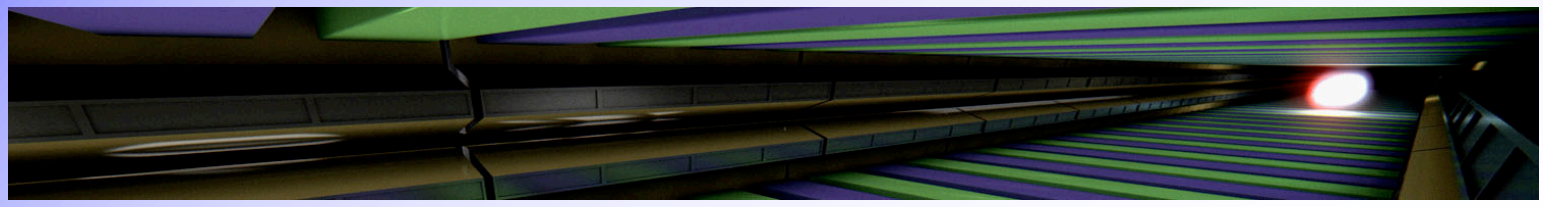
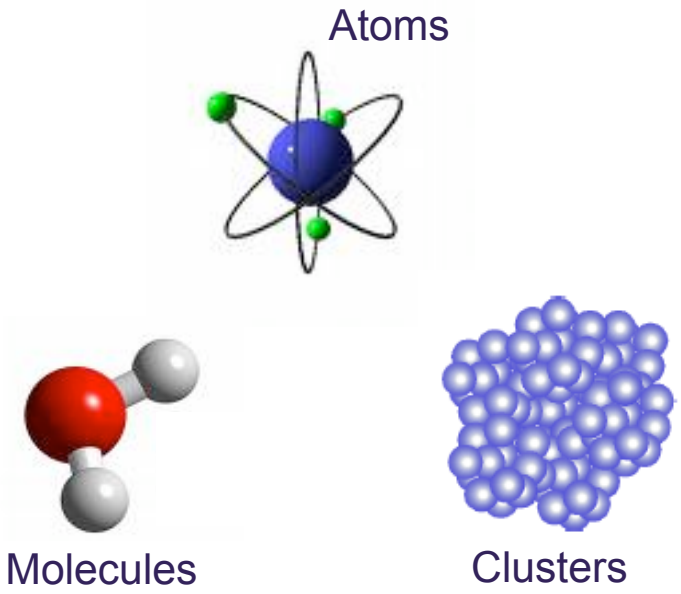


The SQS - Scientific Instrument at the European XFEL

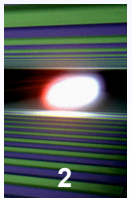
M. Meyer, European XFEL GmbH

“Small Quantum Systems”



European XFEL

OUTLINE



The SQS - Scientific Instrument at the European XFEL

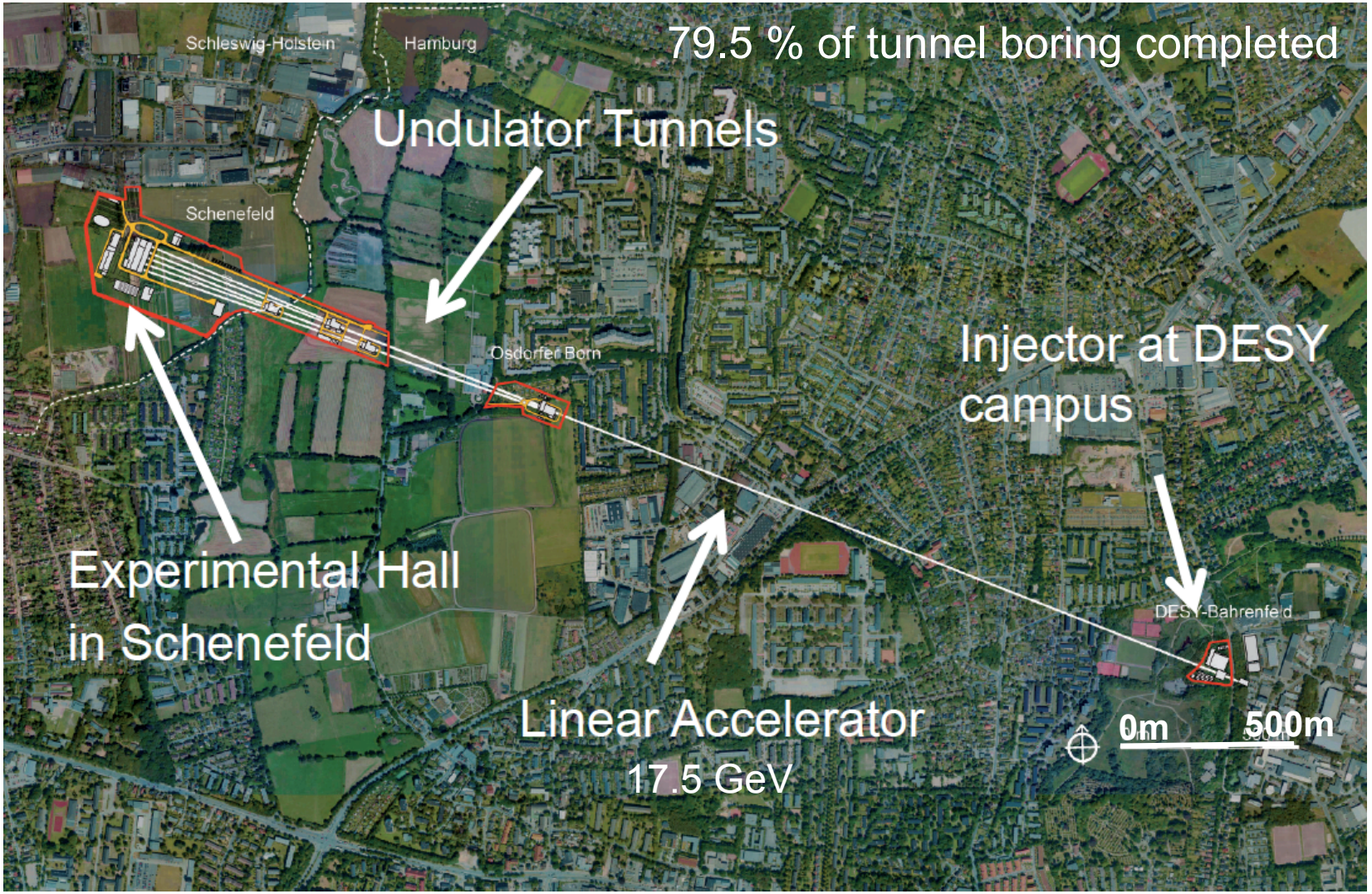
- **Soft X-rays at the European XFEL**
- **Scientific Case for SQS**
- **Instrument Layout**

