



SQS Commissioning and first experiments (SASE-3)

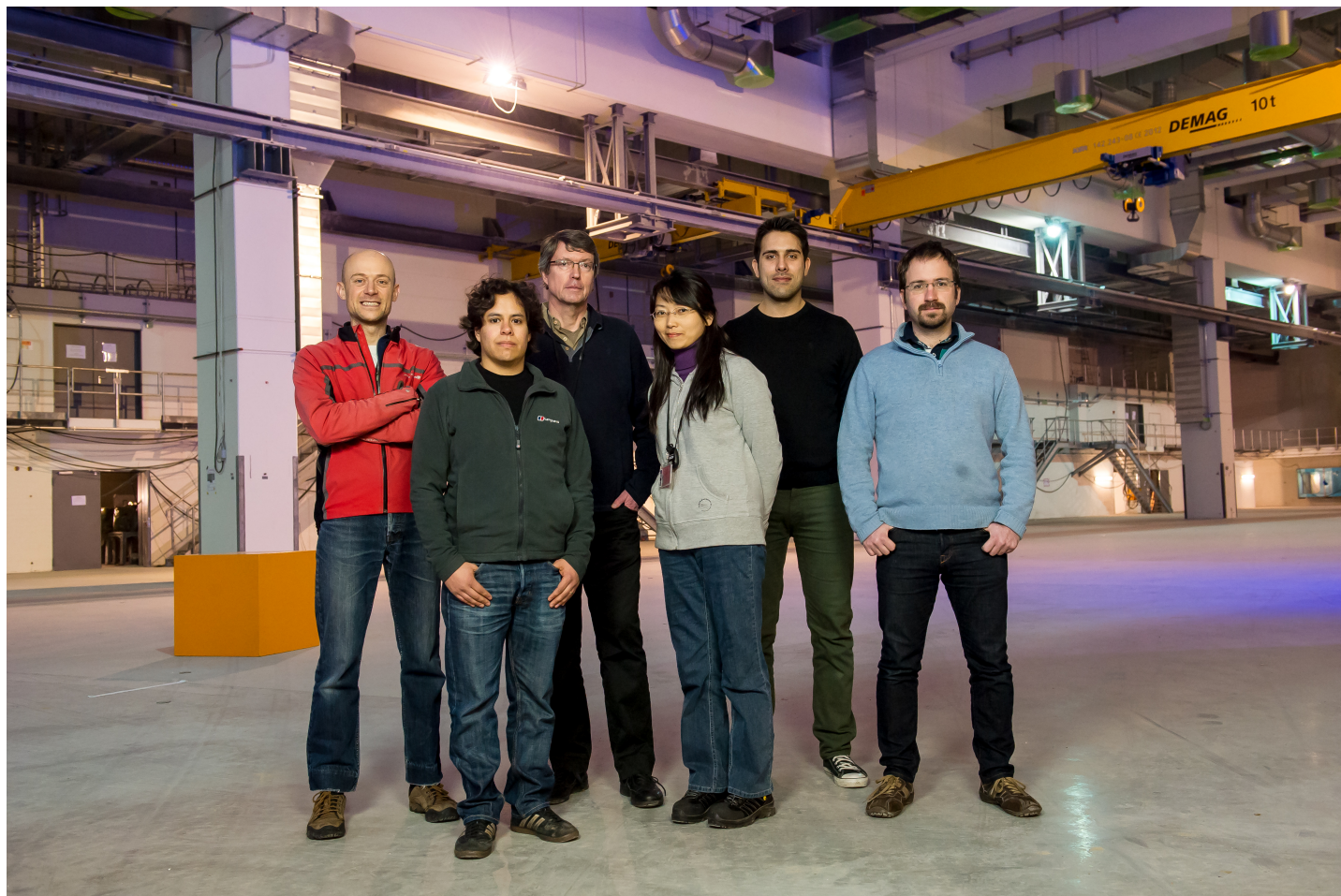
M. Meyer, WP-85 (SQS)

1) SQS installation

- Status and Schedule

2) First experiments

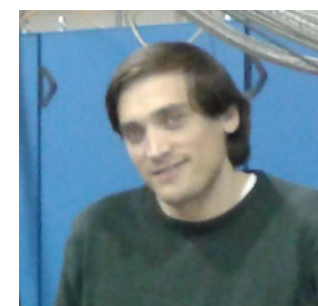
- Commissioning experiments
- First “Science” application
 - 1) Non-linear Processes
 - 2) Molecular Fragmentation



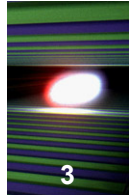
A. de Fanis M. Meyer J. Rafipoor
A. Achner H. Zhang T. Mazza

Since mid 2015:

