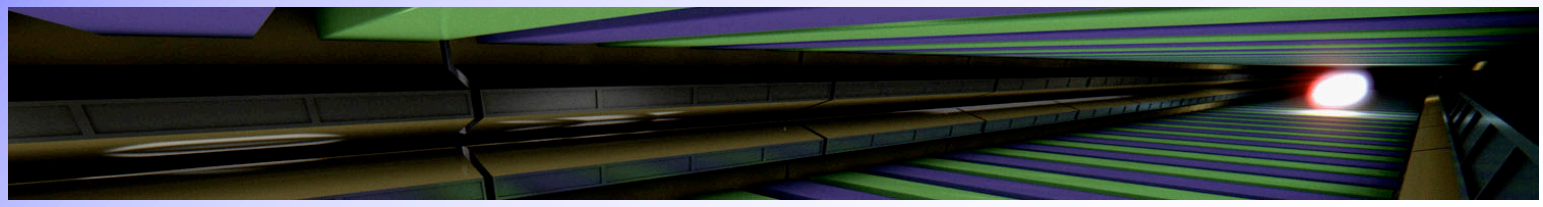
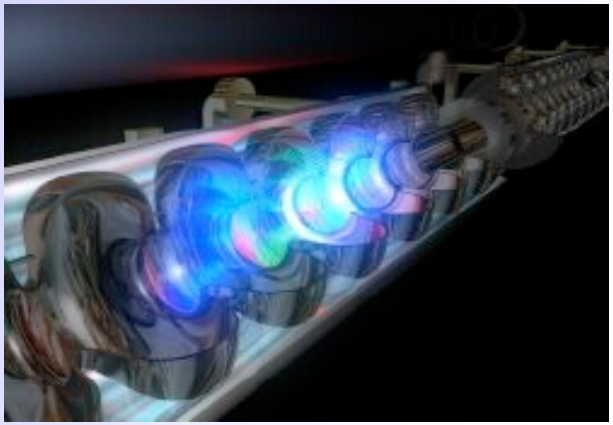


Conceptual Design Report
SQS - Scientific Instrument @ European XFEL

M. Meyer, European XFEL GmbH

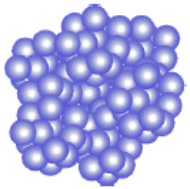
Free Electron Lasers



N x hν

2 - 100fs

"Small Quantum Systems"



Conceptual Design Report
SQS - Scientific Instrument @ European XFEL

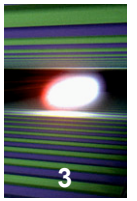
- **Soft X-rays at the European XFEL**
- **Scientific Case for SQS**
- **Instrument Layout**

  beam line, SQS end station, floor plan
- **Infra-structure / Add-ons**

  optical laser, diagnostics, add-on equipment, time line

European XFEL

Definition of the SQS Instrument



Workshops

1) International Workshop on the Science with and the Instrumentation for Small Quantum Systems (SQS) at the European XFEL
University of Aarhus, Denmark, **October 29-31, 2008**

2) International Workshop on Soft X-ray science and instrumentation at the European XFEL
Trieste, Italy, **December 16 - 17, 2010**

Reviews

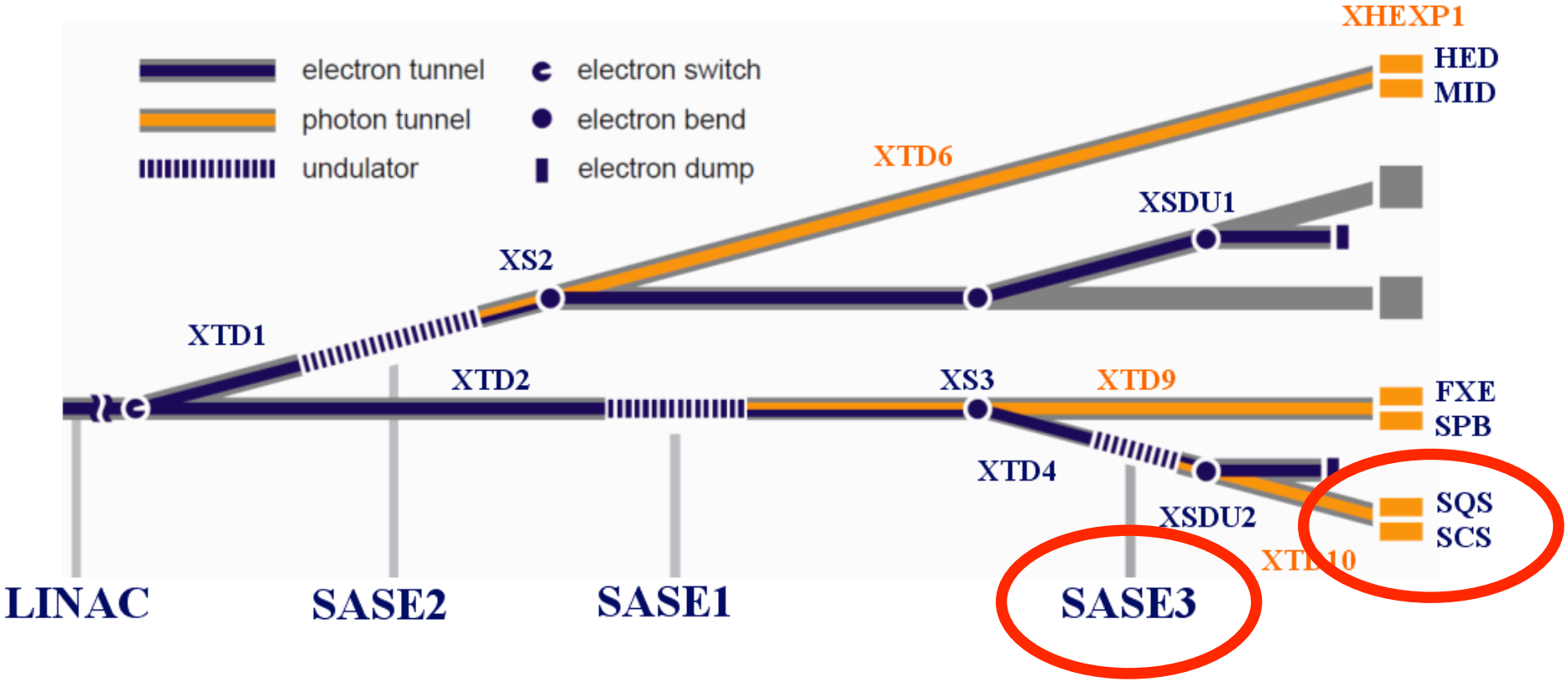
1) Review Meeting of the Advisory and Review Team (SQS-ART)
J.Bozek (SLAC), Th. Möller (TU Berlin), J. Nordgren (U. Uppsala), H. Pedersen (U. Aarhus)
J. Ullrich/A. Rudenko (MPI/CFEL), J. Viefhaus (DESY), M. Vrakking (MBI)
April 6th, 2011

2) Meeting of the Scientific Advisory Committee (SAC) of the European XFEL
April 8th, 2011