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

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

European XFEL

European X-ray Free Electron Laser



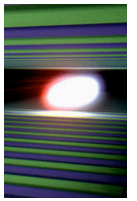
European XFEL

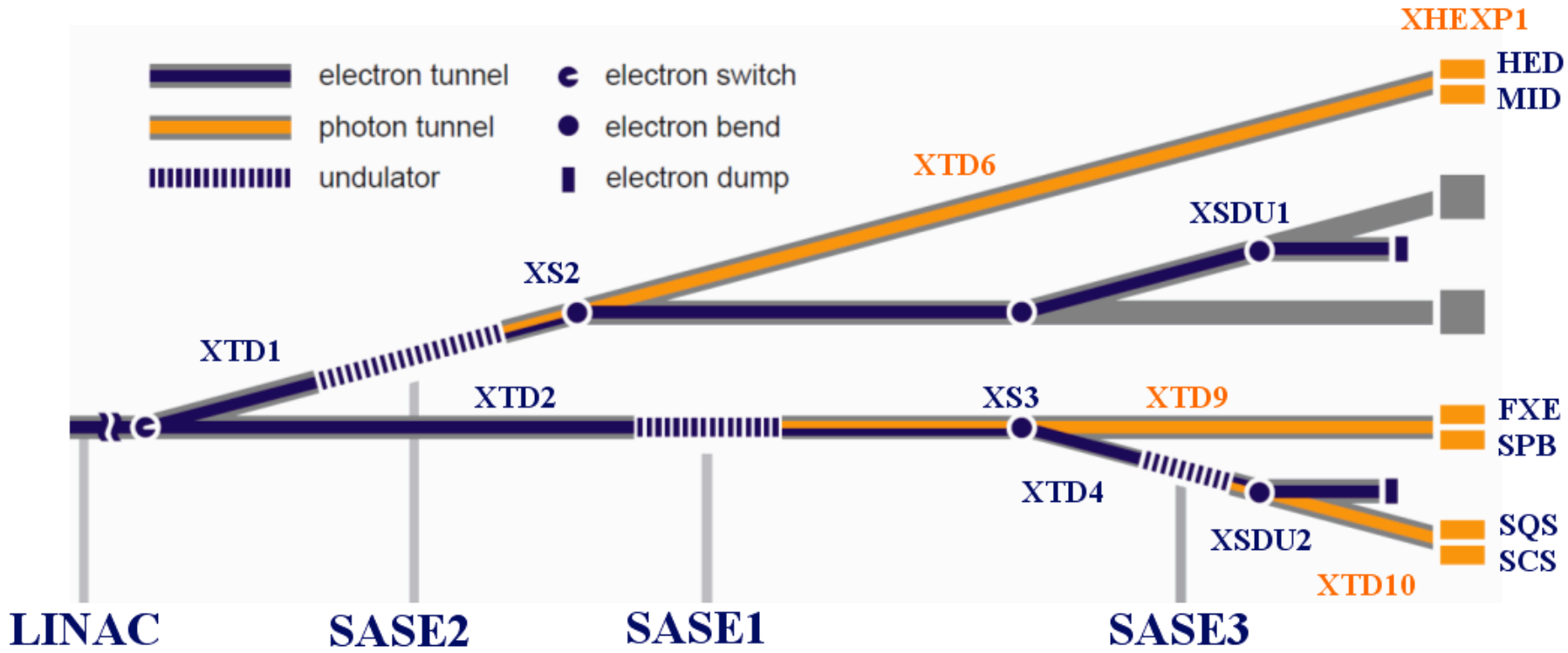
European X-ray Free Electron Laser

European XFEL

European XFEL

Photon beam transport systems





European XFEL

Scientific Instruments

SASE 1 / SASE 2

Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB)

- Structure determination of single particles: atomic clusters, bio-molecules, virus particles, cells.

Materials Imaging & Dynamics (MID)

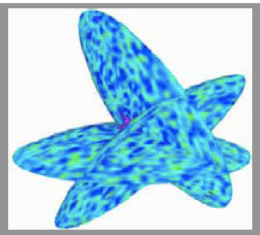
- Structure determination of nano- devices and dynamics at the nanoscale.

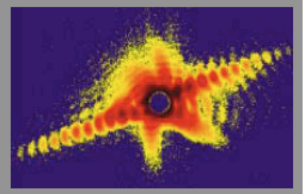
Femtosecond X-ray Experiments (FXE)

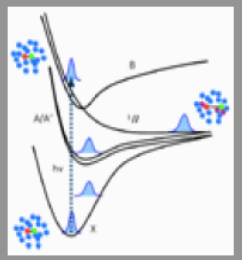
- Time-resolved investigations of the dynamics of solids, liquids, gases

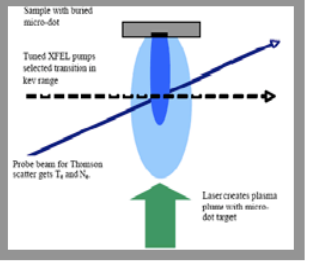
High Energy Density Matter (HED)

- Investigation of matter under extreme conditions using hard x-ray FEL radiation, e.g. probing dense plasmas









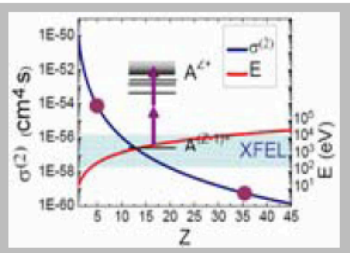
SASE 3

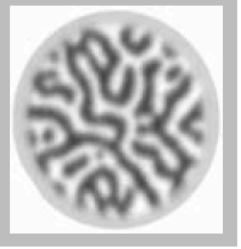
Small Quantum Systems (SQS)

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

Spectroscopy and Coherent Scattering (SCS)