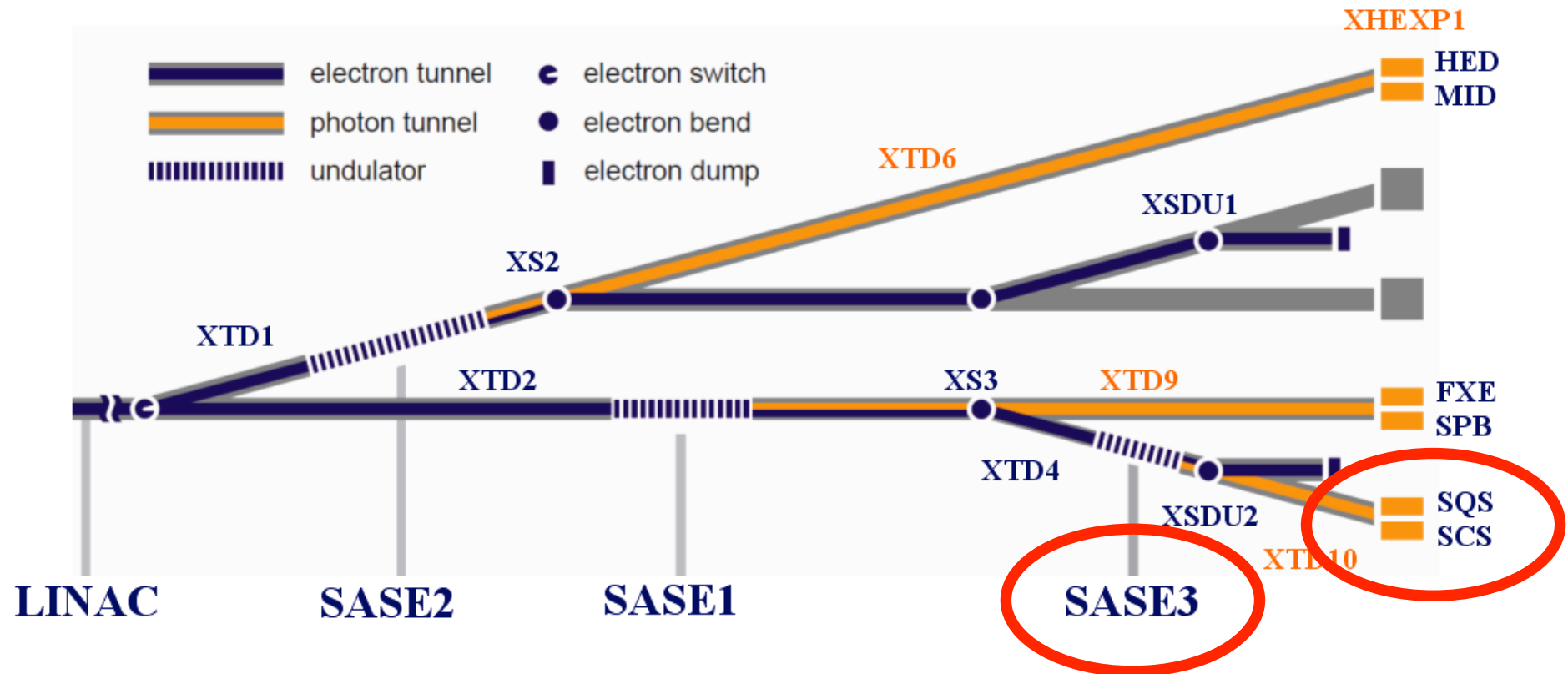
Th. Baumann



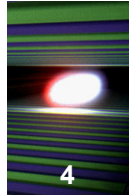
Y. Ovcharenko



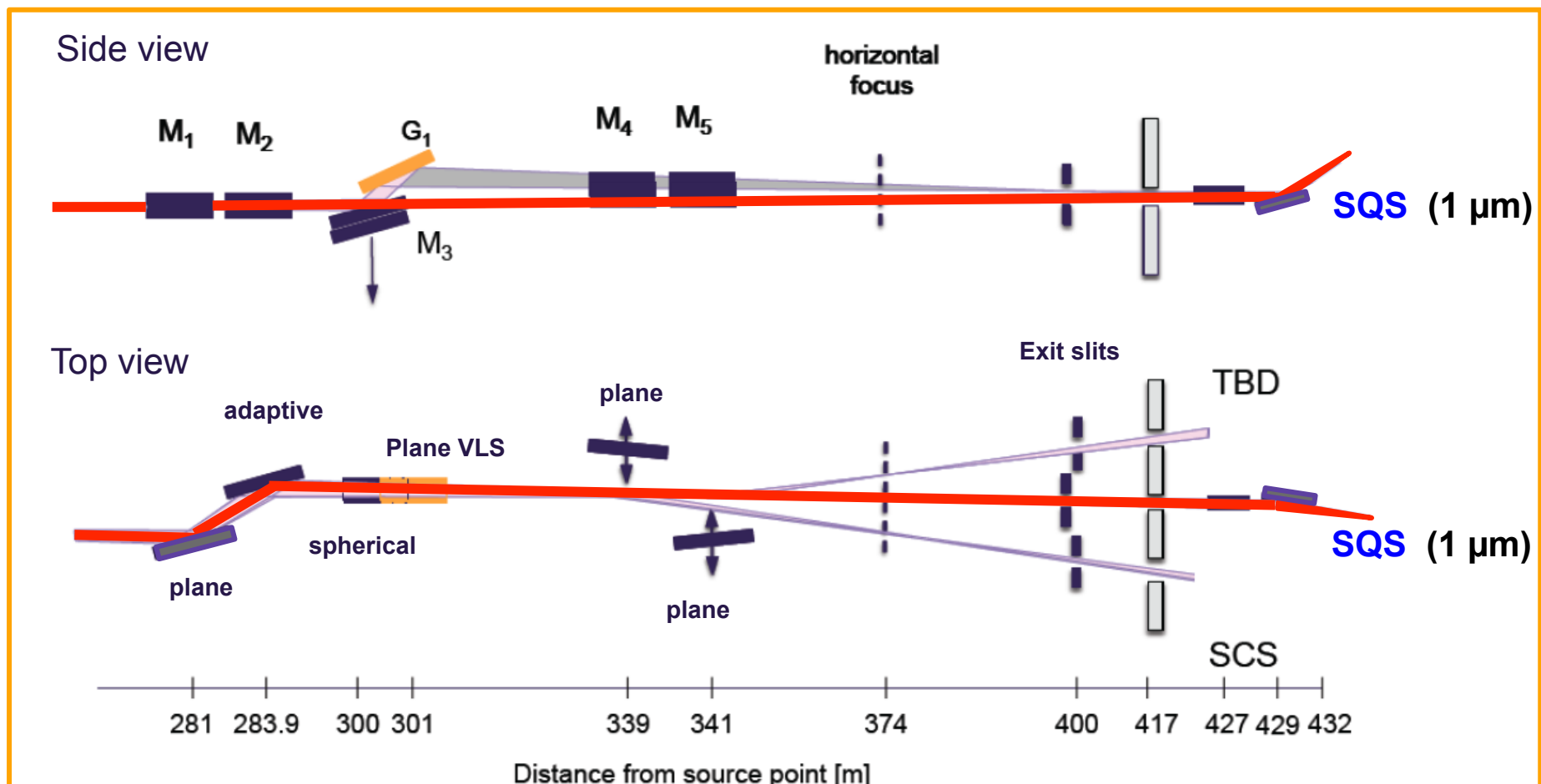
European XFEL



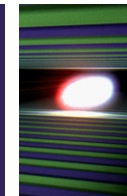
Photon beam transport systems



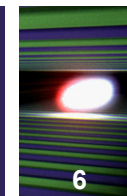
- **direct beam** → **Small Quantum System (SQS)**
- **monochromatized** → **Spectroscopy @ Coherent Scattering (SCS)**