European XFEL

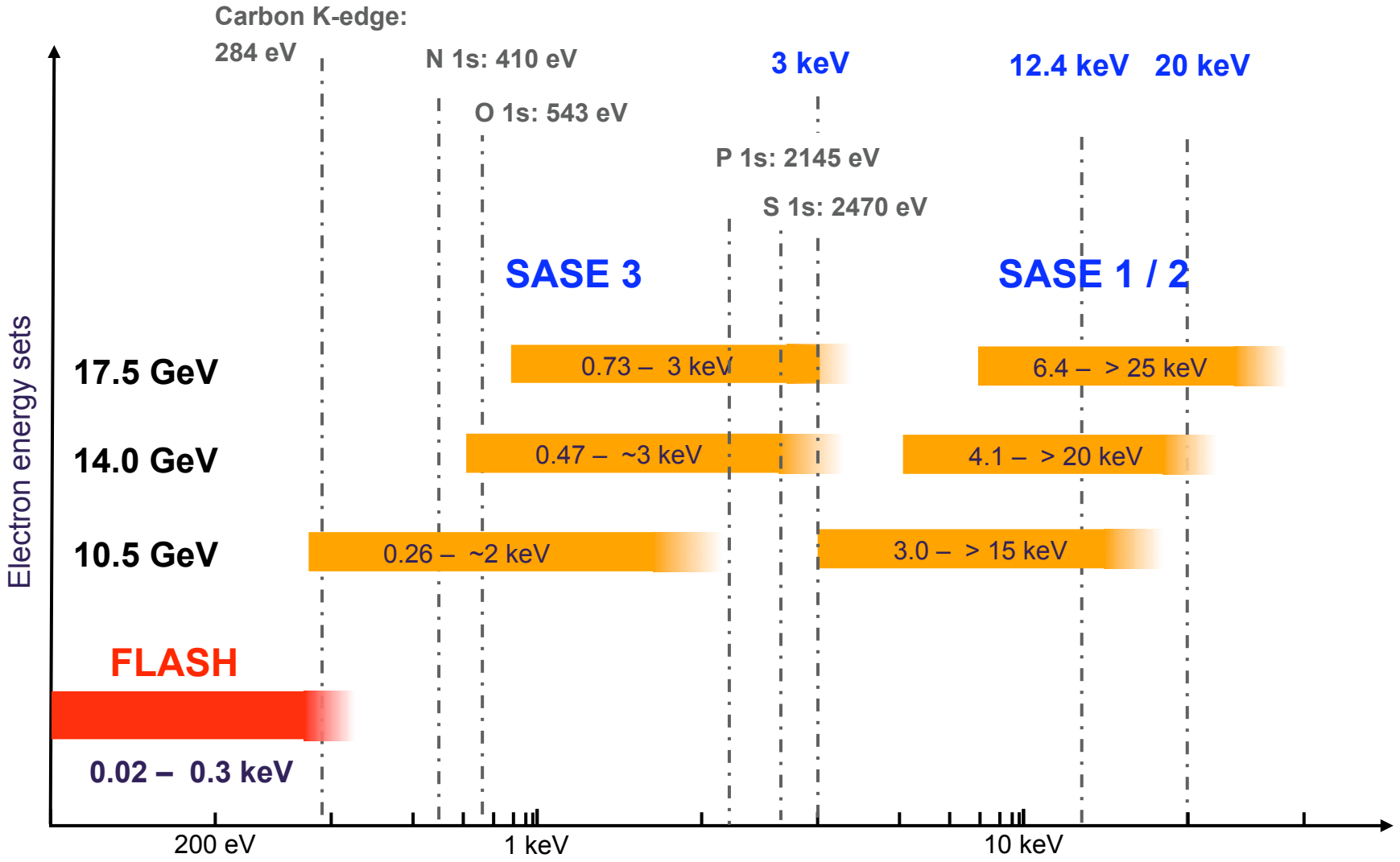
Photon beam transport systems

European XFEL



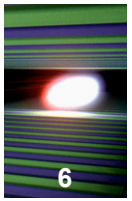
European XFEL

Photon energy ranges



European XFEL

SASE 3 Undulator



General Soft X-Ray radiation parameters

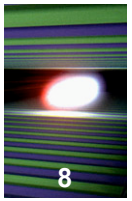
Pulse widths	**2 – 100 fs**	**Coherence time**	0.3 – 1.8 fs
Pulse energy	**0.2 – 11.0 mJ**	**Bandwidth**	0.25 – 0.7 %
Peak power	50 – 120 GW	**Number of photons**	**0.1 – 2 x 10^{14}**
Average power	3 – 300 W	**Average flux of photons**	0.3 – 5.4 x 10^{18}
Beam size	40 – 80 μm	**Average brilliance**	0.03 – 2.6 x 10^{24}
Rep. rate	**10 Hz (2700 pulses in bunch train)**		

Parameter	Unit					
Bunch charge	pC	20	100	250	500	1000
Pulse duration (FWHM)	fs	2	9	23	43	107

Scientific case for SQS Scientific Instrument

European XFEL

Scientific Applications



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

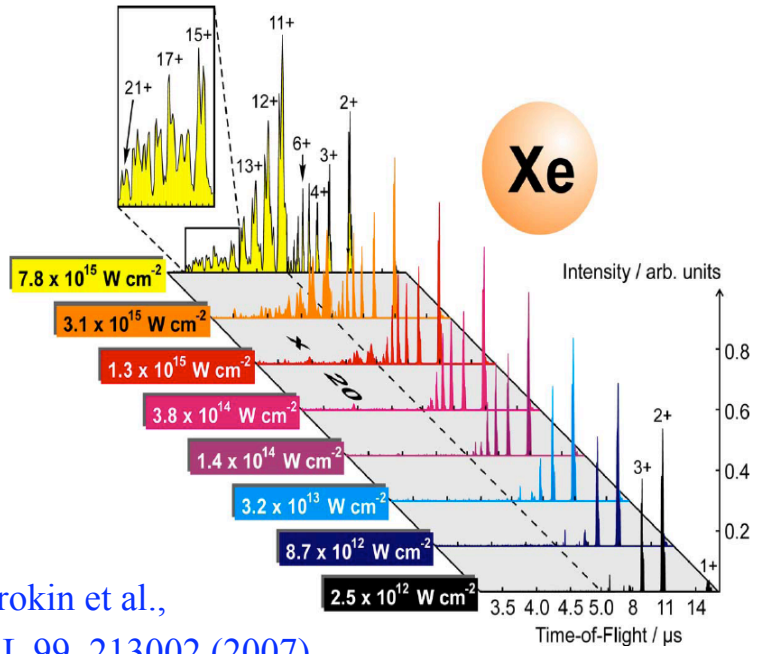
High intensities: $>10^{15}$ W/cm^2	⇨	**Non-linear phenomena** **Multi-photon processes**
Short pulses: 2 - 100 fs	⇨	**Ultra-fast dynamics** **Pump-probe experiments**
High flux $> 10^{12}$ photons / pulse $> 10^{15}$ photons / sec	⇨	**Extremely dilute targets** **Processes with small cross section**
Spatial coherence	⇨	**Coherent Diffraction Imaging**

European XFEL

High repetition rate: < 27000 pulses/ sec	➡	**High data collection rate** **Multi-particle coincidences**

Multi-photon Multiple Ionization

Intense Radiation ⟷ Matter



Sorokin et al.,
PRL 99, 213002 (2007)

FLASH : 93 eV (7.8 x 10^{15} W/cm^2)

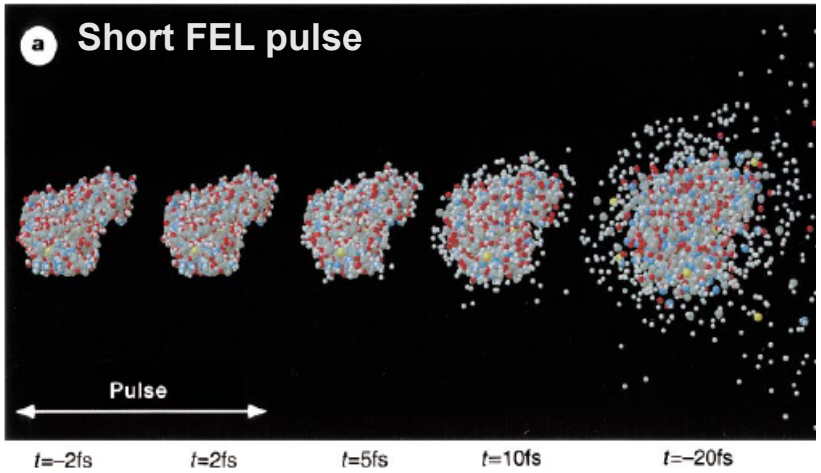
IP(Xe 21+) ≈ 5 keV

Young et al., Nature 466, 56 (2010)