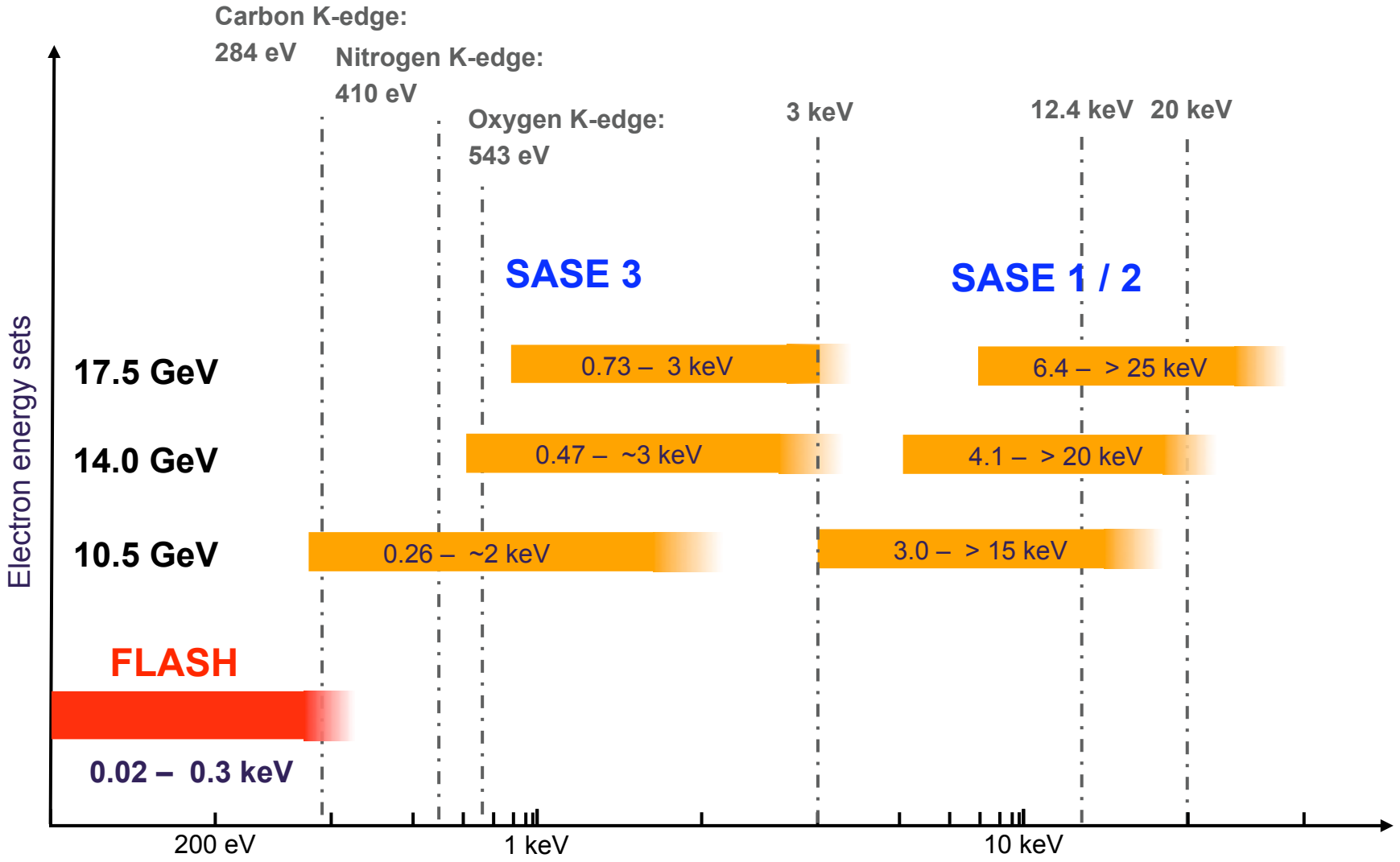
- Structure and dynamics of nano-systems and of non-reproducible biological objects





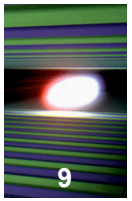
European XFEL

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

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)
April 6th, 2011

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

SQS – Small Quantum Systems –

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

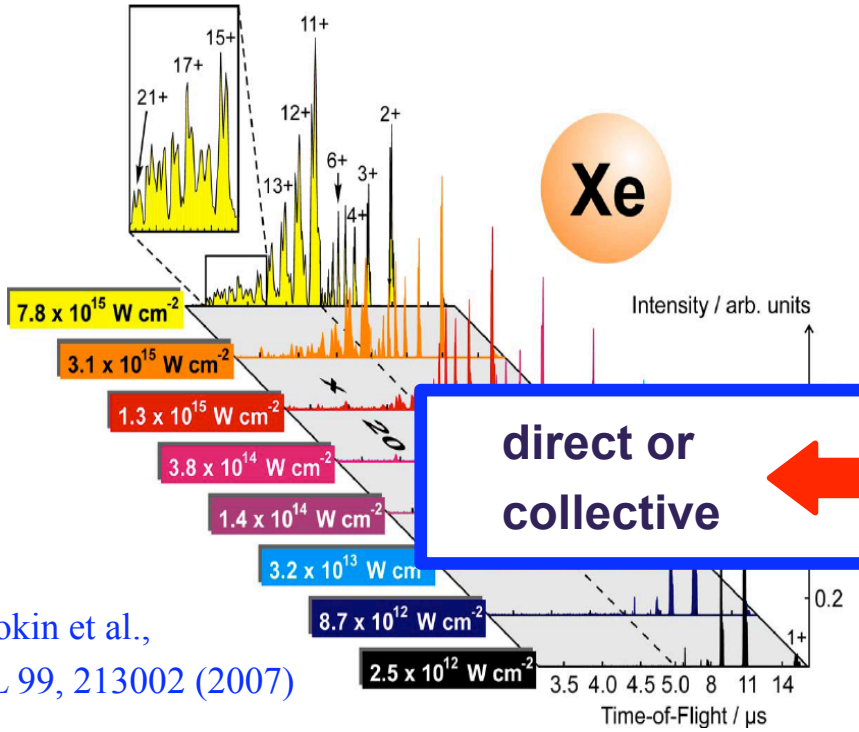
High intensities: $>10^{15}$ W/cm^2	⇨	**Non-linear phenomena, multi-photon**
Short pulses: 2 - 100 fs	⇨	**Ultra-fast dynamics, pump-probe**
High flux $> 10^{12}$ photons / pulse $> 10^{15}$ photons / sec	⇨	**Extremely dilute targets,** **Processes with small cross section**
Spatial coherence	⇨	**Coherent Diffraction Imaging**
Soft X-Ray photon energies	⇨	**Threshold phenomena** C(1s)=290 eV, N(1s)=410eV, O(1s)=560eV