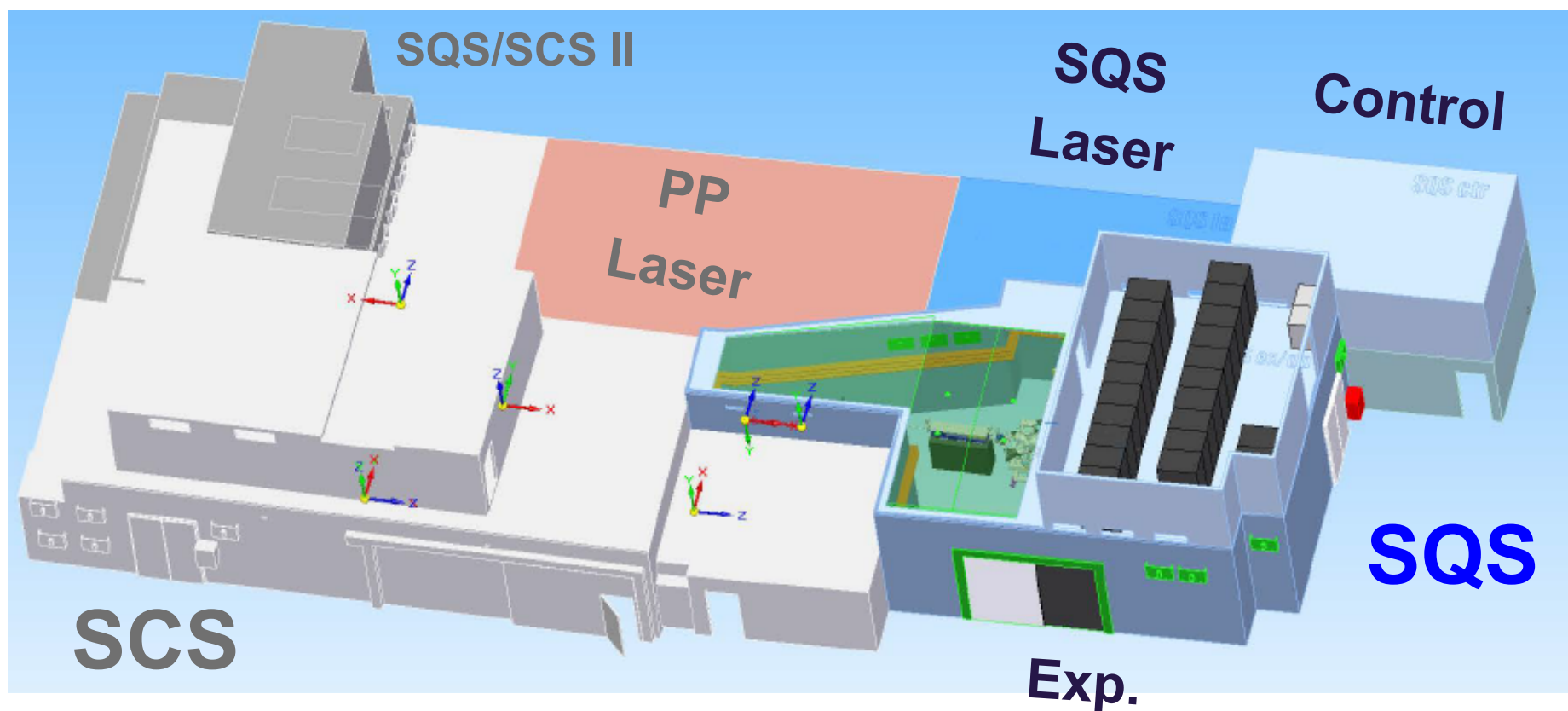
SASE3 – October 2015



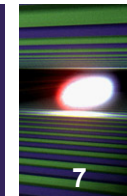
SASE3 Laser Hutches



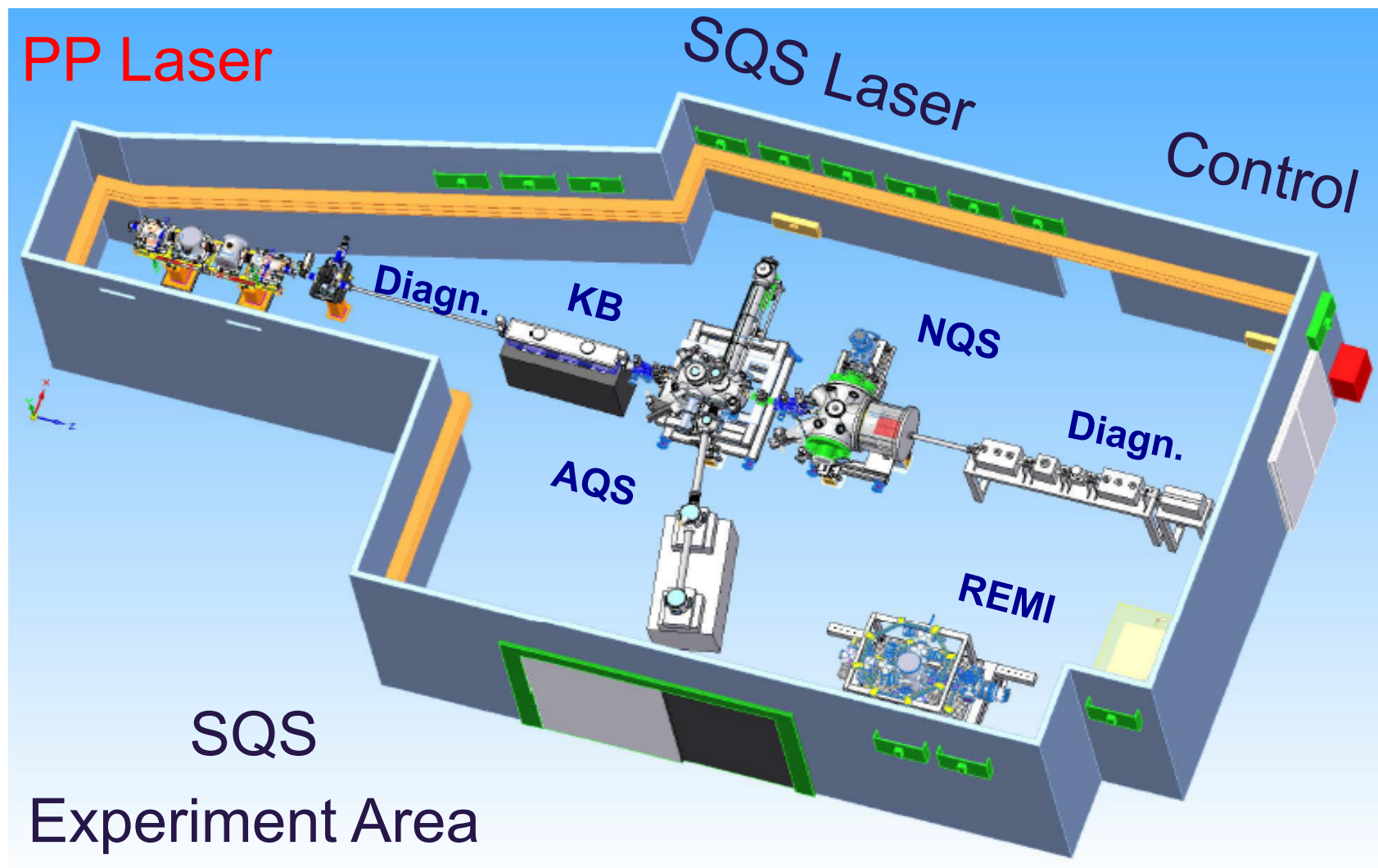
SASE3



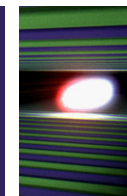
General Layout of SQS Scientific Instrument



7

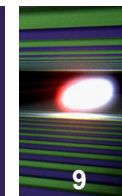


Milestone update (PSPO)

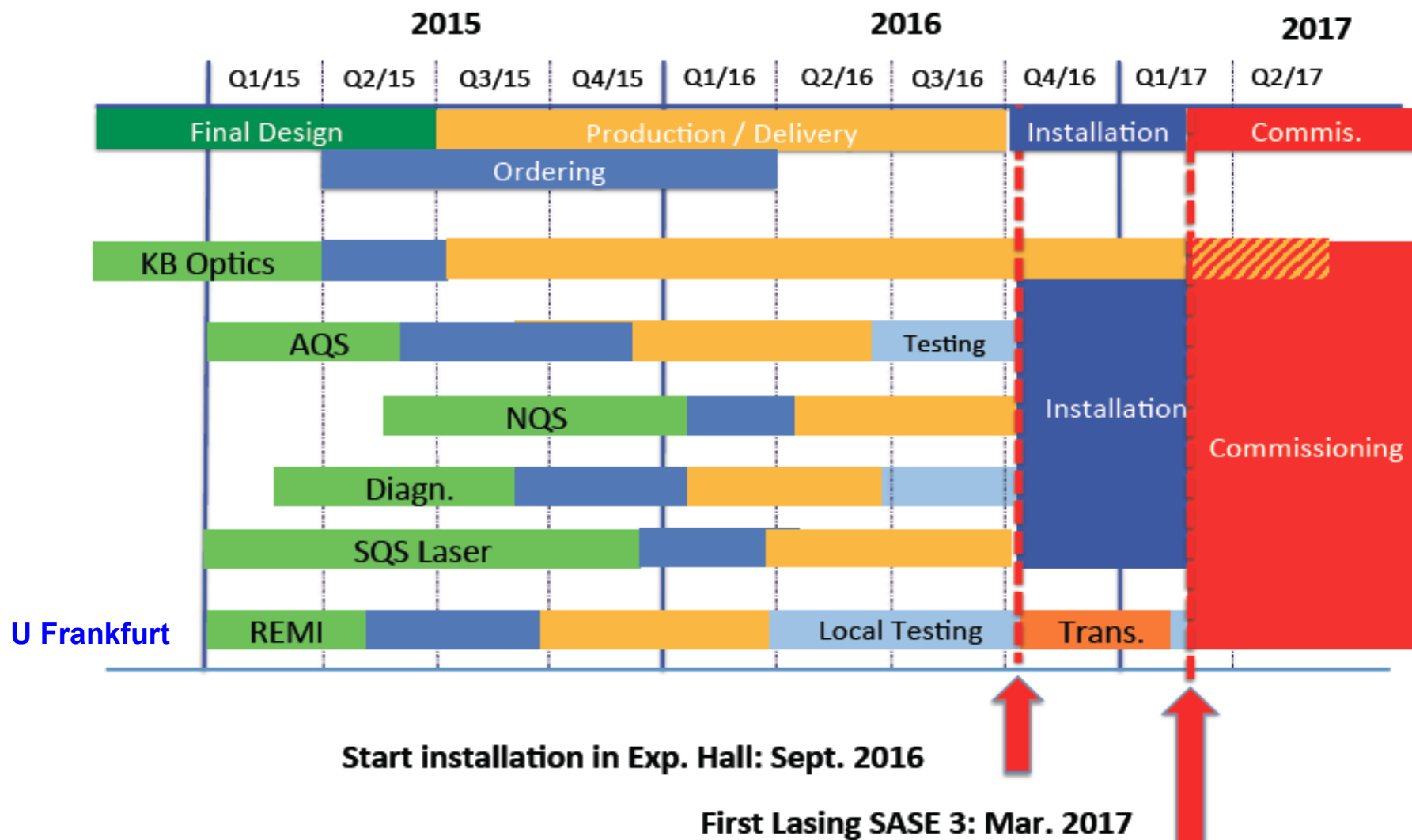


Milestone Name	Date
SASE1	
HUTCH PRR	18.03.2014
SASE1 Hutch construction start	14.04.2015
FXE BIG ITEMS	03.08.2015
SPB/SFX BIG ITEMS	13.07.2015
HUTCH CONSTRUCTION COMPLETE (INSTRUMENT INSTALLATION POSSIBLE)	09.10.2015
INFRASTRUCTURE PRR	25.02.2015
ALL HUTCHES & BASIC INFRASTRUCTURE DONE (INSTALLATION OF SENSITIVE COMPONENTS POSSIBLE)	26.04.2016
COMPLETE HUTCHES AND INFRASTRUCTURE DONE	19.07.2016
SASE3	
HUTCH PRR	17.03.2015
SASE3 Hutch construction start	05.08.2015
HUTCH CONSTRUCTION COMPLETE (INSTRUMENT INSTALLATION POSSIBLE)	11.03.2016
INFRASTRUCTURE PRR	24.09.2015
ALL HUTCHES & BASIC INFRASTRUCTURE DONE (INSTALLATION OF SENSITIVE COMPONENTS POSSIBLE)	28.09.2016
COMPLETE HUTCHES AND INFRASTRUCTURE DONE	23.11.2016
SASE2	
HUTCH PRR	15.10.2015
SASE2 Hutch construction start	23.02.2016
HUTCH CONSTRUCTION COMPLETE (INSTRUMENT INSTALLATION POSSIBLE)	06.07.2016
INFRASTRUCTURE PRR	16.11.2015
ALL HUTCHES & BASIC INFRASTRUCTURE DONE (INSTALLATION OF SENSITIVE COMPONENTS POSSIBLE)	22.11.2016
COMPLETE HUTCHES AND INFRASTRUCTURE DONE	17.01.2017

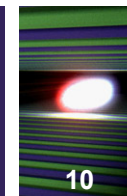
Schedule for SQS Scientific Instrument



9

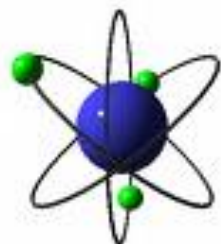


SASE3 & SQS Performances



SASE3	$h\nu = 260 - 3000 \text{ eV}$	$P = 0.2 - 11.0 \text{ mJ}$	Lin./Circ. Pol.
	$\Delta T = 2 - 100 \text{ fs}$	Coherence: 0.96	Split & Delay

Atoms



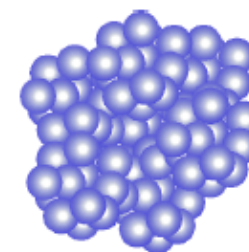
Non-linear phenomena
 $10^{17} - 10^{18} \text{ W / cm}^2$

Molecules



Time-resolved studies
low jitter (<10 fs)

Clusters



Imaging experiments
Spatial coherence

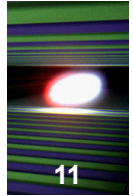
European XFEL

High repetition rate:
< 27000 pulses/ sec



High data collection rate
Multi-particle coincidences

!!!!