LCLS : 800 - 2000 eV (<1 x 10^{18} W/cm^2)

Ne(+) → Ne (10+)

Coulomb explosion of large molecules



R. Neutze et al., *Nature*, 2000, **406**, 752

- **Intensity dependence**
- **Time evolution**
- **Wavelength dependence**

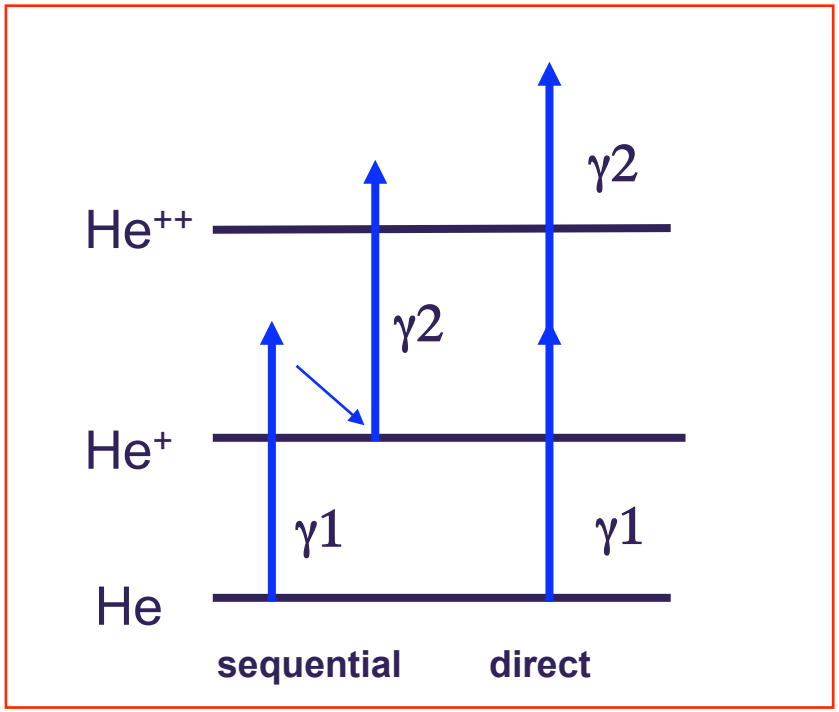
?

European XFEL

Fundamental Processes

Intense Radiation ⟷ Matter

Prototype Studies

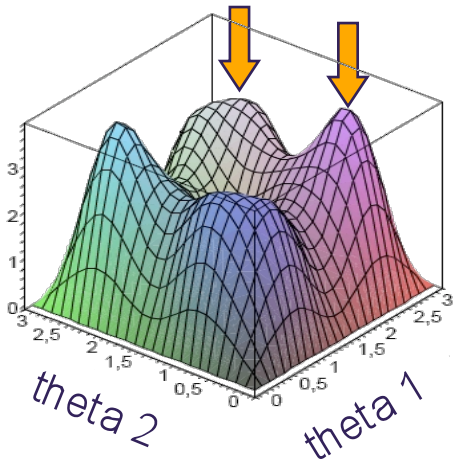


Reaction microscope : full solid angle

but

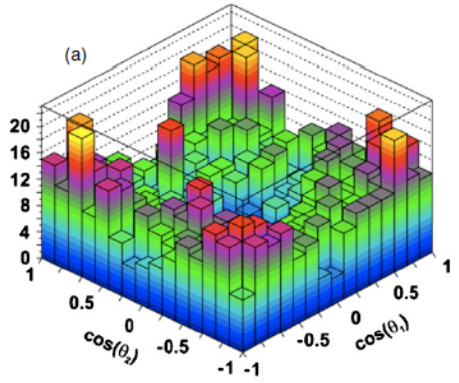
60 Hz ➡ **very limited statistics**

Angular correlation between 2 electrons



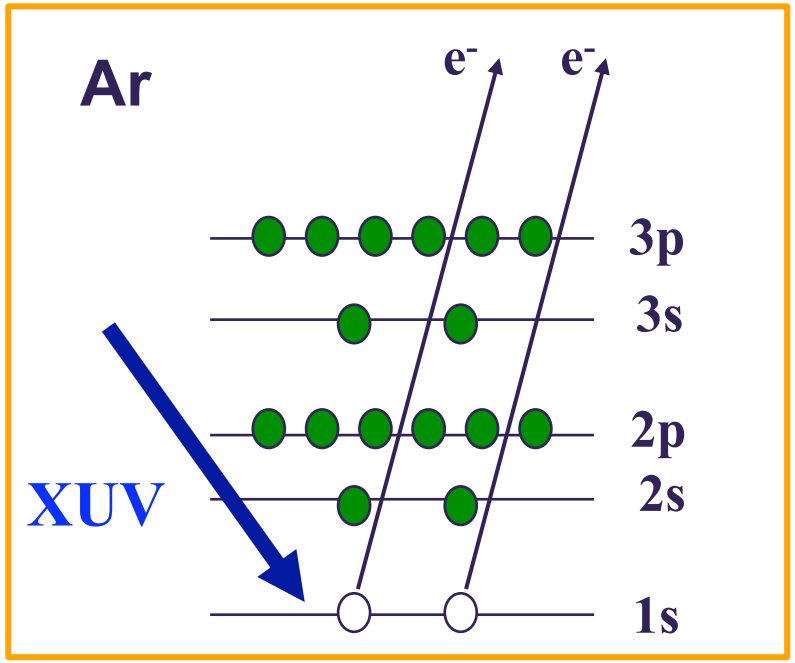
Theory:
Fritzsche et al.
J.Phys.B 41,
165601 (2008)

Experiment:
(FLASH 2008)
Kurka et al.,
J.Phys.B42,
141002 (2009)



Fundamental Processes

Innershell Processes



Double core hole formation

Complex Relaxation Dynamics

- New phenomena -

Electron Spectroscopy

- Detailed information about energy redistribution

Coincidence Spectroscopy

- Dynamical information for correlated electron emission

high rep. rate (27 000 pulses/s)

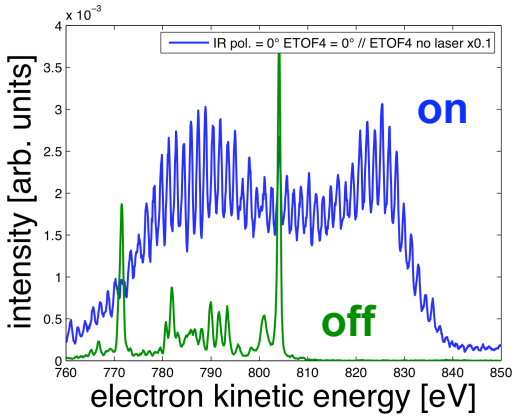
Fluorescence Spectroscopy

- High resolution data unperturbed by space charges

European XFEL

Ultrafast Dynamics (Pump – Probe)