European XFEL

Non-linear Processes

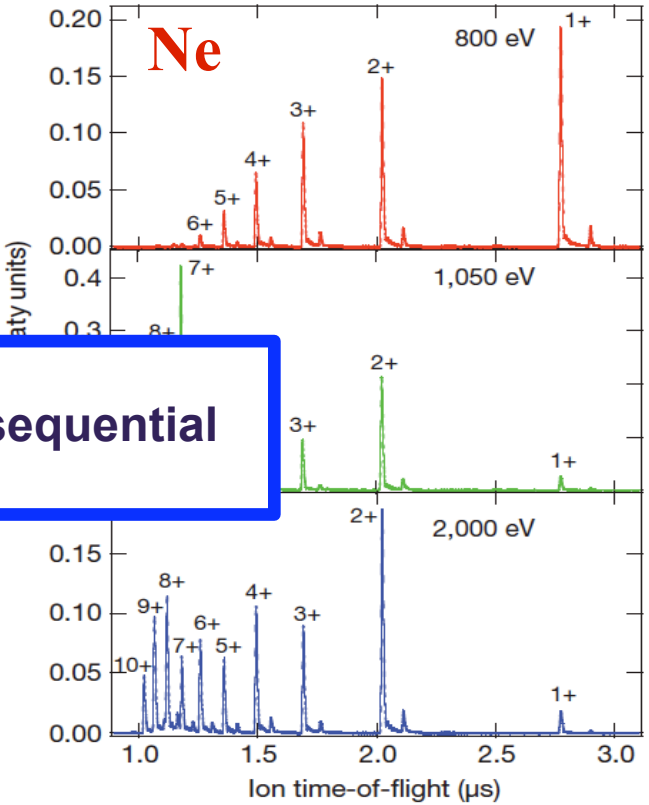
Multi-Photon Multiple Ionization

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



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

direct or collective ⟷ **sequential**



FLASH : 93 eV

focus 2.6 µm: 7.8 x 10^{15} W / cm^2

IP(Xe 21+) ≈ 5 keV

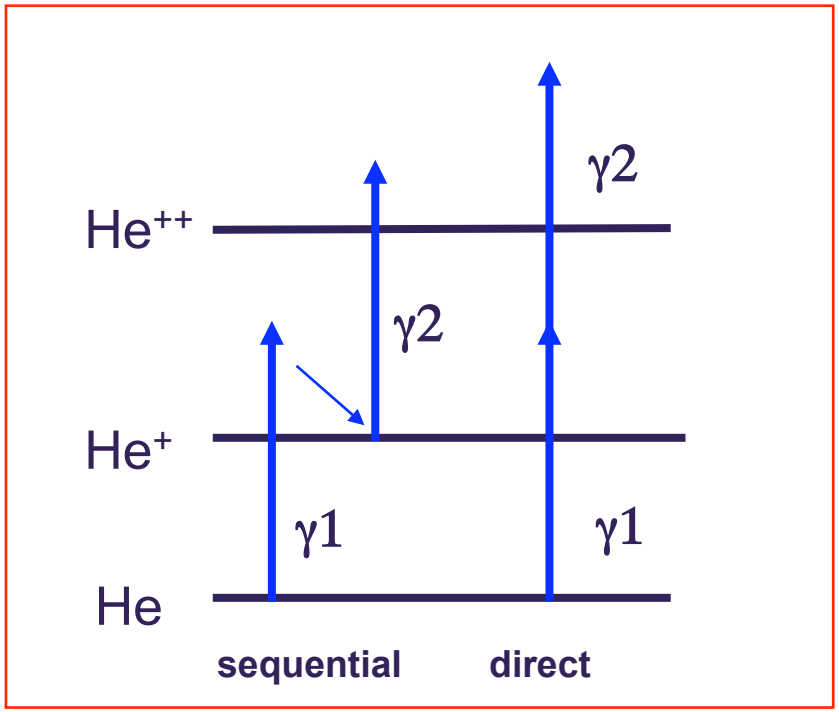
LCLS : 800 - 2000 eV

< 1 x 10^{18} W / cm^2

Non-linear Processes

Fundamental Processes

2-Photon Double Ionization

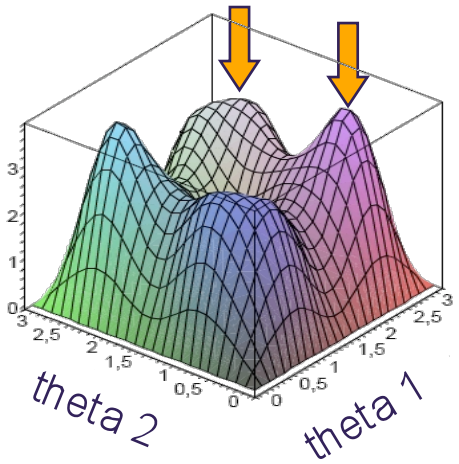


Reaction microscope : full solid angle

but

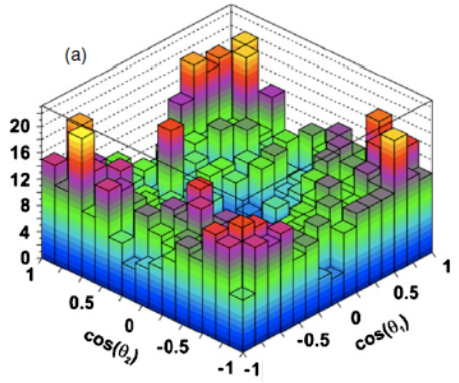
60 Hz → **very limited statistics**

Angular correlation between 2 electrons



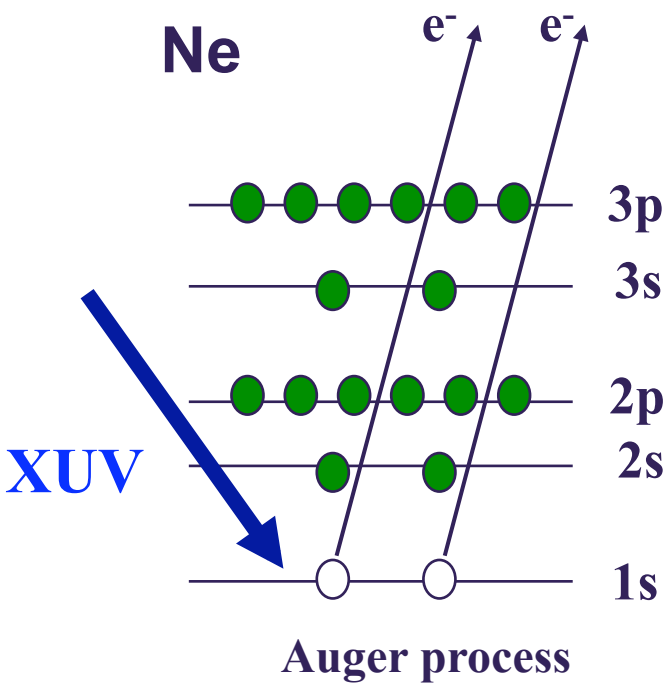
Theory:
Fritzsche,
Grum-Grzhimailo,
Gryzlova, Kabachnik
J.Phys.B 41,
165601 (2008)

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

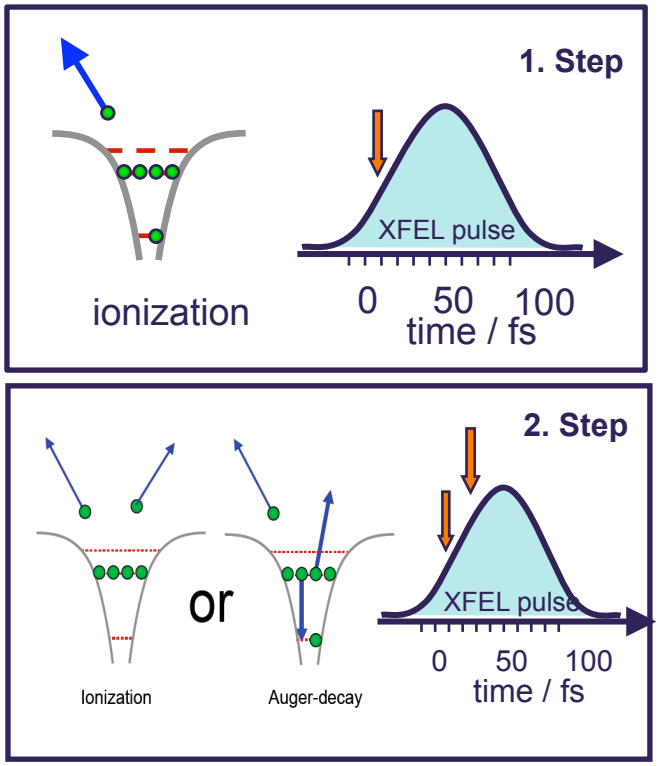


Innershell Processes

Direct



Sequential



Comparable time scales

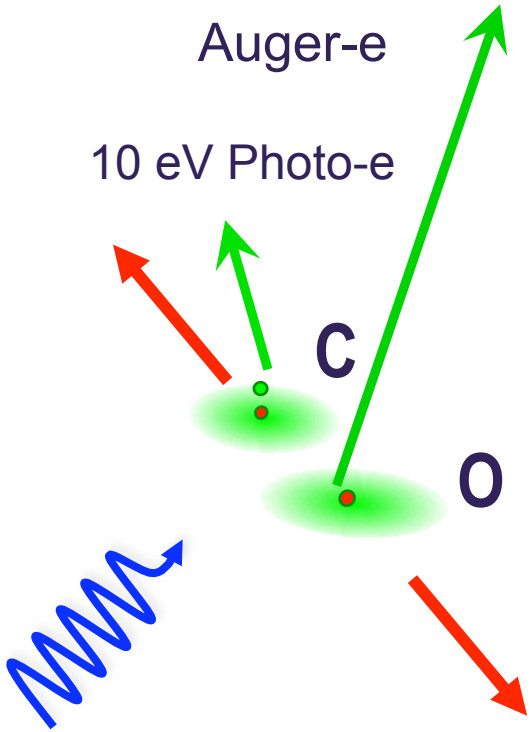
Complex Decay Dynamics

→ **e-e coincidences**

high rep. rate (27 000 pulses/s)