- **SQS & SCS (SASE3)**
 - First Lasing March 2017
 - Early user operation from October 2017

“Day – one” parameter: SASE3

Rep. rate : 100 kHz

Photon energy: 1.0 – 1.5 keV

Pulse energy: up to 3 mJ

Pulse duration: 50 fs

Electron beam energy: 17.5 GeV

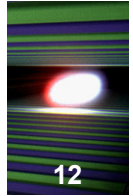
Shifts 2017 for SASE3 (SQS)

(no parallel operation)

Commissioning (total): 150 shifts (12 hours)

SQS Instrument : ≈ 25 shifts
(including beam transport)

“friendly” user operation : ≈ 10 shifts



■ 1) Non-linear processes

Multi-photon processes

Nonlinear: Signal $\sim I^N$

Intensity

$$I \sim \frac{\text{pulse energy [J]}}{\text{pulse duration [sec]} \times \text{focus area [cm}^2\text{]}}$$

Example: 10 μ J, 10 fs, 10 μ m
 $\sim 10^{15}$ W/cm²

“Day – one” parameter: SASE3

Rep. rate : 100 kHz

Photon energy: 1.0 – 1.5 keV

Pulse energy (P): up to 3 mJ

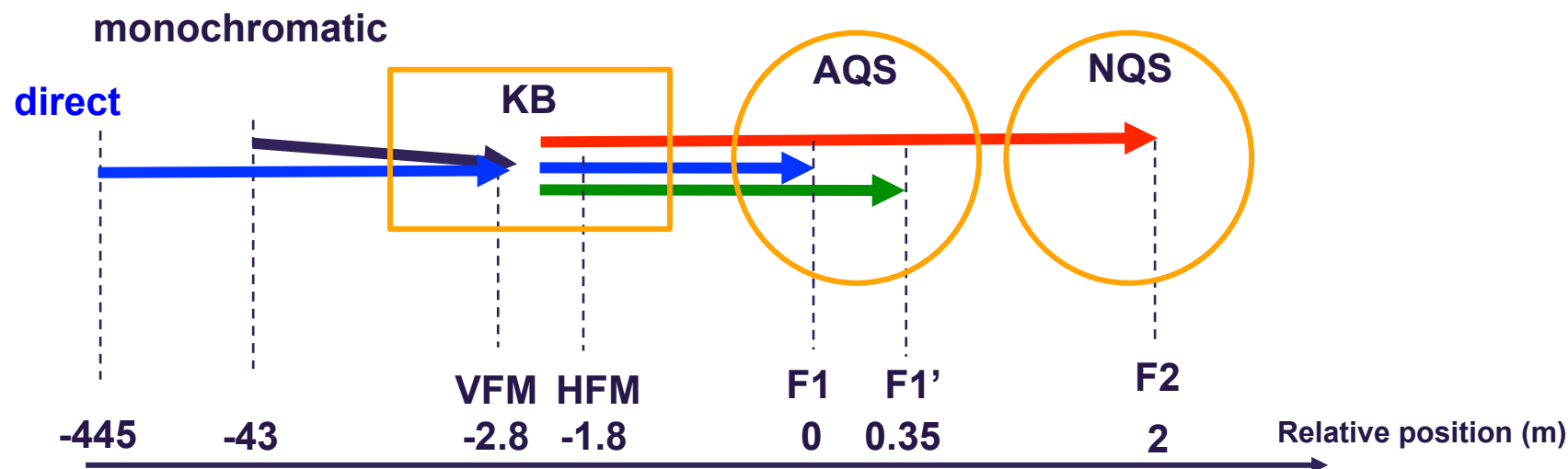
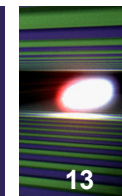
Pulse duration (T): 50 fs

SQS KB system:

Focus diameter: 1 micron

6×10^{18} W/cm²

KB focusing optics (in coll. with WP-73)



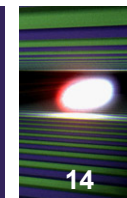
Requirements

- 3 interaction points
- ≤ 1 micron focus
- variable focus size
- high transmission
- large wavelength range

Challenges

- Bendable mirrors
- Length 800 mm
- Large bending range
- Slope error 50 nrad
- Cooling system

Simulations for KB optics (Mechanical benders)



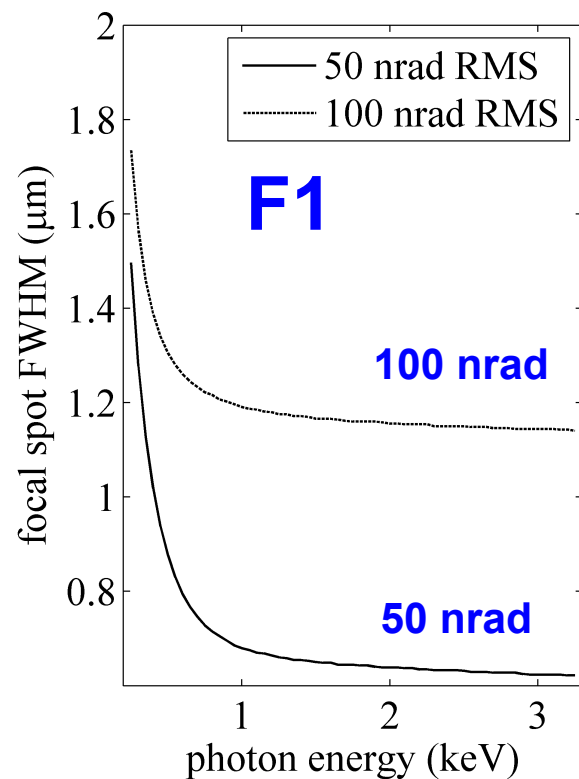
Bending range: VFM 600 – 1100 m
HFM 400 – 850 m