Atomic photoionization in strong 'overlapping' optical fields

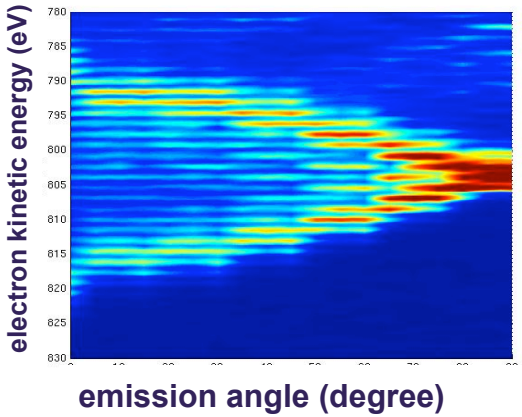


HR - AES

LCLS: 1 keV, 2-5 fs

τ (Ne 1s) = 2.4fs

T (800nm) = 2.6fs

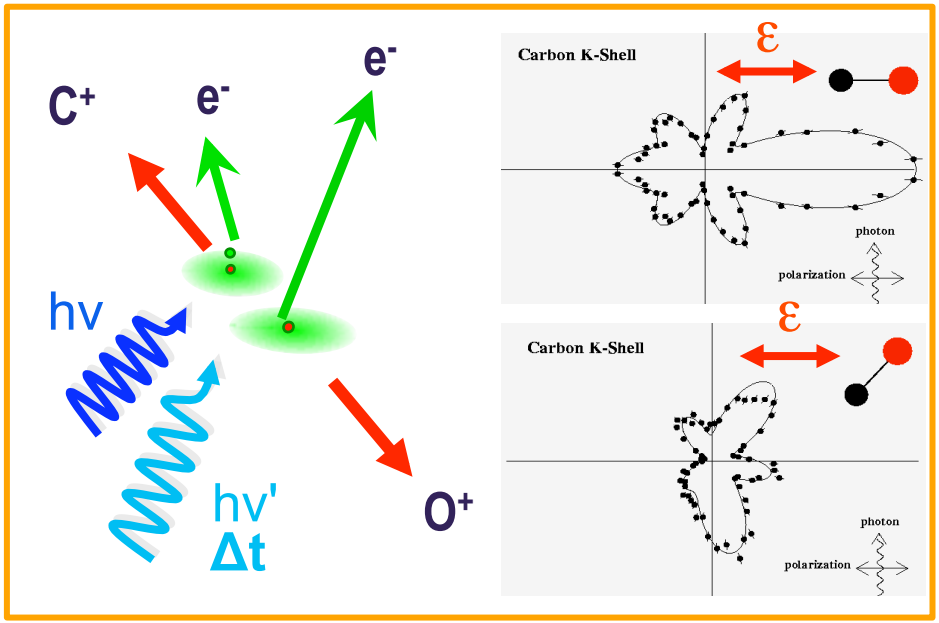


Angular distribution

Meyer et al., PRL108 (2012)

Kazansky, Kabachnik, JPB43, 035601 (2010)

Molecular dissociation dynamics



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

electron – ion – ion **coincidences**

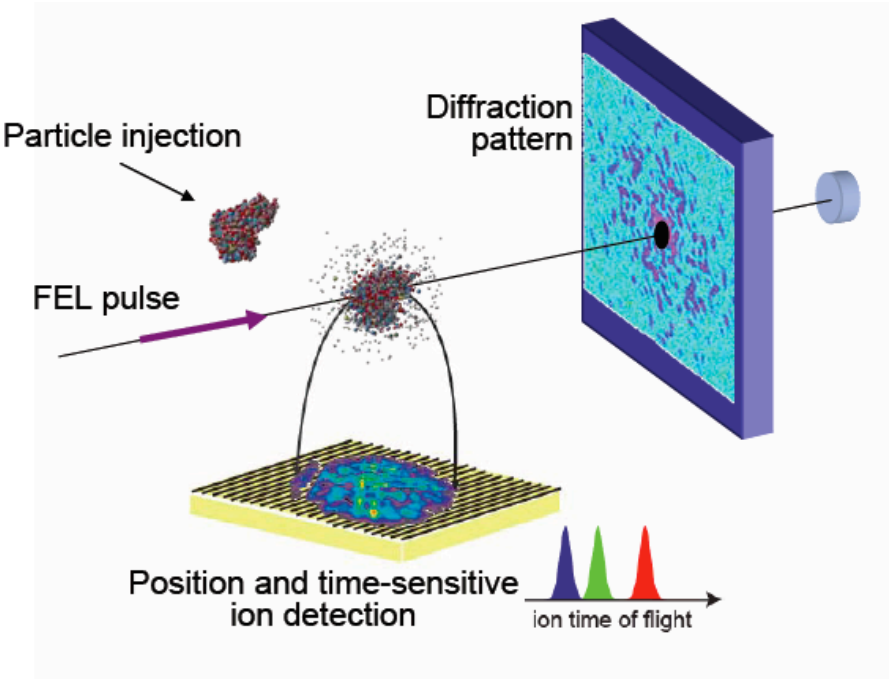
1 pulse = 1 event !!

FEL (fs) → Dynamical information!!!