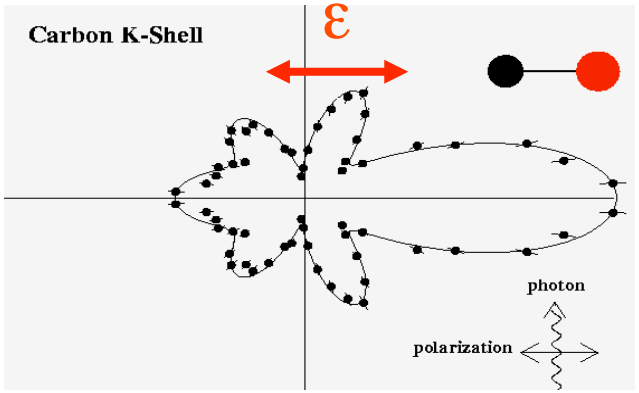
Ultra-fast processes

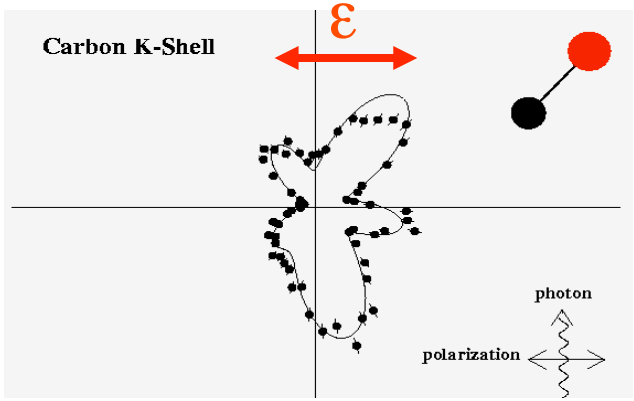
Molecular Dissociation Dynamics



Landers & Dörner

PRL 87 (2001)





Coincidences:

electron – ion –ion

1 pulse = 1 event !!

COLTRIMS:

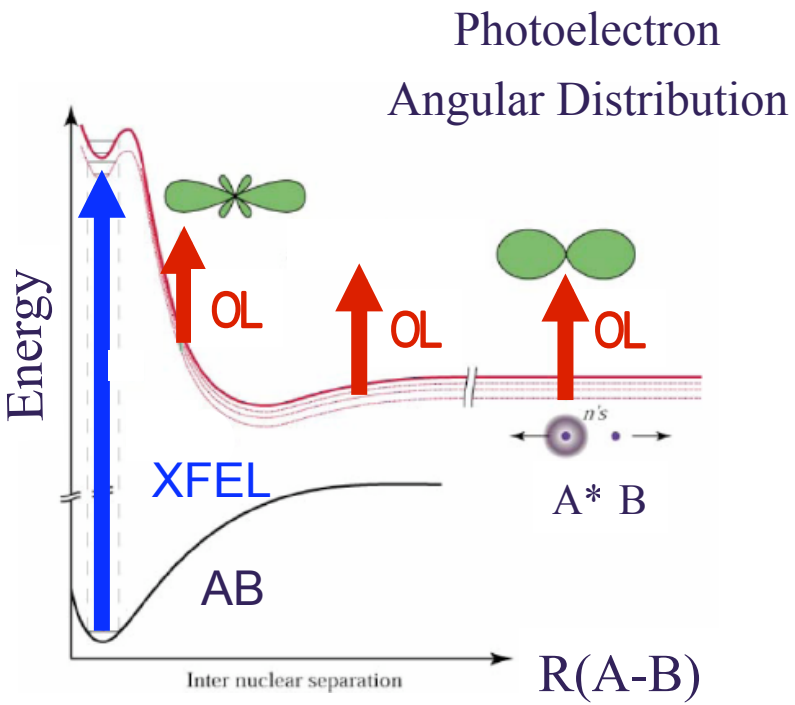
high collection efficiency

ALS:

MHz rep. rate

~~**fs-dynamics**~~

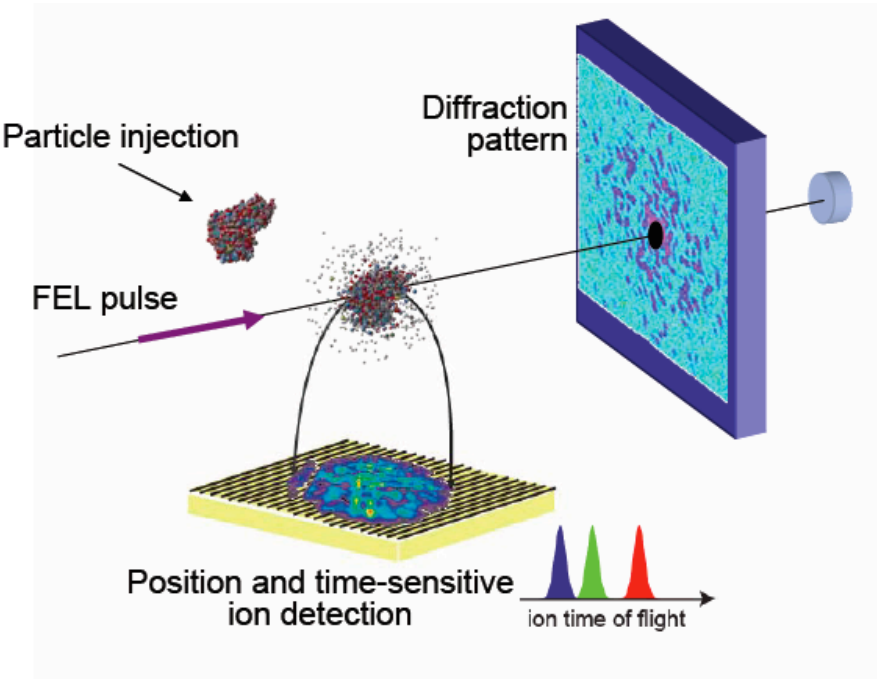
Diatomic molecules



"element specific" pump or probe

Complex Molecules

Ullrich et al. , ASG MPI Heidelberg



complete characterization = multiple coincidences

coincidences: ➡ **high (> kHz) repetition rate**

European XFEL

Two-color Pump-Probe Experiments

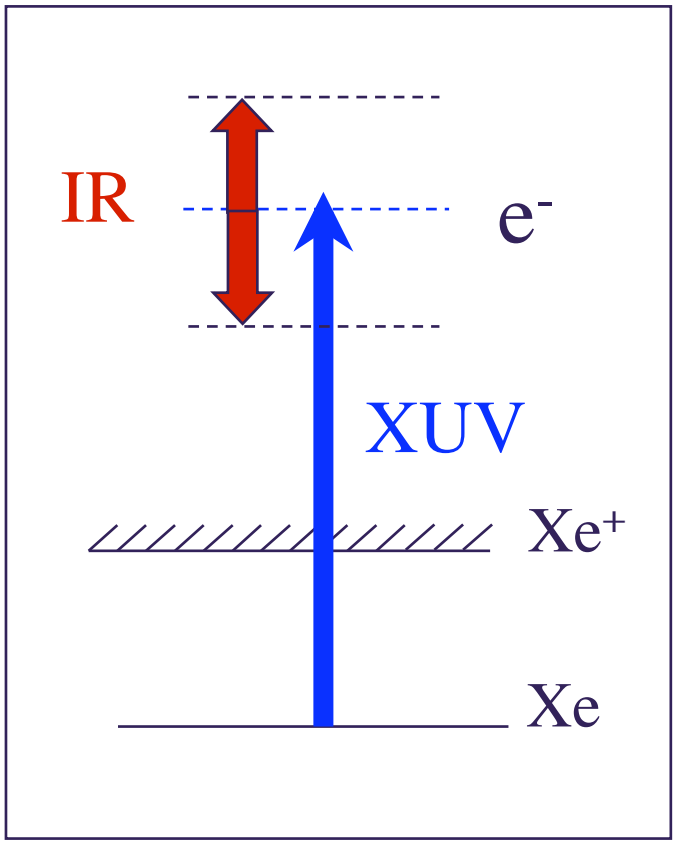
FLASH

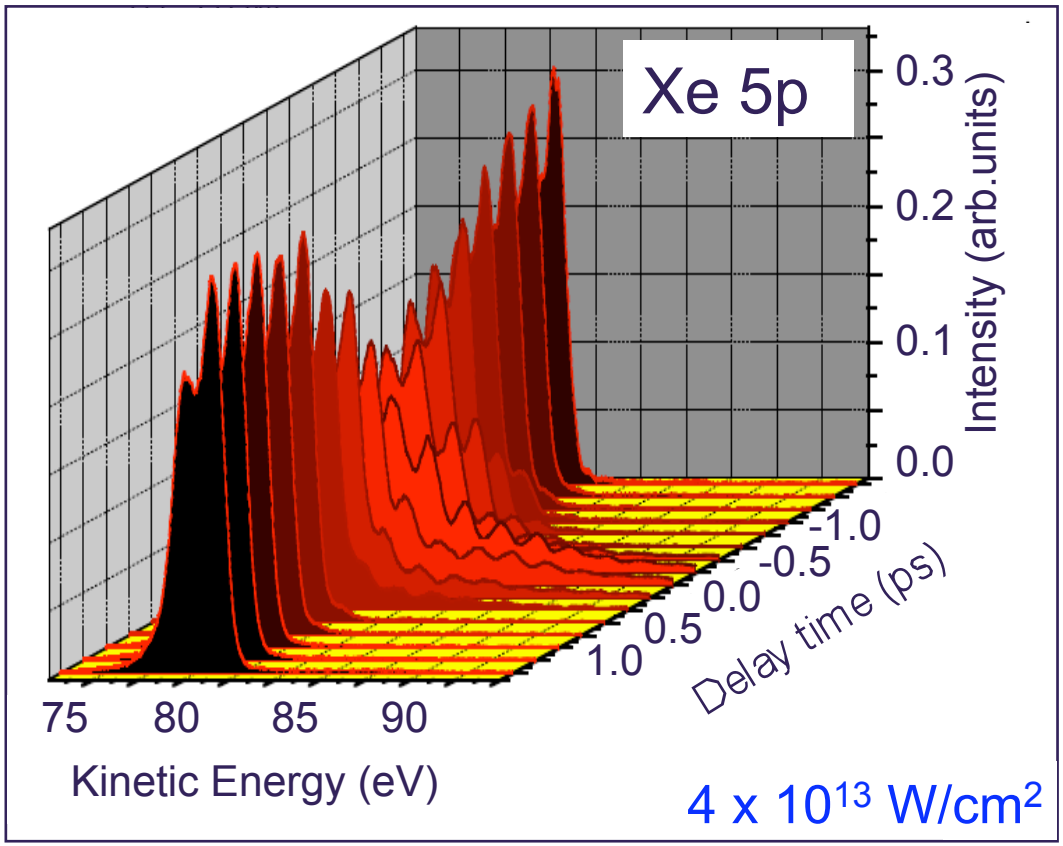
Intense Laser (> 10^{10} W/cm^2)

FLASH: 13.7 nm, 30 μJ, 50 μm focus, 20 fs

Opt. Laser : 800 nm, ≤ 4 mJ, 50 μm focus, 120 fs

Free-Free transitions

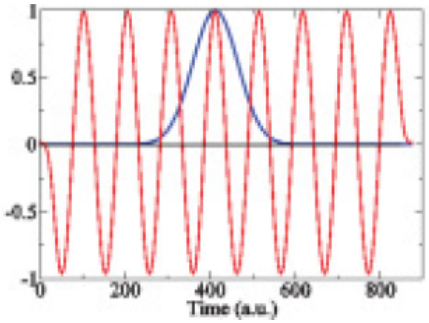




Example: Two-color Pump-Probe

Optically induced electron interferences in the angular distribution

Auger lifetime similar to optical cycle

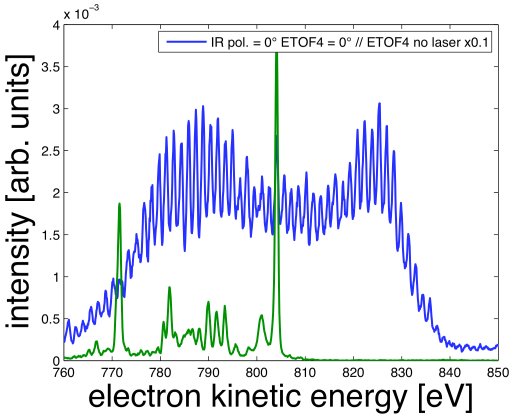


Core hole lifetime **LCLS: 1 keV, 2-5 fs**

τ (Ne 1s) = 2.4fs

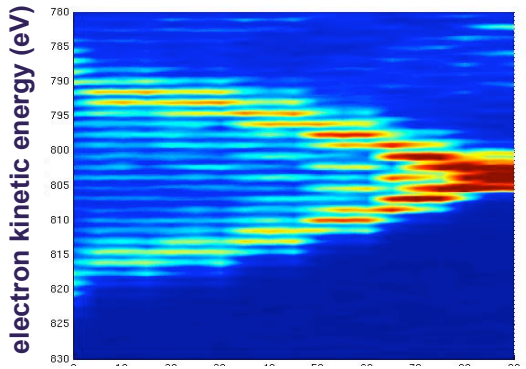
Optical cylce

T (800nm) = 2.6fs



HR - Electron spectroscopy

Ne



Angular distribution

Meyer et al., LCLS_Nov/2010

A.K. Kazansky, N.M. Kabachnik, JPB 43, 035601 (2010)

