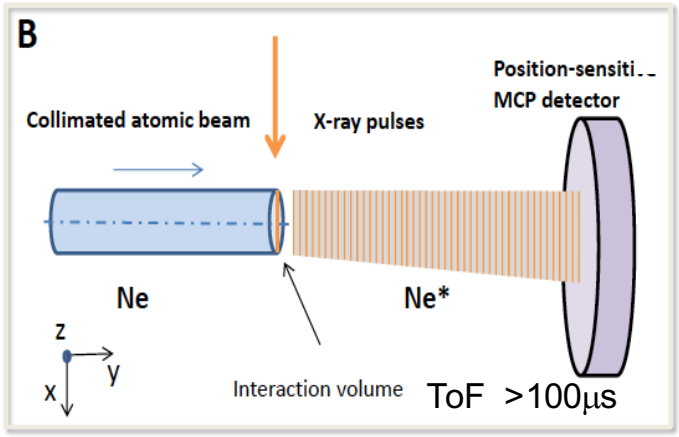
860 eV

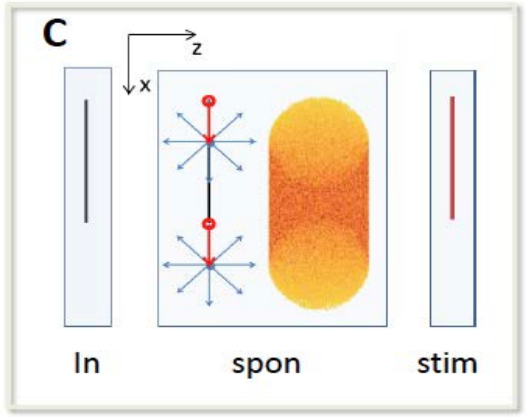
855 eV

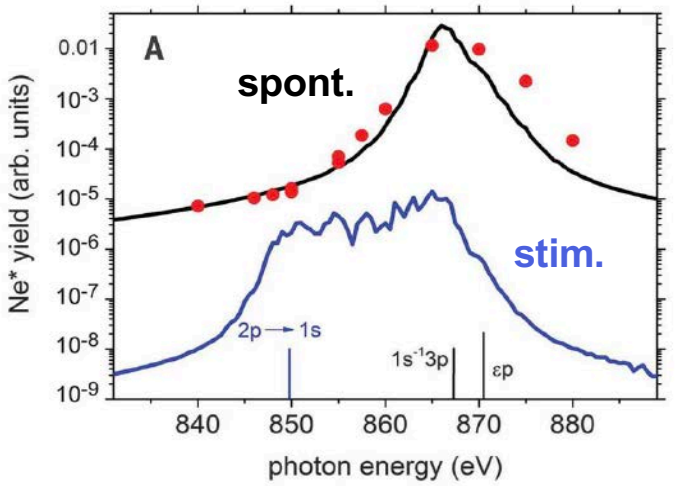


Ne* yield









Main experimental tools at SQS:

AQS: Electron Spectroscopy
Ion Spectroscopy
Metastable neutral atoms

REMI: Electron-Ion Coincidences
Momentum spectroscopy

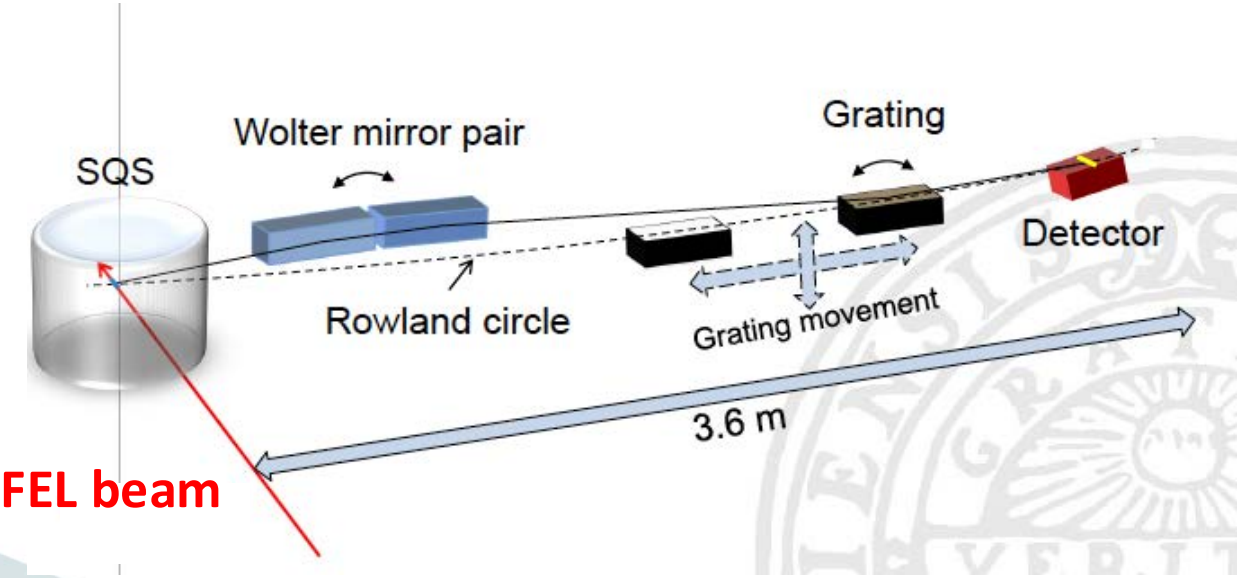
NQS: Ion Spectroscopy
Coherent Diffraction Imaging