European XFEL

Ultra-fast processes

Complex molecules



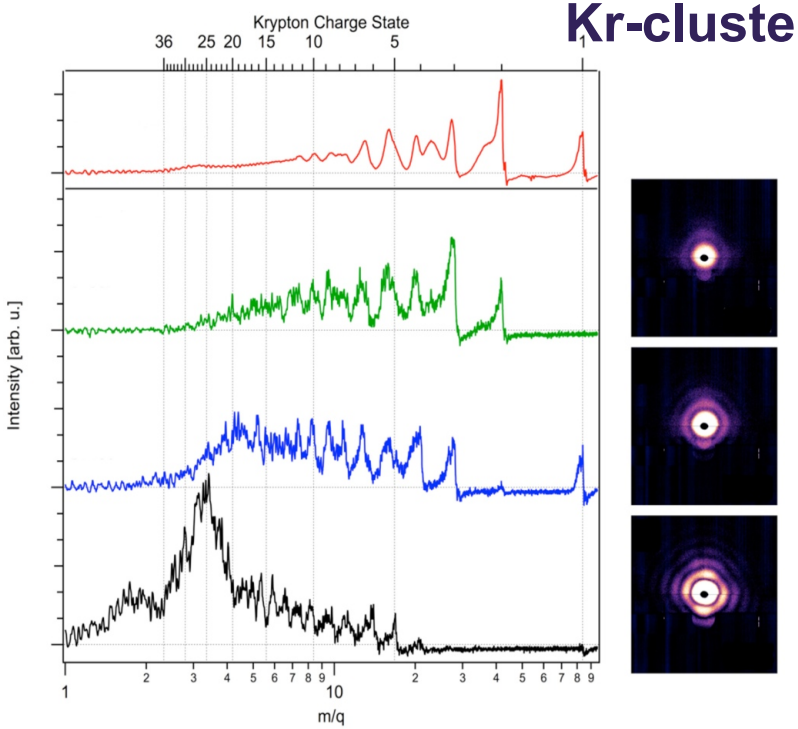
Ullrich et al., ASG MPI Heidelberg

photon – ion – ion **coincidences**

27 000 pulses / sec

Size dependence of multiple ionization in clusters

Kr-cluster



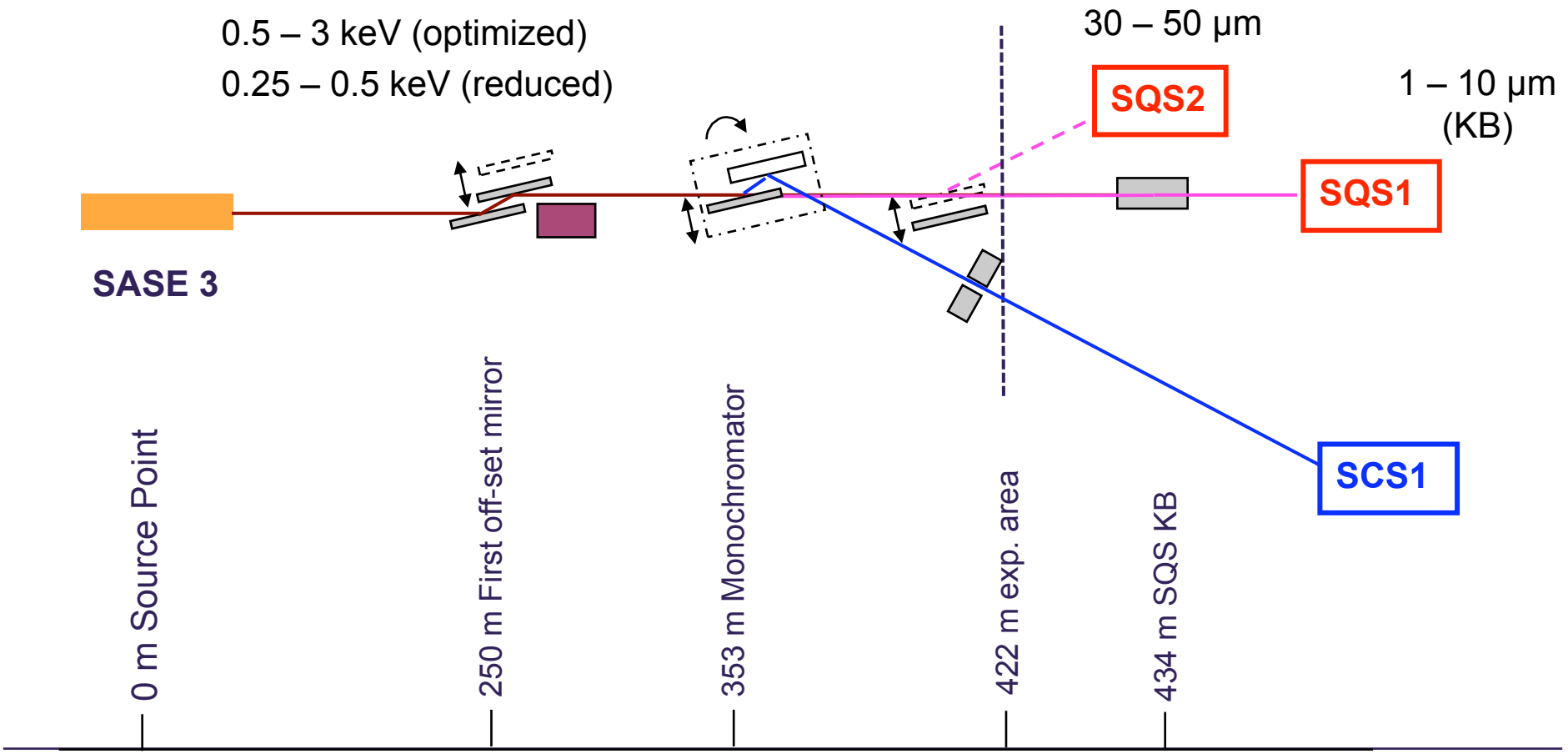
LCLS: 1.5 keV, 3 mJ

Principal investigator:
Christoph Bostedt
(LCLS)

General Layout of SQS Scientific Instrument

Optical layout of the beam transport system (H. Sinn)

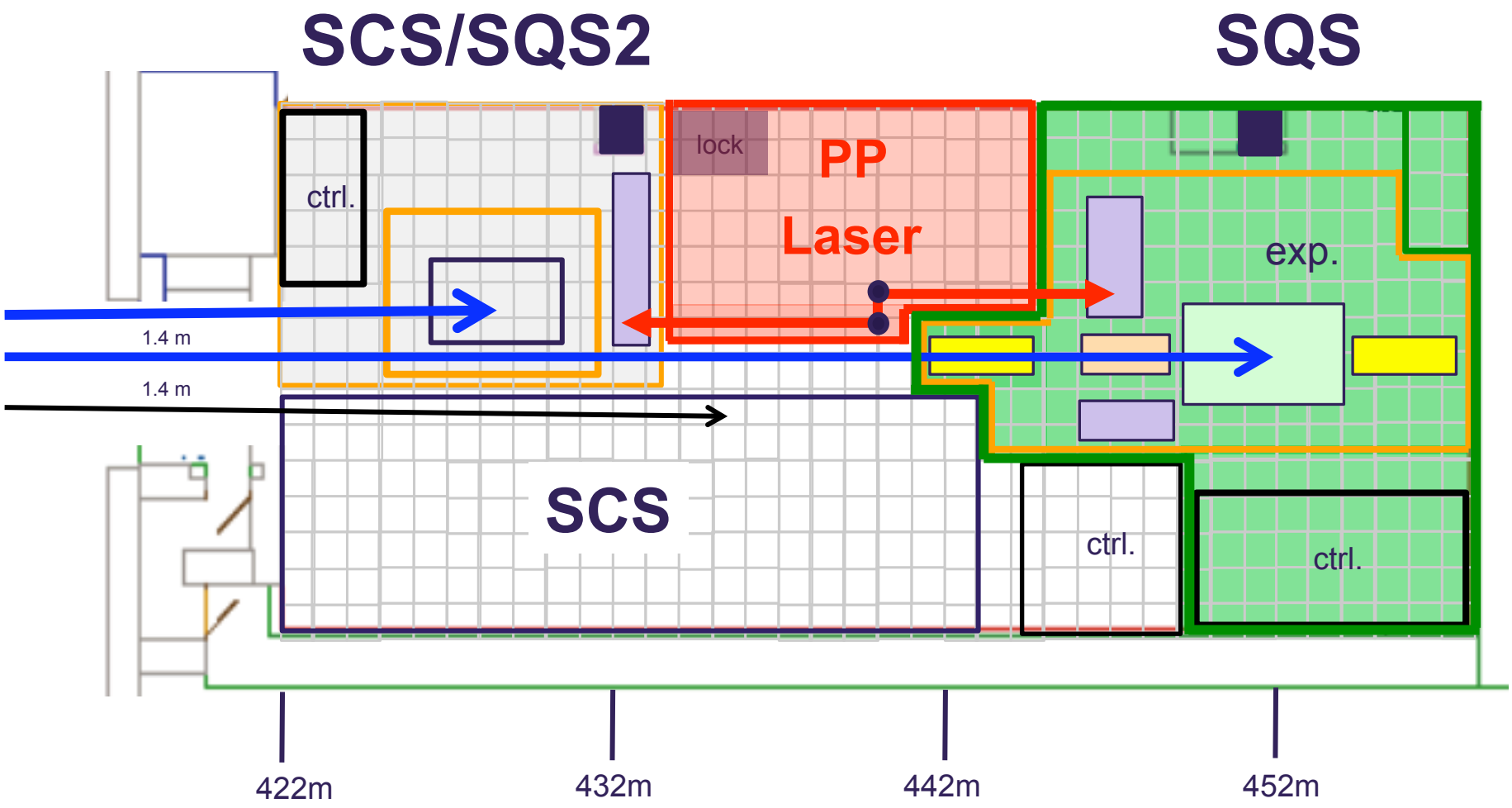
- direct beam → Small Quantum System (SQS)
- monochromatized → Spectroscopy @ Coherent Scattering (SCS)