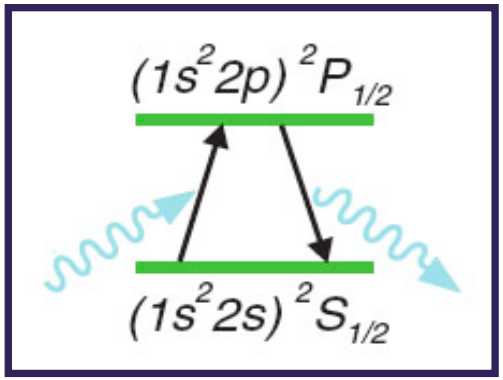
European XFEL

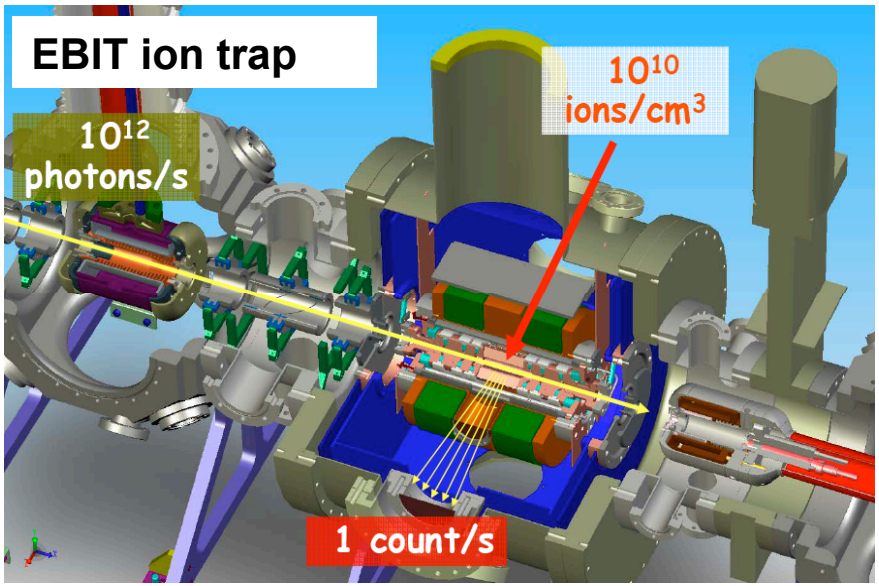
High flux studies

FLASH

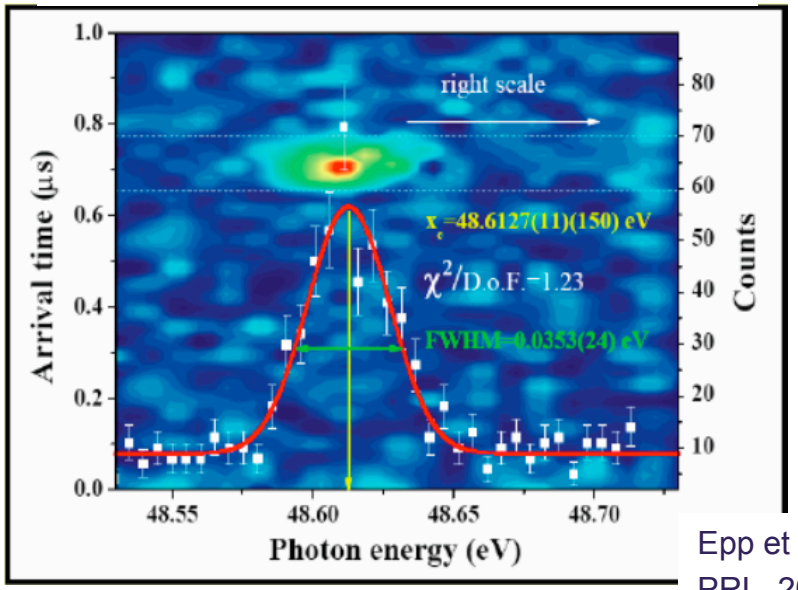
J.Crespo Lopez-Urrutia et al. ,
MPI Heidelberg

- **Ionic targets**
  - highly charged ions
  - non-linear processes
  - test of fundamental laws
- **Laser cooled atoms**