Perfect shape only for **ONE** position

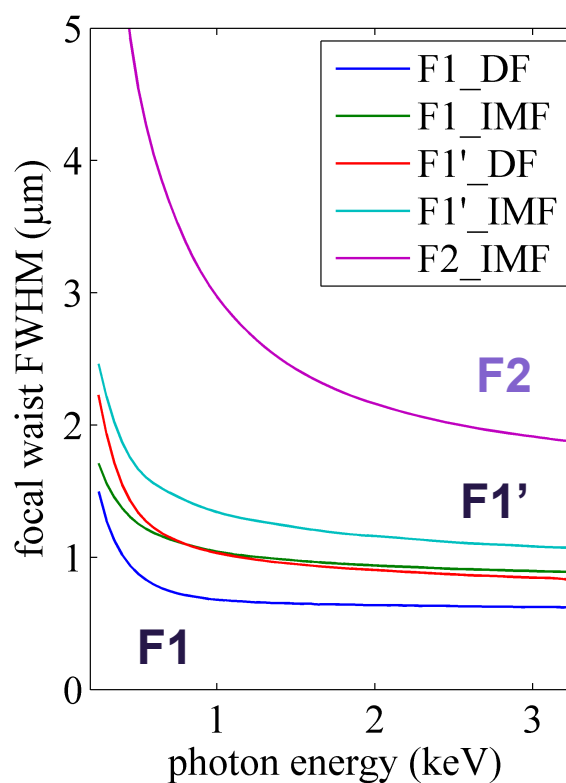
T. Mazza
WP85

Direct / Intermediate

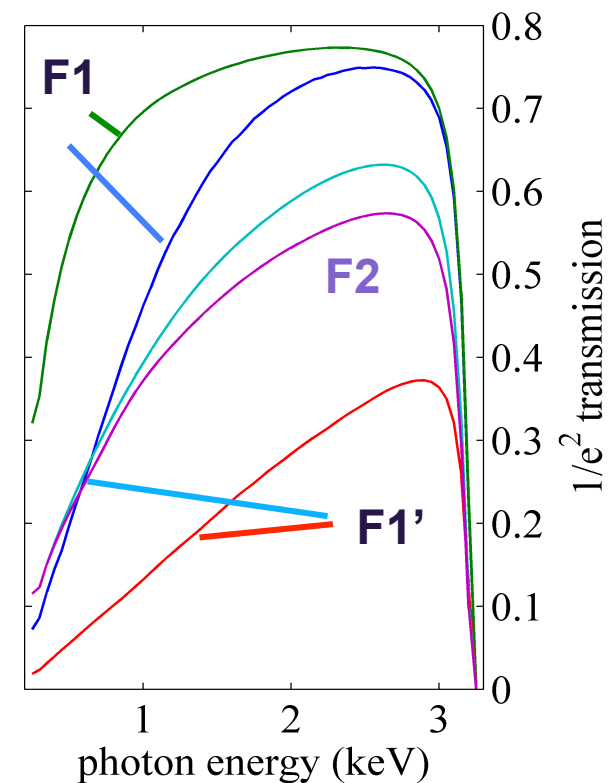
Focus size



Focus size

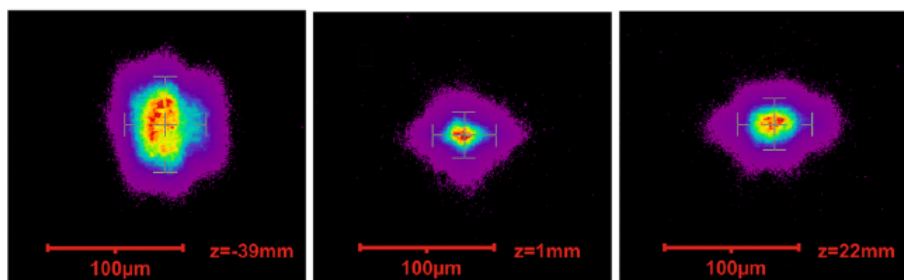


Transmission



■ Characterization of KB performances

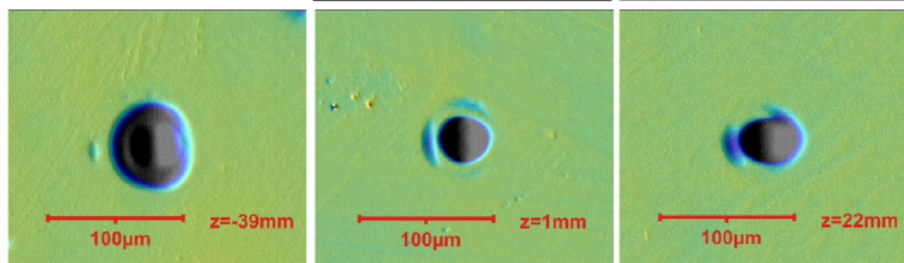
■ Hartmann-type wavefront sensor



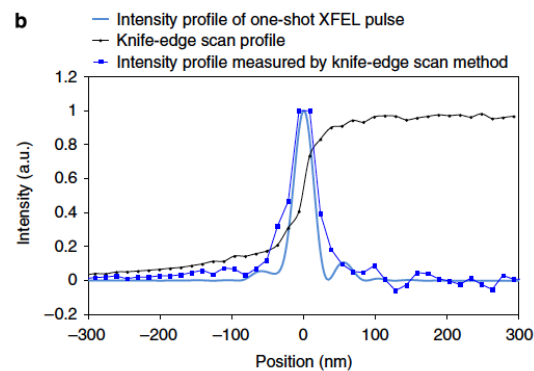
FLASH:

B. Flöter et al.,
NJP 12, 83015,
2010

■ PMMA Imprints

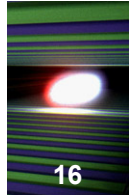


■ Knife edge scan



SACLA

H. Mimura et al.,
Nat.Comm. 5, 3539,
2014

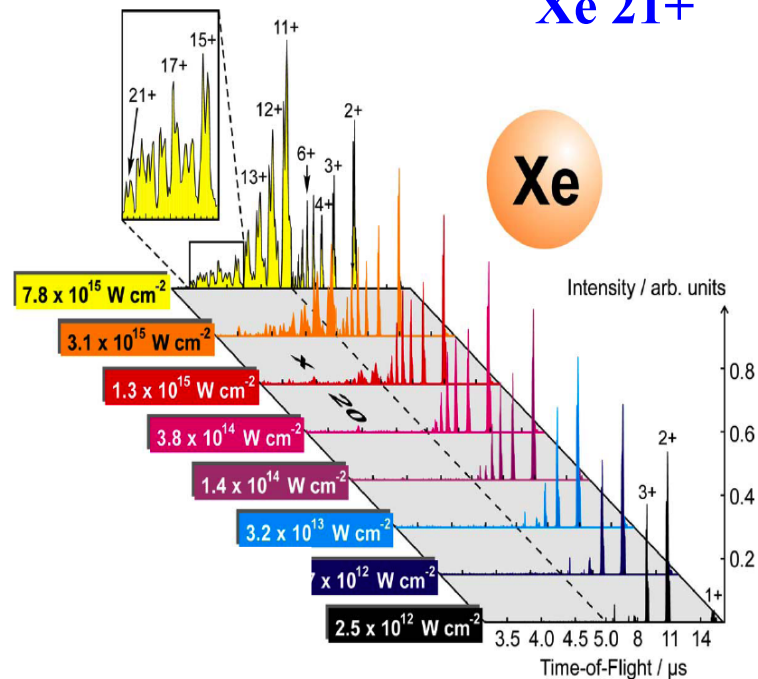


■ Reference for SQS performance cf. LCLS, FLASH

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

$h\nu = 93$ eV

Xe 21+



7.8×10^{15} W/cm²

6×10^{18} W/cm²

1×10^{17} W/cm²

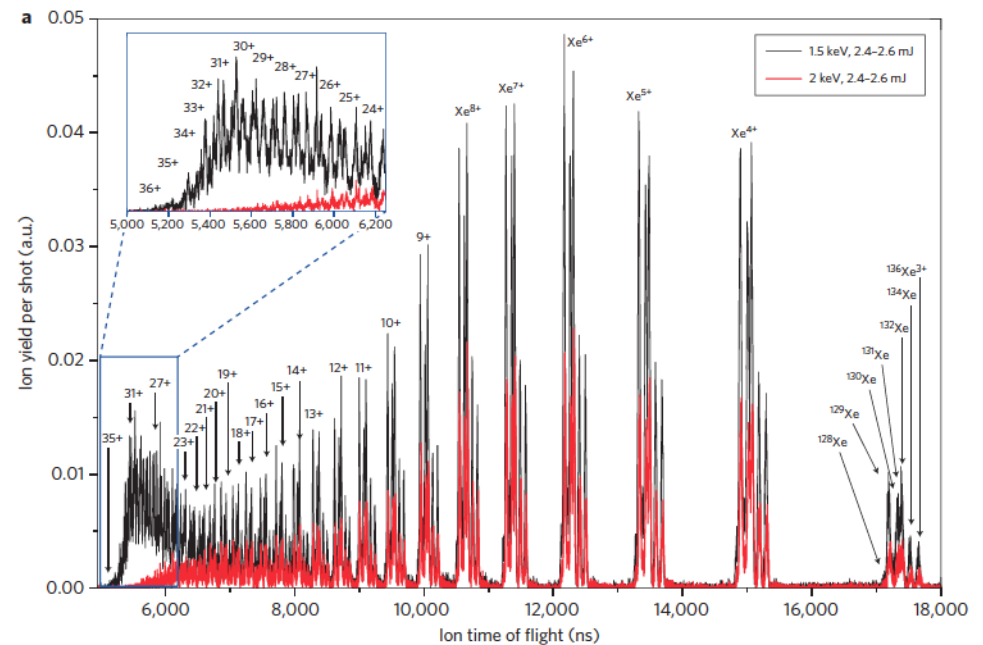
λ (LCLS) = 0.8 nm

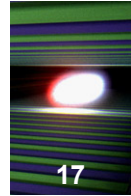
Rudek et al., Nat.Phot. 6,
858 (2012)