European XFEL

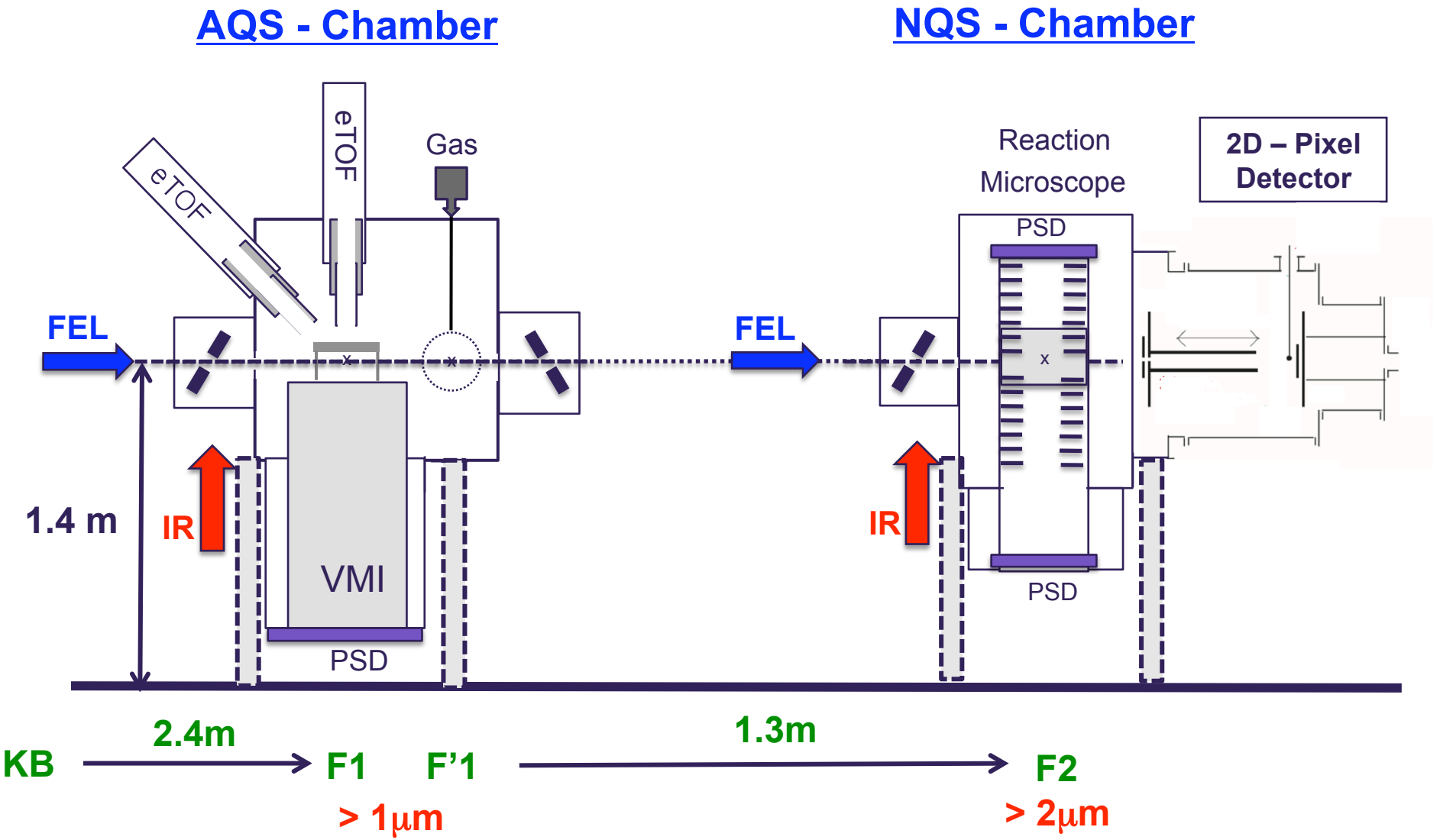
Floor plan (SASE3)

15 x 36 = 540 m²



European XFEL

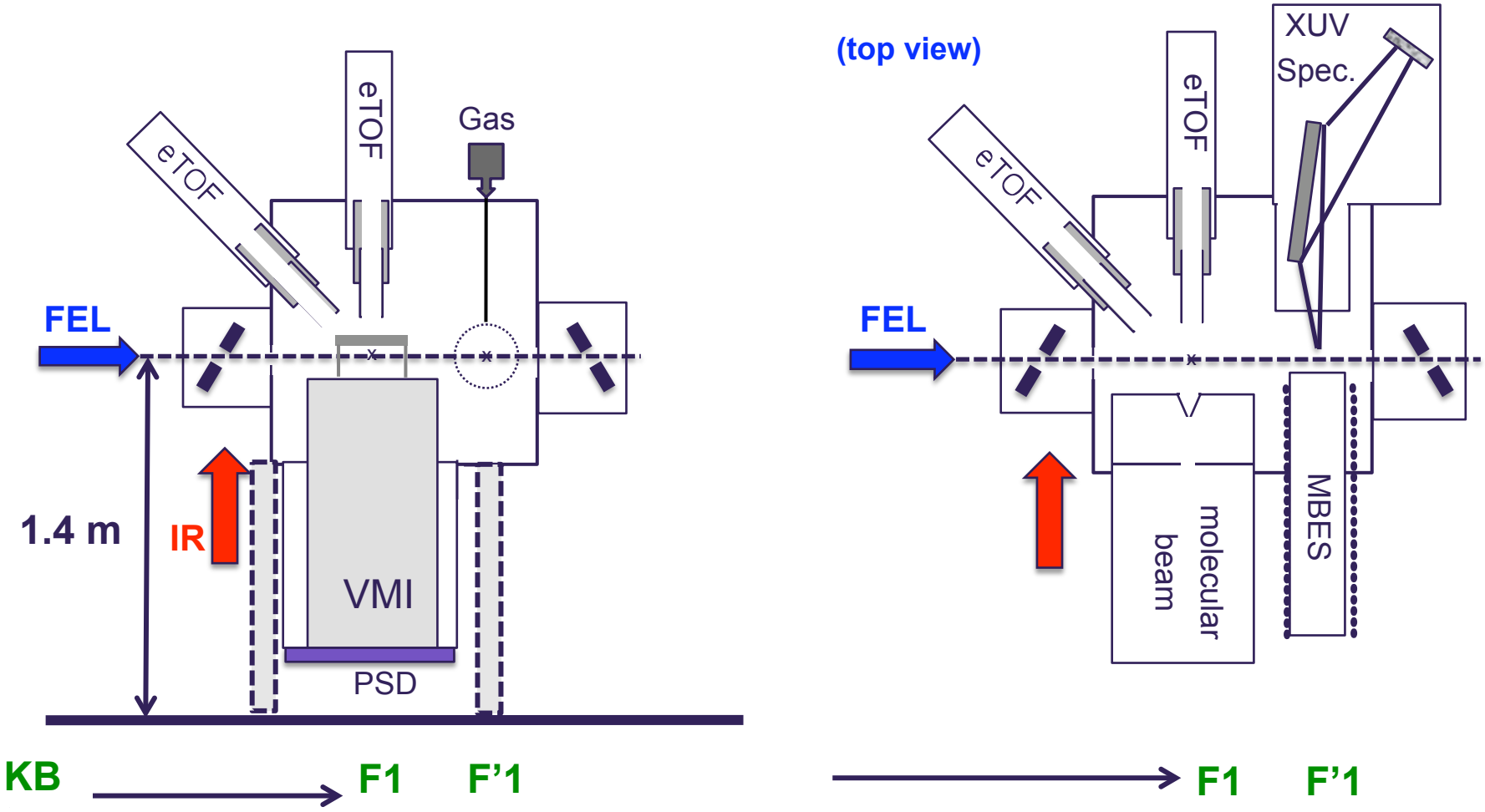
SQS end-station



European XFEL

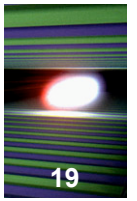
SQS end-station

AQS – Atomic-like Quantum Systems



European XFEL

Analyzers and Detectors



AQS - Chamber

1. **HR-electron Time-of-Flight (eTOF)**
   - angle-resolved spectroscopy
   - **1D – MCP - detector**

     $E / \Delta E > 10^4$
     acceptance 5% of 4π
     e – e – coincidences (5 eTOFs)

2. **Magnetic Bottle Electron Spectrometer**
   - single shot capability
   - **1D – MCP - detector**

     $E / \Delta E > 10^2$
     acceptance < 2π
     e – ion – coincidences

3. **Velocity-Map-Imaging (VMI)**
   - full angular information
   - **2D – delay-line - detector**