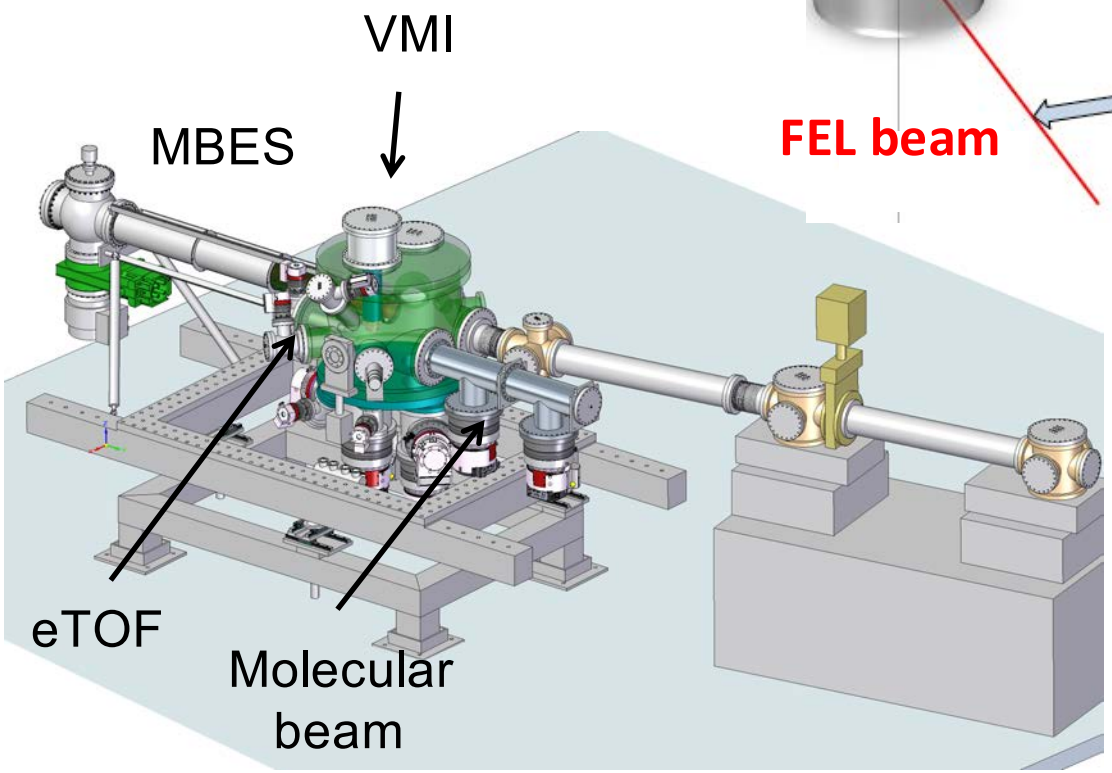
→ **Photon Spectroscopy ??**

AQS: XUV 1D Imaging spectrometer

M. Meyer, XFEL UM2014

In-Kind Contribution:
J. Nordgren, J-E. Rubensson,
Uppsala University, Sweden

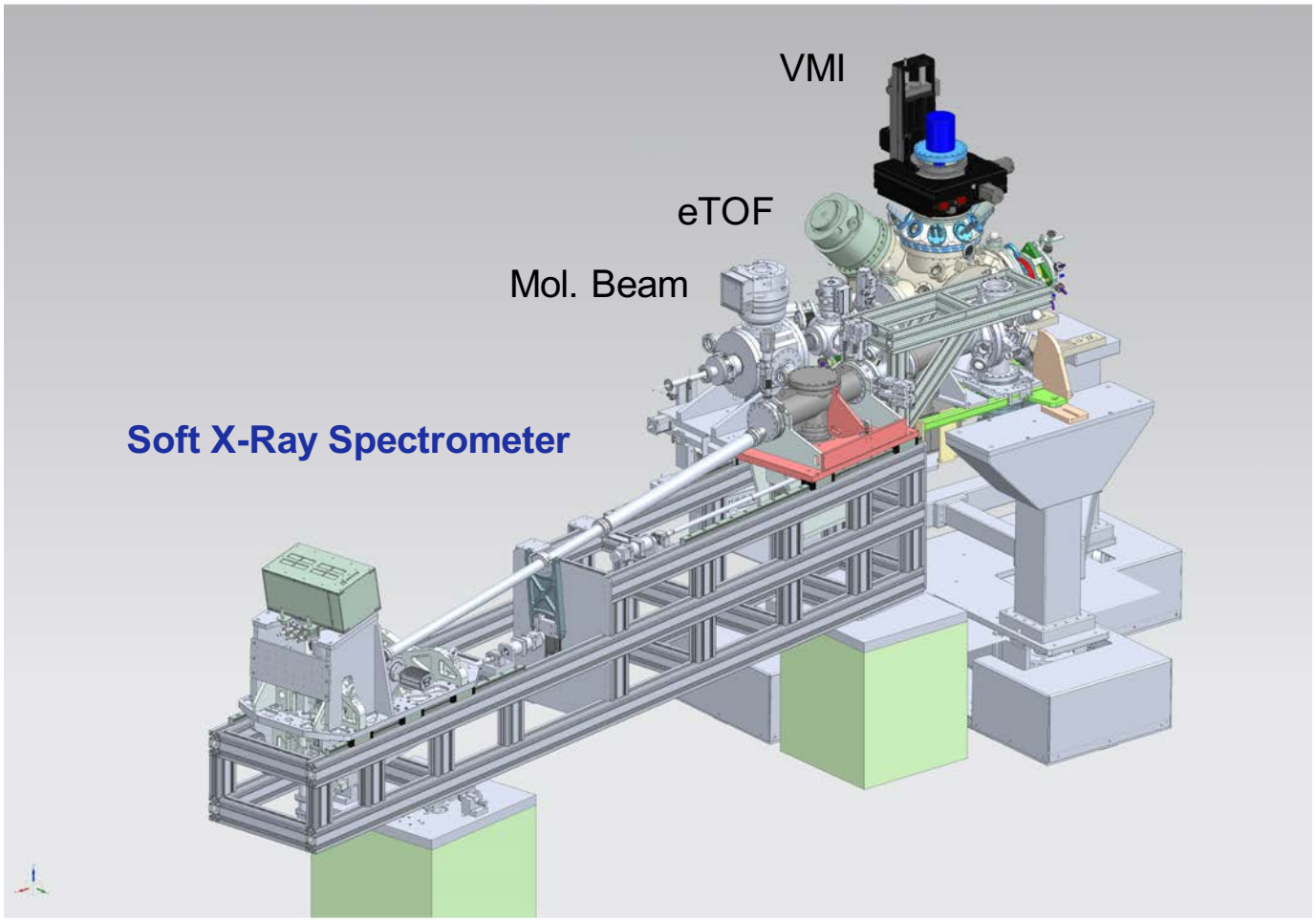




Optimized Design
Spectral resolution: 10 - 50 meV
Spatial resolutions: 2 µm
Single pulse sensitivity