$h\nu = 1.5$ keV

$h\nu = 2.0$ keV

Xe 35+





■ Multiple ionization of atoms

“Day – one” parameter: SASE3

Rep. rate : 100 kHz

Photon energy: 1.0 – 1.5 keV

Pulse energy (P): up to 3 mJ

Pulse duration (T): 50 fs

Focus diameter: 1 micron

$$I(\text{SQS}) \leq 6 \times 10^{18} \text{ W/cm}^2$$

Rep. rate : **< 100 kHz**

1.0 – 1.5 keV

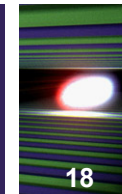
P > 3 mJ

T : 50 fs

Focus diameter: 1 micron

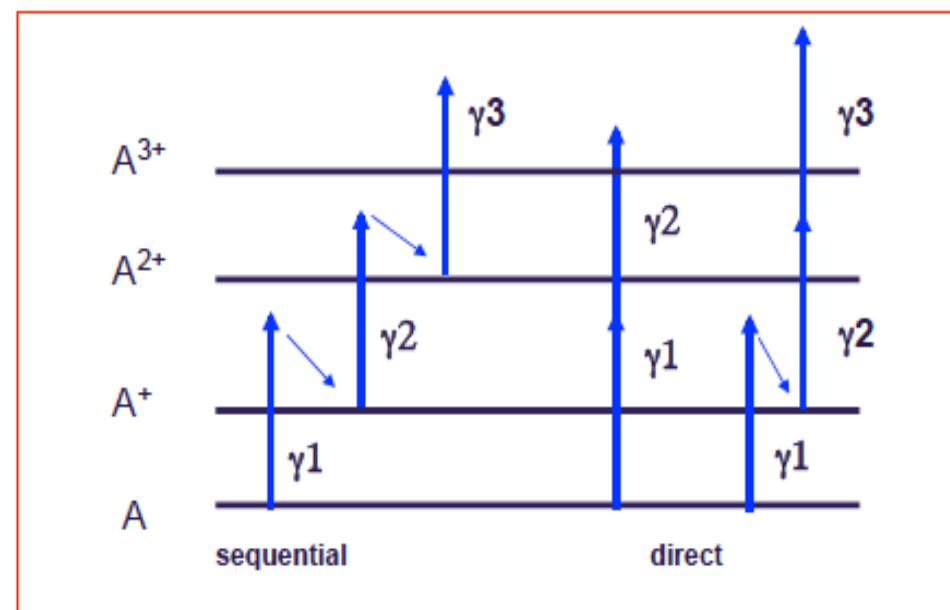
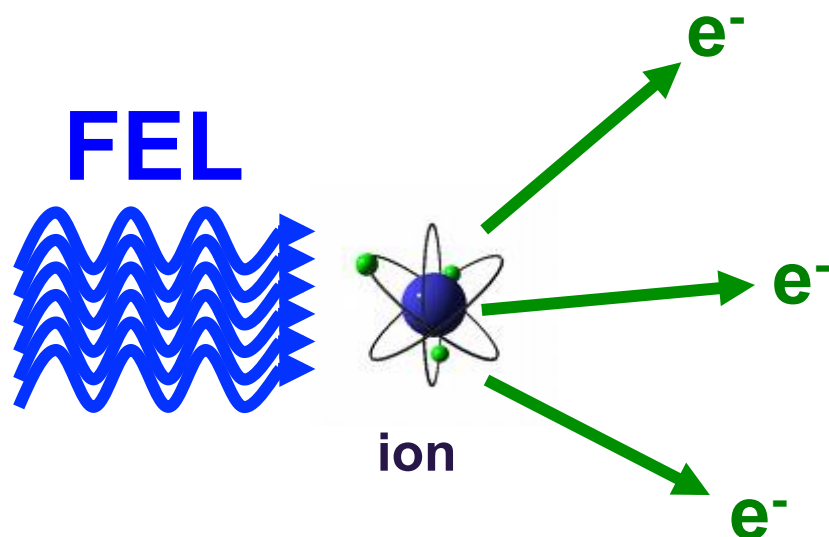
$$I(\text{SQS}) > 6 \times 10^{18} \text{ W/cm}^2$$



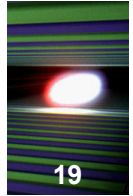


■ Electron – Ion Coincidences (atoms)

- Dynamical information -
- Determination of ionization pathways -



First „science“ experiments at SQS



- **Electron – Ion Coincidences** (atoms)
 - Dynamical information -
 - Determination of ionization pathways -

Requirements:

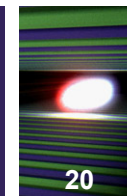
Unambiguous correlation between electron and ion

→ 1 photon-atom interaction per pulse

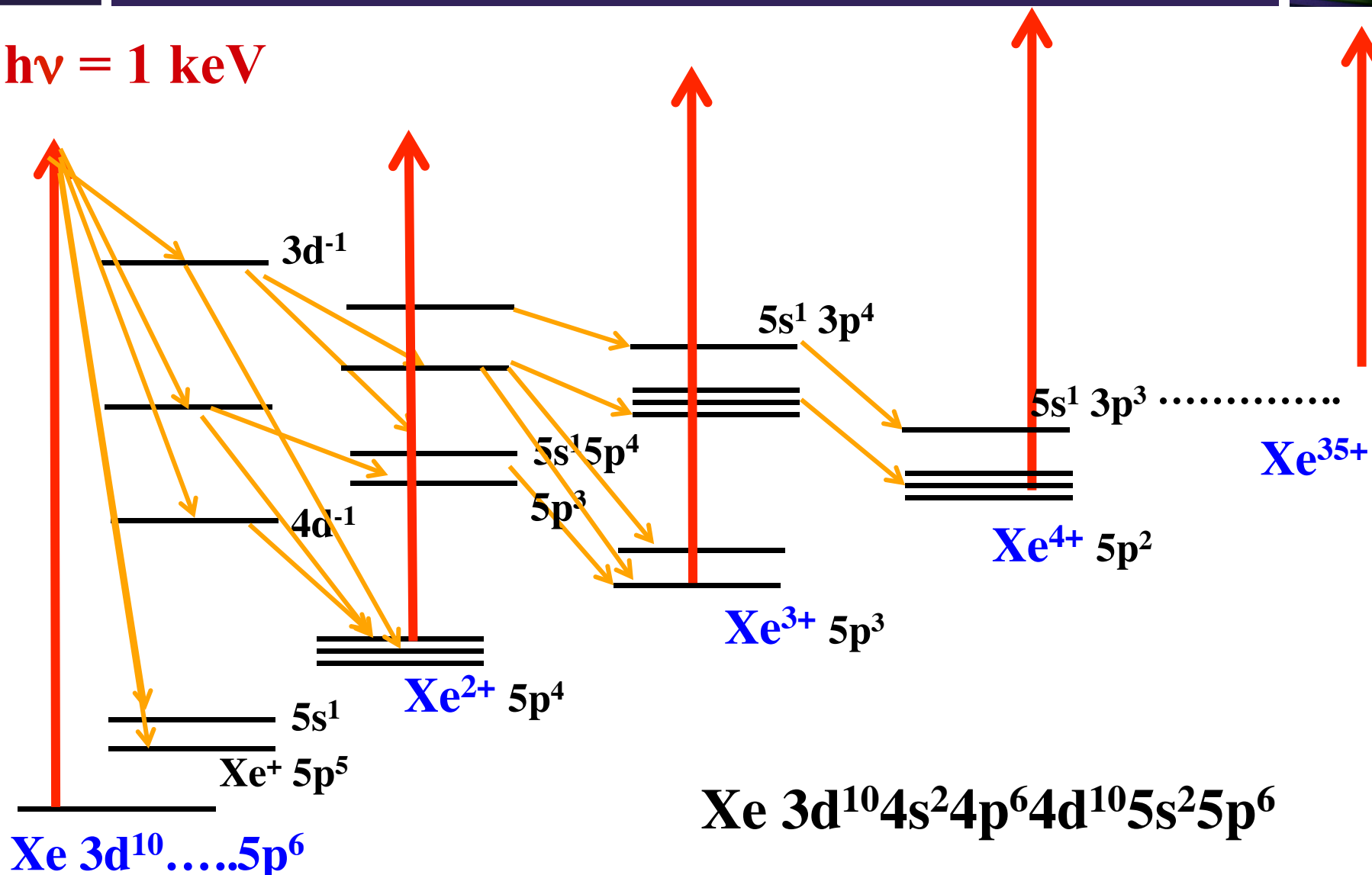
Electron spectra: Time-of-flight $E(\text{kin}) > 13 \text{ eV} \rightarrow < 220 \text{ ns}$