     $E / \Delta E > 10^2$
     acceptance 4π
     e – ion - coincidences

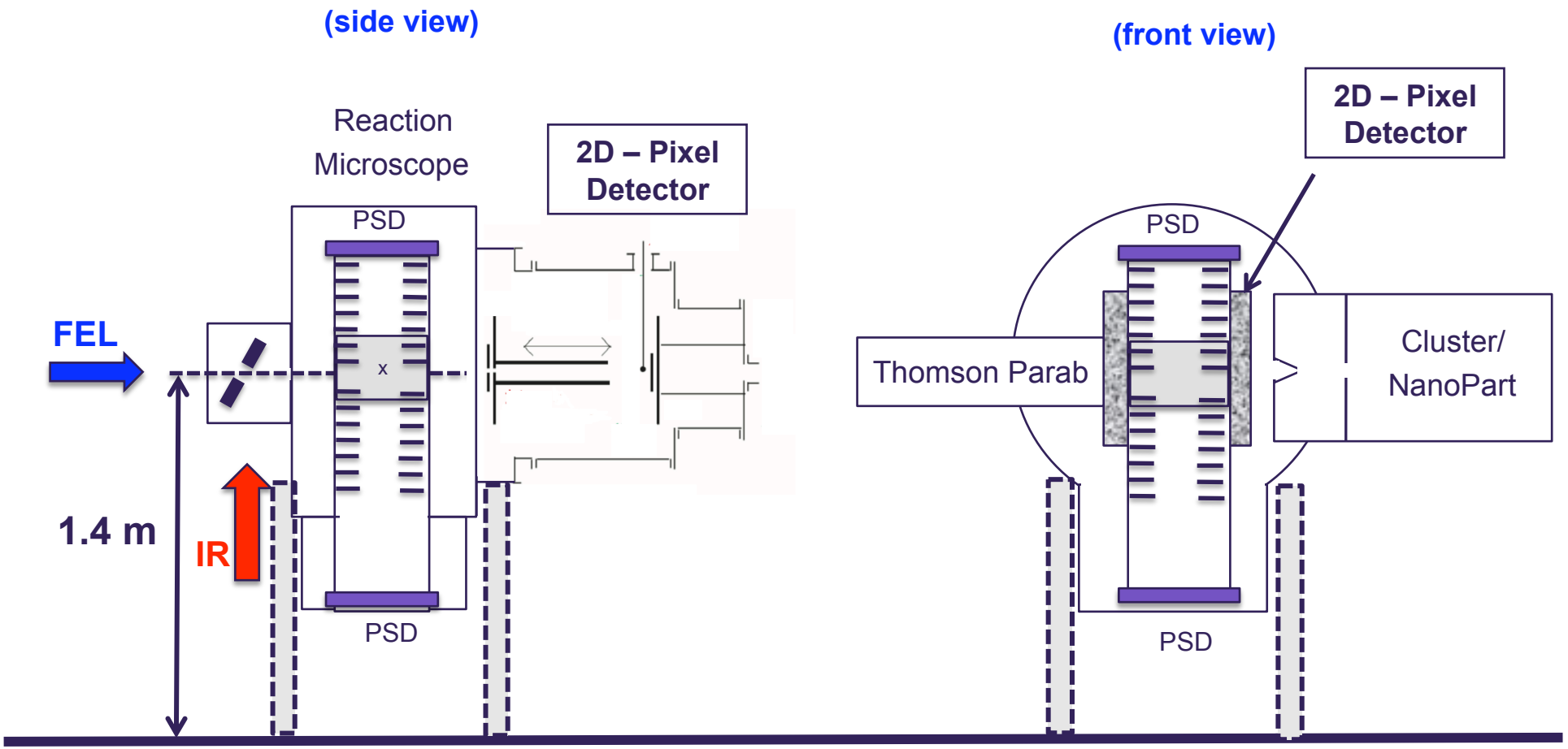
4. **XUV fluorescence spectrometer**
   - high spectral resolution
   - **2D - CCD**

     $E / \Delta E > 10^4$
     acceptance <1% of 4π

European XFEL

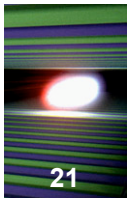
SQS end-station

NQS - Nano-size Quantum Systems



European XFEL

Analyzers and Detectors



NQS - Chamber

1. **Reaction Microscope**
   - angle-resolved spectroscopy
   - **2D – delay-line – detector**

     $E / \Delta E > 10^2$
     acceptance 4π
     e-ion-fluo-coincidences

2. **Time-Of-Flight**
   - electron kinetic energies
   - **1D – MCP - detector**

     $E / \Delta E > 10^3$
     acceptance ~5% of 4π
     e-ion-fluo-coincidences

3. **Thomson Parabola**
   - high recoil energies
   - **2D - CCD**

     acceptance <1% of 4π

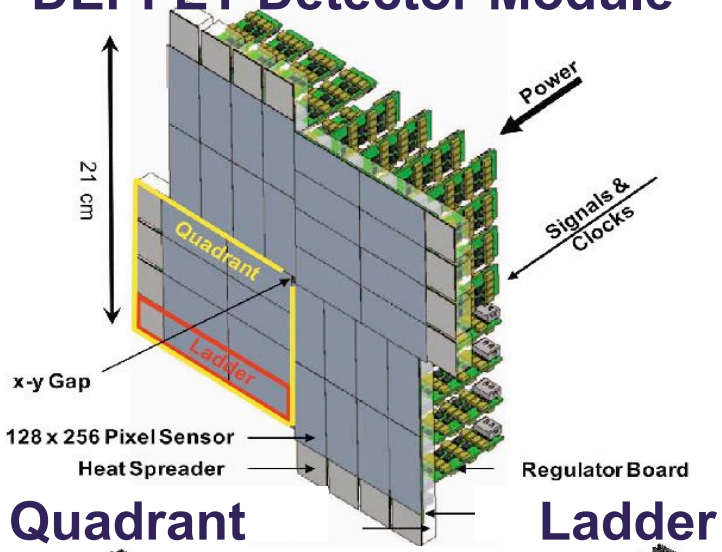
4. **2D Pixel detector**
   - imaging experiments
   - **DSSC or fast CCD**

     < 10 nm spatial resolution
     e-ion-fluo-coincidences

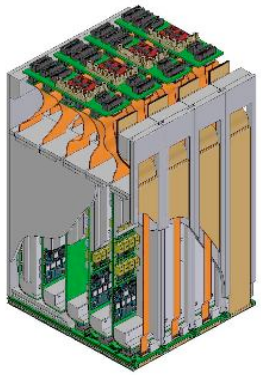
European XFEL

DSSC 1 M Pixel Detector Module (M. Kuster)

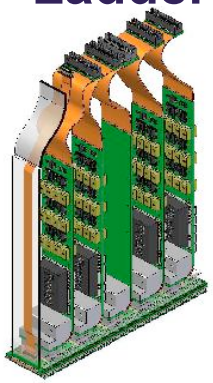
DEPFET Detector Module



Quadrant



Ladder



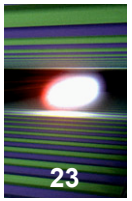
Key Detector Parameters

- Goal: Single photon sensitivity
  5 σ @1 keV and 4.5 MHz
- Energy range
  0.5 – 6 (25) keV
- Dynamic range
  > 6000 photons/pixel/pulse @1 keV
- Single photon sensitivity
  5 σ @ 1 keV (5 MHz)
  5 σ @ 0.5 keV (≤ 2.5 MHz)
- Number of storage cells 576
- Smallest detector unit “ladder
  128 x 512 pixels
- 4 ladders built on quadrant
- 4 quadrants = 1k x 1k detector

Porro et al. NIM A (2010) vol. 624 pp. 509

Data transfer rate: 1 GB / train (10 GB / s)

Optical Laser (M. Lederer)



Collaboration DESY, European XFEL, CFEL

Intra-Burst:

- 2700 pulses
- $f_{intra\text{-}burst}$ = 0.1…4.5 MHz
- **1mJ per pulse at 1MHz**
- τ_{FWHM} = 10 … 100fs
- ≈ 10 fs jitter (rms)

„Burst Energy“: ... 1J
„Burst-Power“: … 1kW
„Average Power“: … 10W

Pump-Probe Laser	Alignment Laser
1 - 4.5 MHz rep. rate	100 kHz rep. rate
0.2 – 1 mJ pulse energy	1 – 250 mJ pulse energy
10 - 100 fs pulse duration	30 fs / 1 ns pulse duration
< 10 fs synchronization	< 10 fs synchronization

SQS Specific

- OPA (200 – 3000 nm)
- variable polarization
- THz radiation
- beam characterization
- pulse stretcher

Option: 800 nm, 100 kHz, 20 – 100fs, 10mJ
1030 nm, 100 kHz, 1 ns, 250 mJ

FEL beam parameters for experiments

single shot / "on-line"

1. pulse energy: ± 1% (rel.)