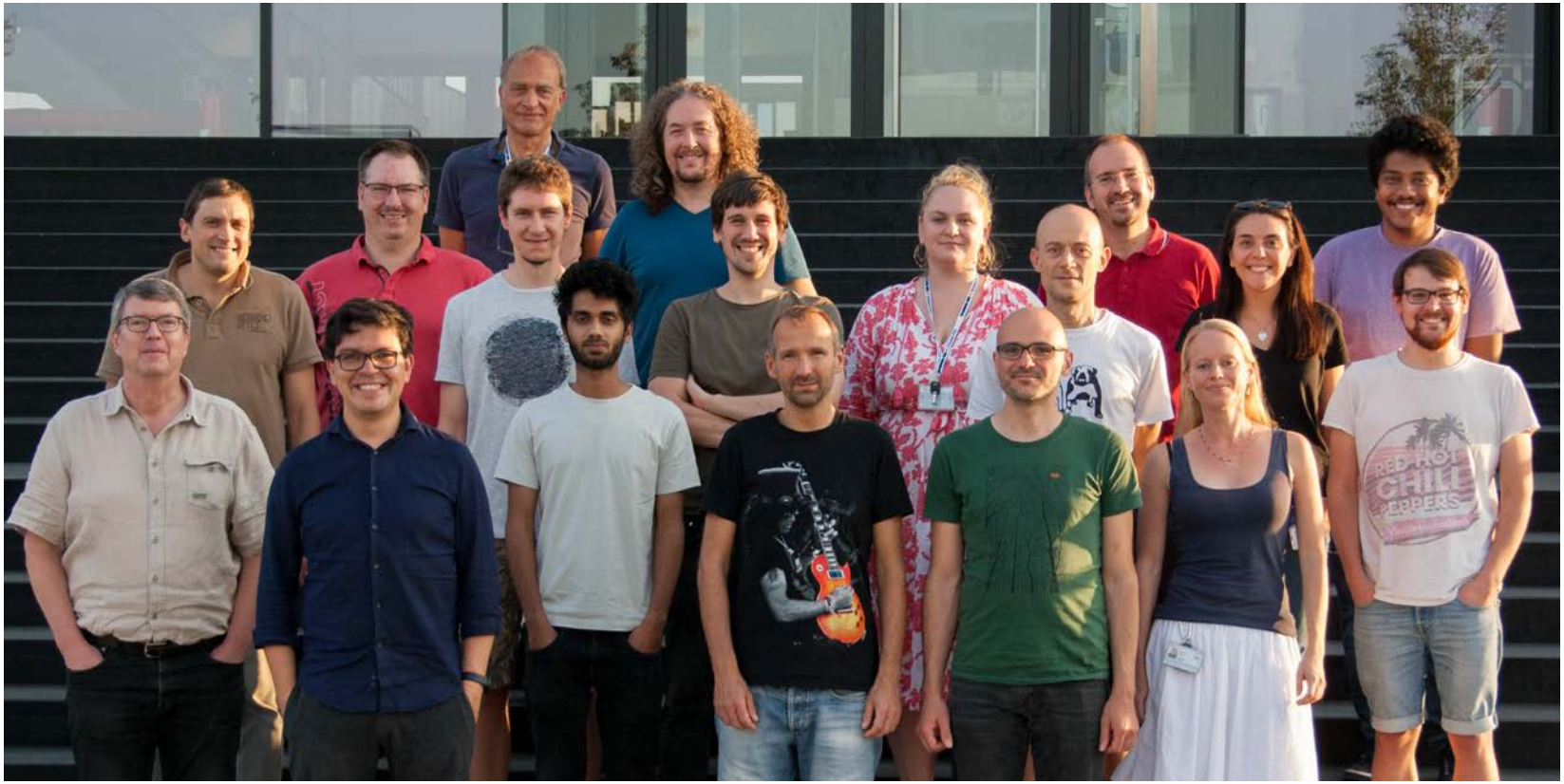
New detector development
MCP with multi-parallel delay-line readout (WP-75)

AQS chamber with XUV 1D Imaging spectrometer



SQS team

Sept 2021



T. Baumann
R. Boll
A. De Fanis
S. Dold
M. Lüdeke

T. Jahnke
T. Mazza
M. Meyer
J. Montano
T. Mullins

Y. Ovcharenko
N. Rennhack
D. Rivas
S. Usenko
M. Peter
R. Hartmann (guest)

PhD students
V. Music
A. Rörig
R. Wagner
A. Alangattuthodi
S. Sasikumar


SQS
Thank you for your attention !!!