Ion spectra: Time-of-flight $\text{Xe (m/q)} < 136 \rightarrow < 10 \mu\text{s}$

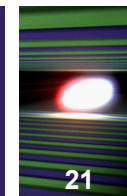
SQS: Coincidence method



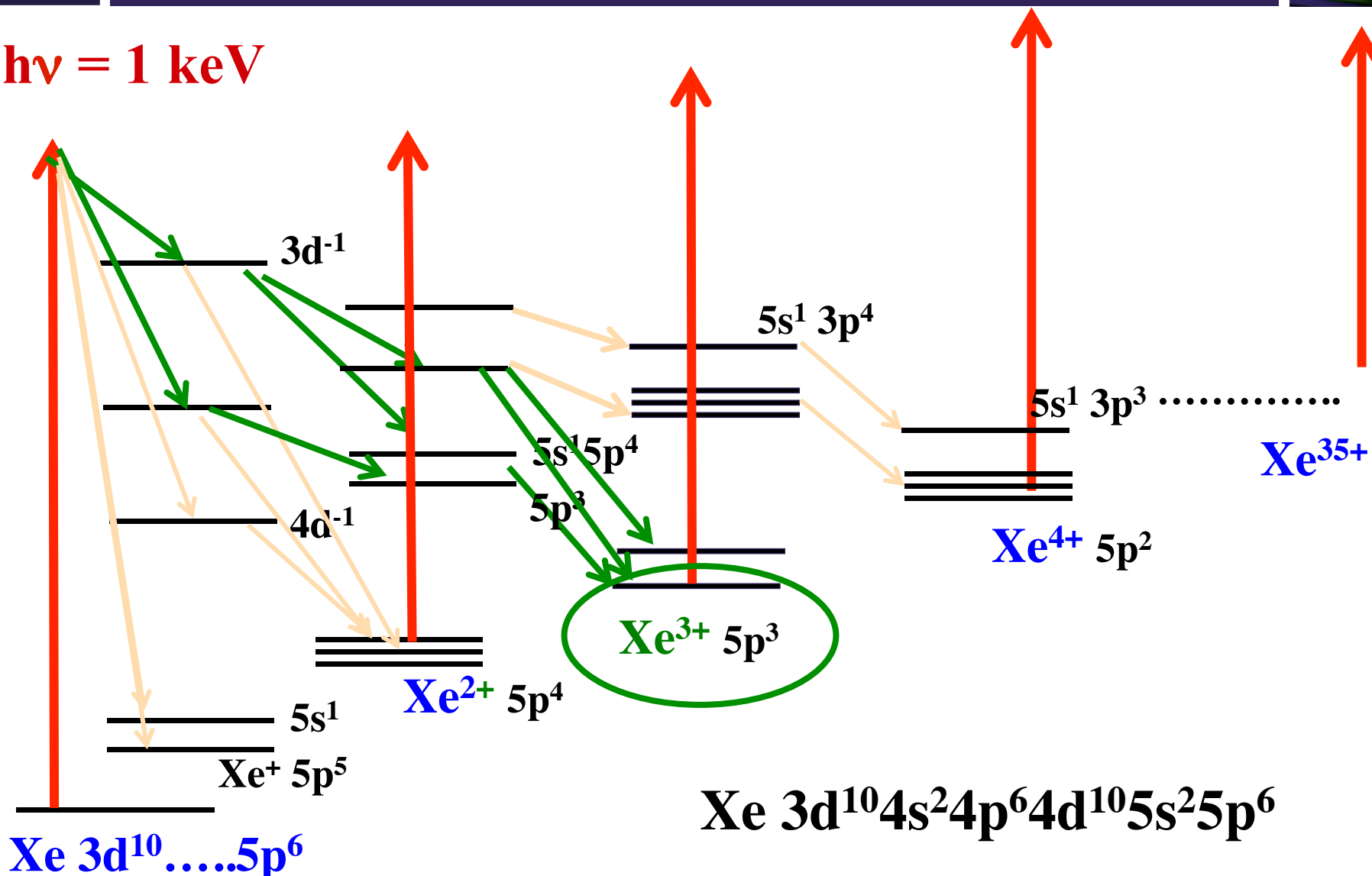
$h\nu = 1 \text{ keV}$



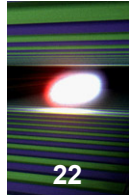
SQS: Coincidence method



$h\nu = 1 \text{ keV}$

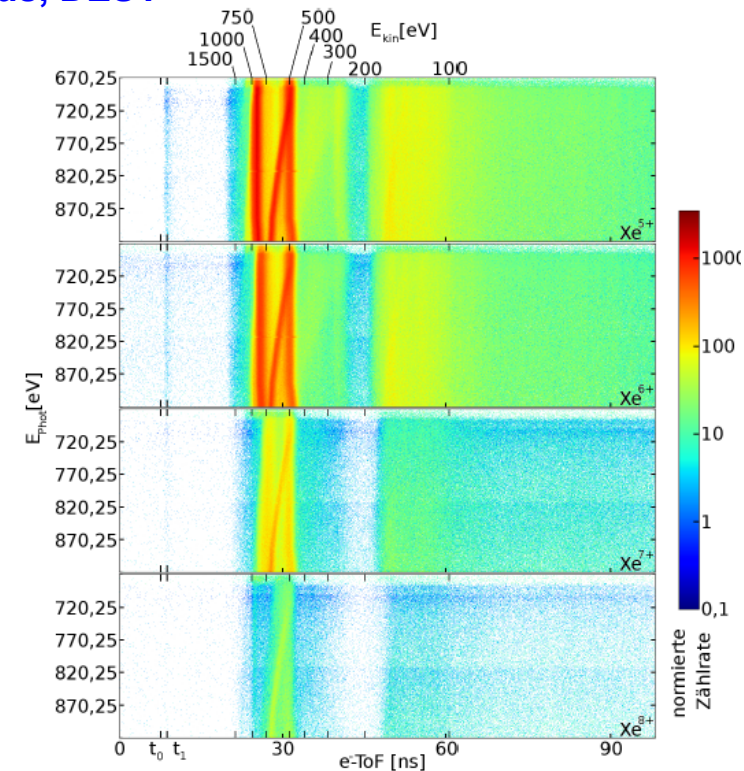
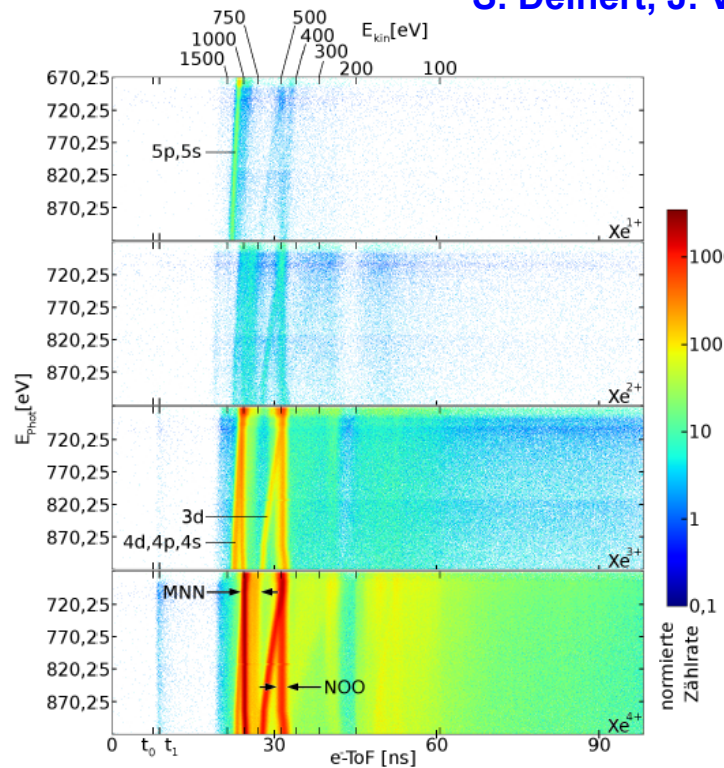


Coincidences : Xe (PETRA III)



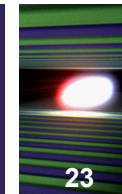
Synchrotron (MHz) – linear one-photon processes ($< \text{Xe}^{8+}$)

S. Deinert, J. Viefhaus, DESY



→ European XFEL – new regime / new dynamics

“non-linear multi-photon ionization”



“ions”

AQS: Atomic-like Quantum Systems

Targets: atoms & small molecules

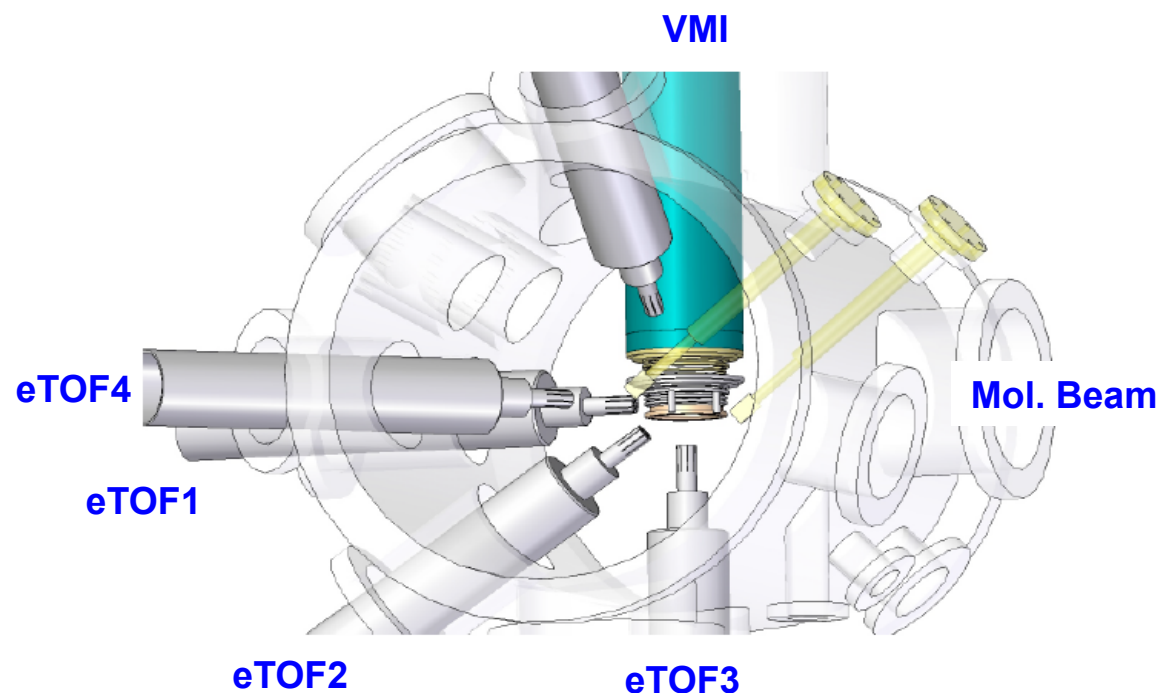
Molecular beam

Vacuum: 10^{-11} mbar

Focus: $\leq 1 \mu\text{m} \rightarrow 50 \mu\text{m}$

electrons, ions, photons

- HR electron spectroscopy
- Angle-resolved spectroscopy
 - Non-dipole studies
- HR fluorescence spectroscopy
 - e / e – coincidences
 - e / ion - coincidences



“electrons”

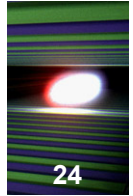
Dipole plane

eTOF1 = 0°

eTOF2 = 54.7°

eTOF3 = 90°

First „science“ experiments at SQS



■ Electron – Ion Coincidences (atoms)