   Gas Monitor Detector (GMD)

2. arrival time: < 10fs

   Reflectivity change (10 Hz),

   THz – electron streaking

3. wavelength: $\Delta\lambda / \lambda = 10^{-3}$

   Photoelectron Spectrometer

4. spectral profile: $\Delta\lambda / \lambda = 10^{-4}$

   VLS-grating monochromator

"off-line"

5. pulse duration: ΔT = < 10 fs

   auto-correlator

   cross-correlation

6. spatial profile

   extended beam on CCD

7. temporal profile

   N.N., THz electron streaking ?

8. beam position: 1 μm

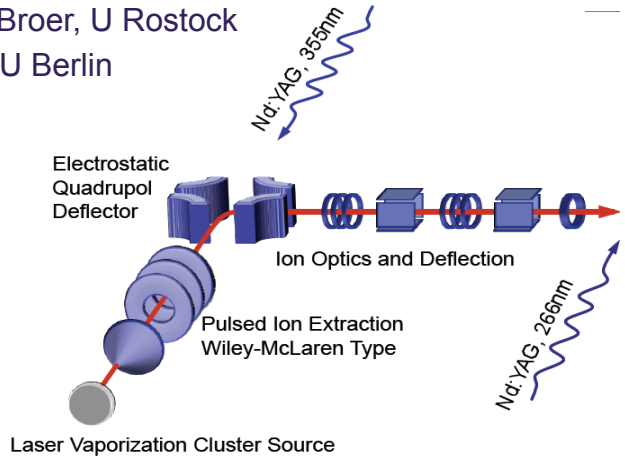
   YAG screens

European XFEL

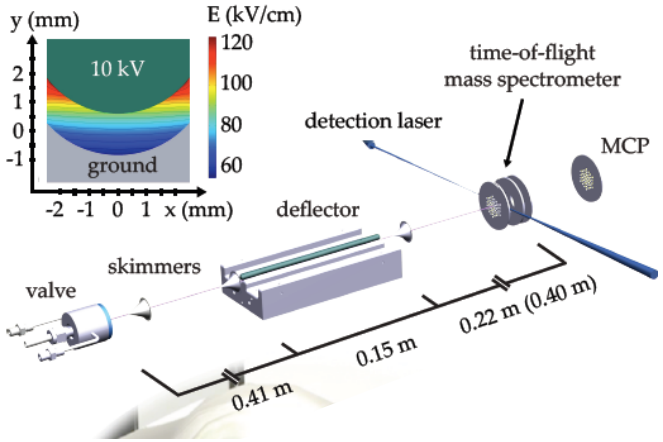
Add-on Equipment

1) Mass selected Cluster Source

Meiwes-Broer, U Rostock
Möller, TU Berlin



2) State-, size, and isomer-selected samples of polar molecules and clusters

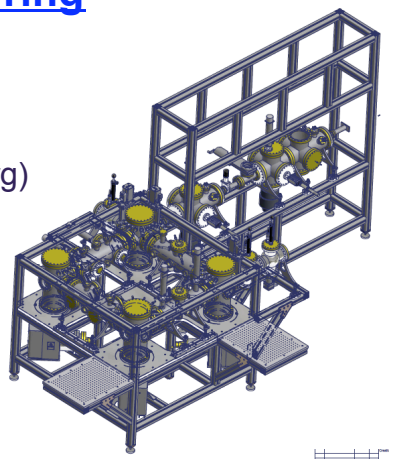


Küpper,
CFEL, Hamburg

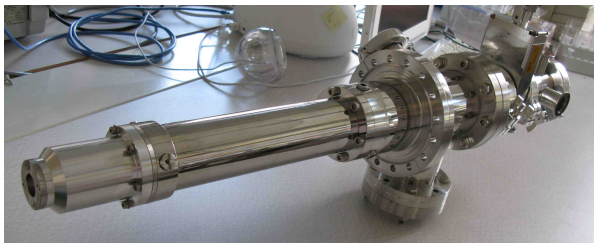
3) Ion storage ring

Pedersen (Aarhus)
Wolf (MPI Heidelberg)
Crespo (MPI Heidelberg)

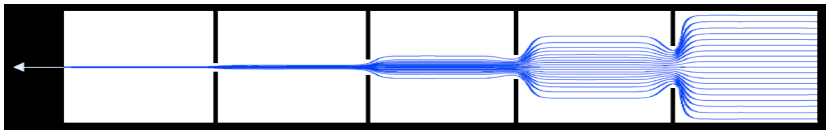
2.7 x 4.4 m^2



4) Injector for biological samples



Schulz,
European XFEL,
Univ. Uppsala



SQS Scientific Instrument: Status report and User participation

Room 2.26, AER 19, Start at 2:00 pm

14h00 – 14h10	Introduction	Michael Meyer (European XFEL)
14h10 – 14h30	Cluster source for SQS	Thomas Möller (TU Berlin)
14h30 – 14h50	COMO (Controlled Molecules)	Jochen Küpper (CFEL Hamburg)
14h50 – 15h10	Nano-particle & Bio-molecule source	Joachim Schulz (European XFEL)
15h10 – 16h30	Discussion of SQS – Conceptual Design & Summary	Michael Meyer
16h30 – 17h00	Coffee Break	

Seminar room 3.11, AER 19 (together with hRIXS Consortium Meeting)

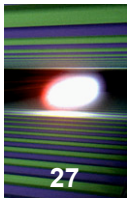
17h00 – 17h25	SASE 3 and beamline layout	Harald Sinn (European XFEL)
17h25 – 17h45	Soft X-ray detectors at European XFEL	Andreas Koch (European XFEL)

Room 2.26, AER 19

18h00 – 19h00 (optional)	Discussion of SQS - CDR (continued)	Michael Meyer

European XFEL

Timeline

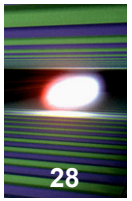


SQS Instrument https://www.xfel.eu/research/instruments/sqs

Conceptual Design Report	April 2011
Consultation of user community	> April 2011
Technical Design Report	end 2012
Start of sending out orders	early 2013
Definition, organization of add-on equipment	2013
Reception, test and assembly	mid 2013
Installation in experimental hall	mid 2014
Ready for beam	spring 2015

European XFEL

Acknowledgement



European XFEL

Paul Radcliffe, Tommaso Mazza	SQS Scientific Instrument
Jerome Gaudin, Harald Sinn	X-ray Optics & Transport
Chris Youngman, Krzystof Wrona	DAQ & Control Systems
Markus Kuster	Detector Development
Max Lederer	Optical Lasers
Jan Grünert	Photon Diagnostics
Adrian Mancuso	SPB Scientific Instrument
Serguei Molodtsov, Thomas Tschentscher	Scientific Directors

Thank you
for your attention!


European XFEL