- Dynamical information -
- Ionization pathways -

“Day – one” parameter: SASE3

Rep. rate : 100 kHz

Photon energy: 1.0 – 1.5 keV

Pulse energy (P): up to 3 mJ

Pulse duration (T): 50 fs

Focus diameter: 1 micron

Rep. rate : **> 100 kHz**

1.0 – 1.5 keV

P > 3 mJ

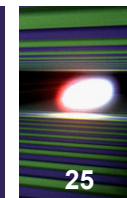
T : 50 fs

Focus diameter: 1 micron

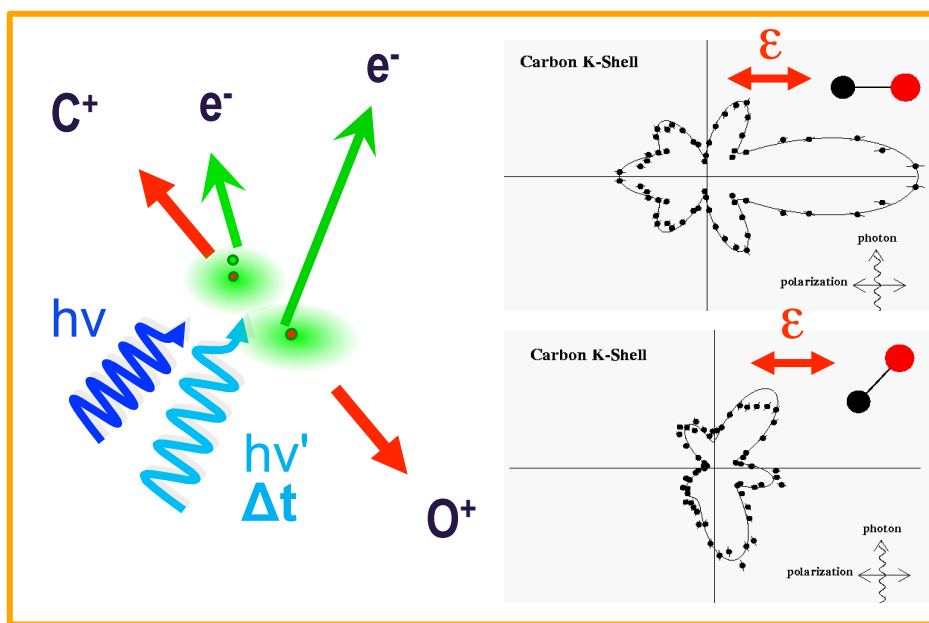


$$I(\text{SQS}) \leq 6 \times 10^{18} \text{ W/cm}^2$$

Second „science“ experiments at SQS



- **Electron – Ion Coincidences (molecules)**
 - **Dissociation Channel** -
 - **Temporal evolution of bond breaking** -



Landers & Dörner PRL **87** (2001), 013002

electron – ion – ion **coincidences**

1 pulse = 1 event !!

Dissociation dynamics (ALS)
“linear”

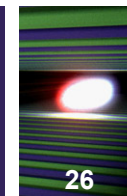
European FEL

→ “non-linear”

→ **Pump-Probe**
fs – dynamics

Temporal evolution
Molecular alignment
Intense fields

Second „science“ experiments at SQS



■ Electron – Ion Coincidences (molecules)

- Dissociation Channel -
- Temporal evolution of bond breaking -

“Small“ molecules: N_2 , O_2 , CO , CO_2 , N_2O , CH_4 , C_{60} ,

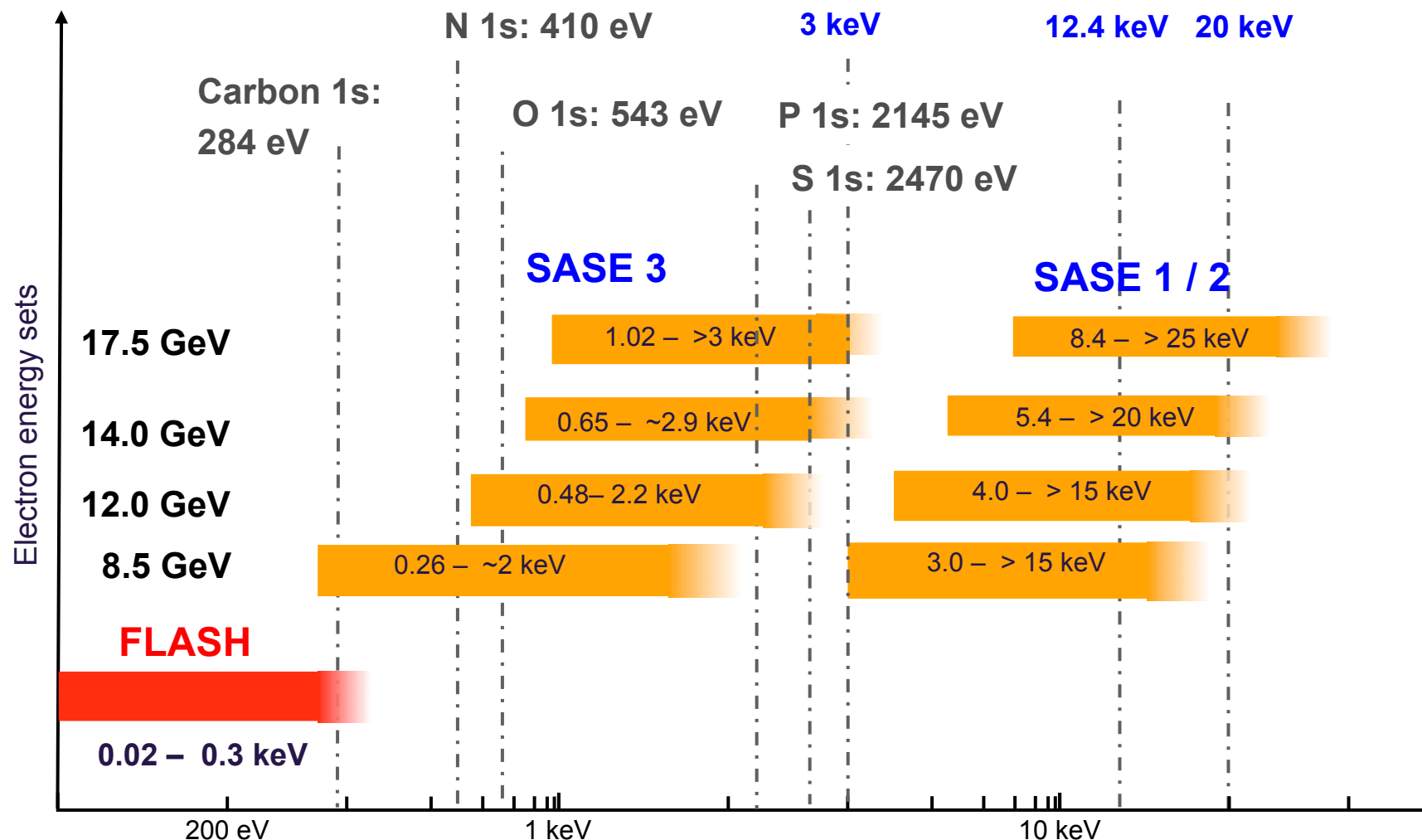
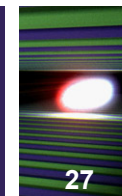
Electron spectra: Time-of-flight $E(\text{kin}) > 13 \text{ eV} \rightarrow < 220 \text{ ns}$

Ion spectra: Time-of-flight $m/q (\text{CO}_2) < 44 \rightarrow < 10 \mu\text{s}$

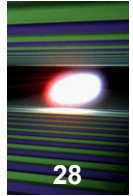
Site specific excitation of localized core (1s) electrons

C-1s: 290 eV, N-1s: 410 eV, O-1s: 560 eV

Photon energy ranges



Second „science“ experiments at SQS



■ Electron – Ion Coincidences (molecules)

- Dynamical information -
- Fragmentation pathways -

“Day – one” parameter: SASE3

Rep. rate : 100 kHz

Photon energy: 1.0 – 1.5 keV

Pulse energy (P): up to 3 mJ

Pulse duration (T): 50 fs

Focus diameter: 1 micron

Electron beam energy: 8.5 GeV



Rep. rate : **> 100 kHz**

0.25 – 1.5 keV

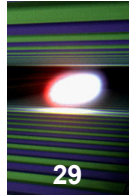
P < 3 mJ

T < 50 fs

Focus diameter: 1 micron

Early stage of operation:

surface contamination !!



- **Commissioning experiments**

- **SQS Reference for non-linear processes**

e.g. Xe multiple ionization

“intensity”

- **First “Science” application**

- 1) **Non-linear Processes**

- **SQS coincidence performances**

“repetition rate”

e.g. first state-resolved ion spectra of Xe multiple ionization

- 2) **Molecular Fragmentation**

- **SQS XUV & coincidence performances**

“soft X-rays”

e.g. first “site-selective” molecular dynamics

European XFEL