2s $^2S_{1/2}$ - 2p $^2P_{1/2}$ line of Li-like Fe^{23+}

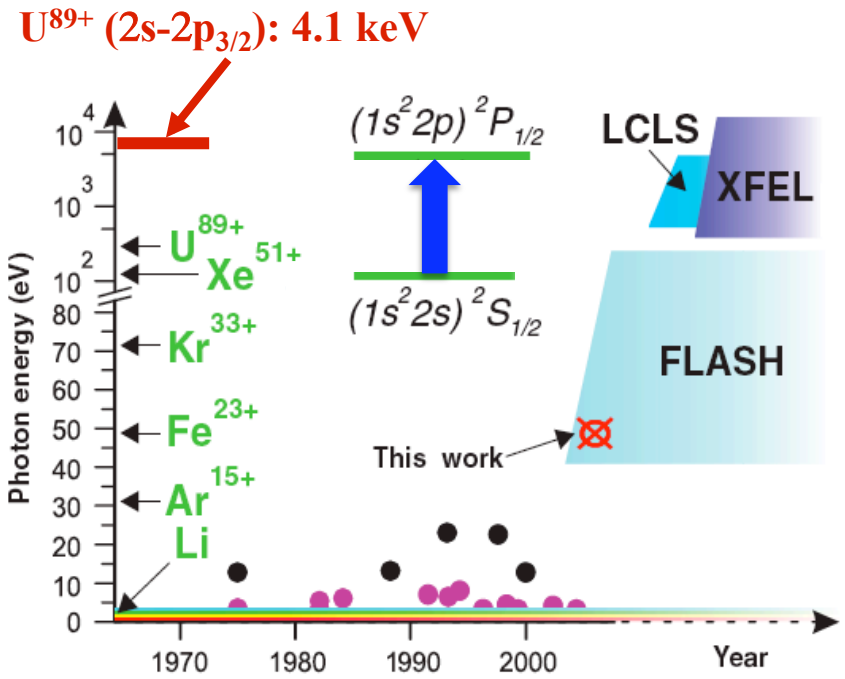


Epp et al.
PRL, 2007

High flux & Non-linear studies

European XFEL

Lamb-shift in HCI



With increasing charge state: J. Crespo

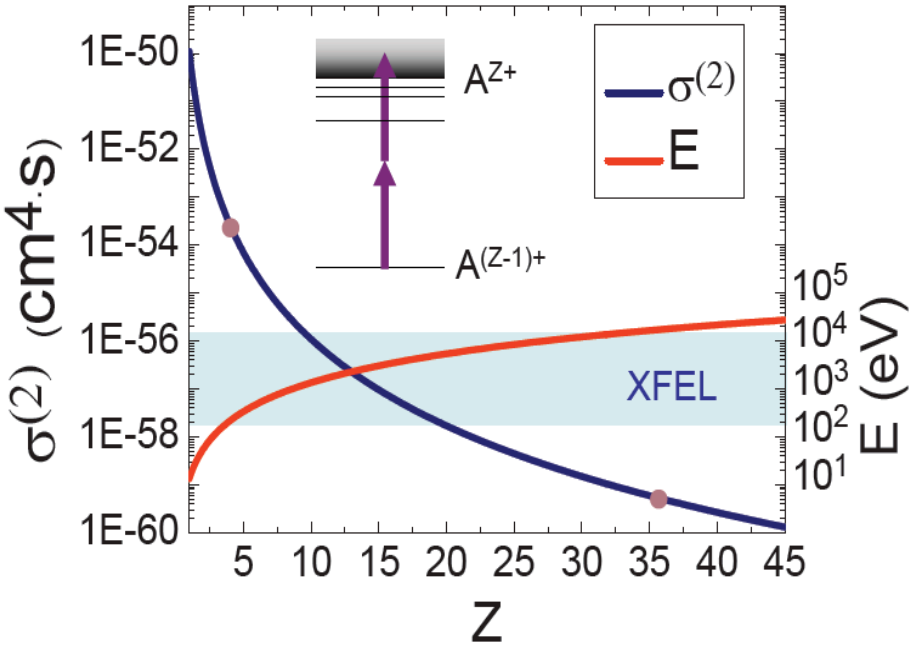
- growing excitation/ ionization energies

  10 eV → **130 keV**

- diminishing cross sections

  10^{-16} cm^2 → 10^{-24}cm^2

Two-Photon Ionization of H-like Ions



For: 1keV D. Charalambidis

Interaction Volume: $V_{int} \simeq 10^{-6}$cm^3

Atomic Density: 10^{12} atoms/cm^3

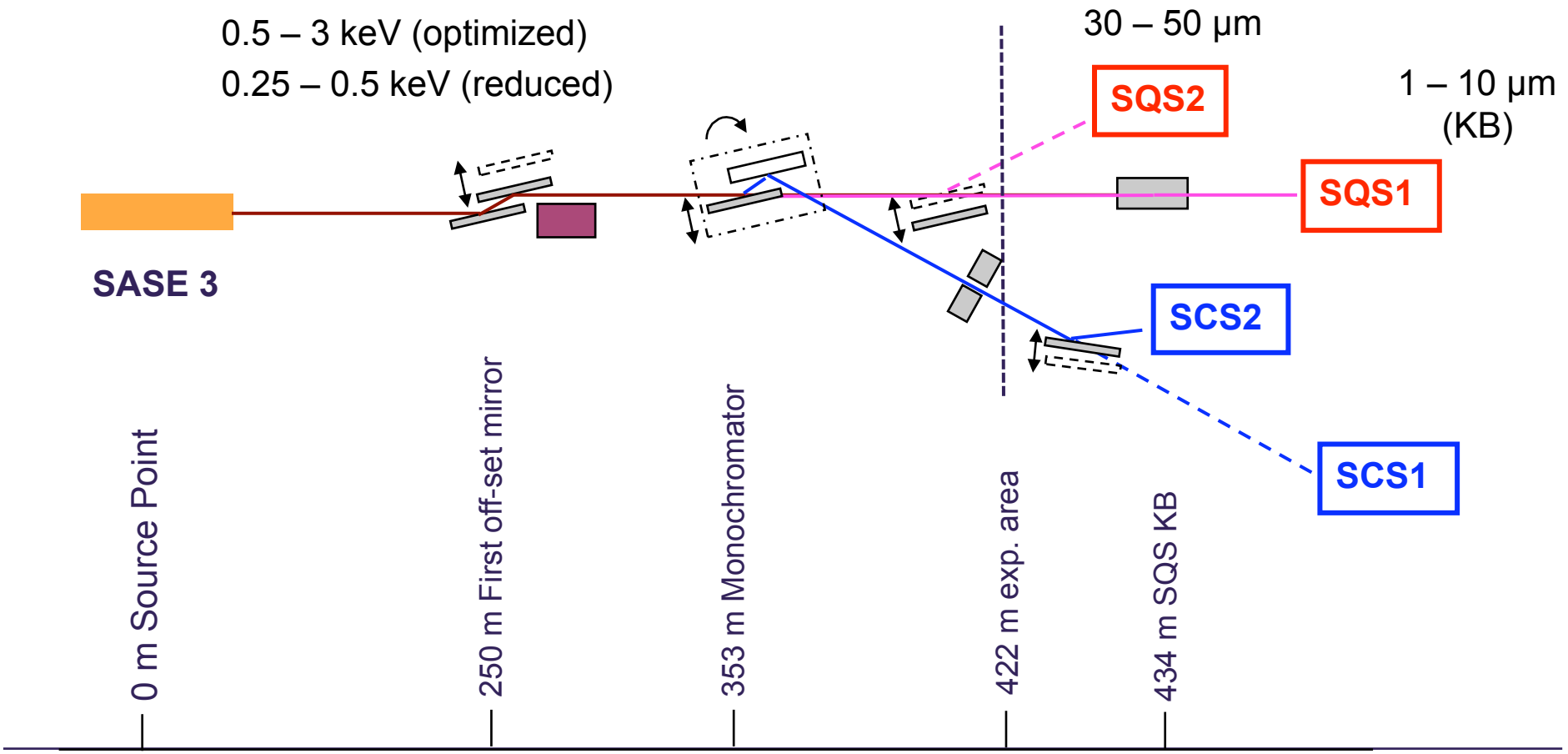
100fs pulses, 3250 pulses/bunch, 10Hz bunch rep rate

⇒ **Mean Ionization Rate: ~10 ions/sec**

General Layout of SQS Scientific Instrument

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

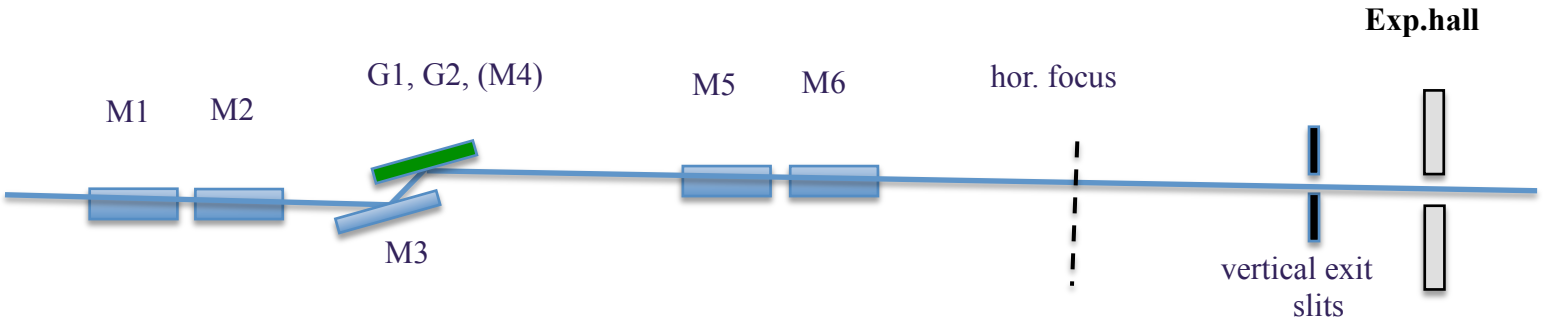
- direct beam → Small Quantum System (SQS)
- monochromatized → Spectroscopy @ Coherent Scattering (SCS)



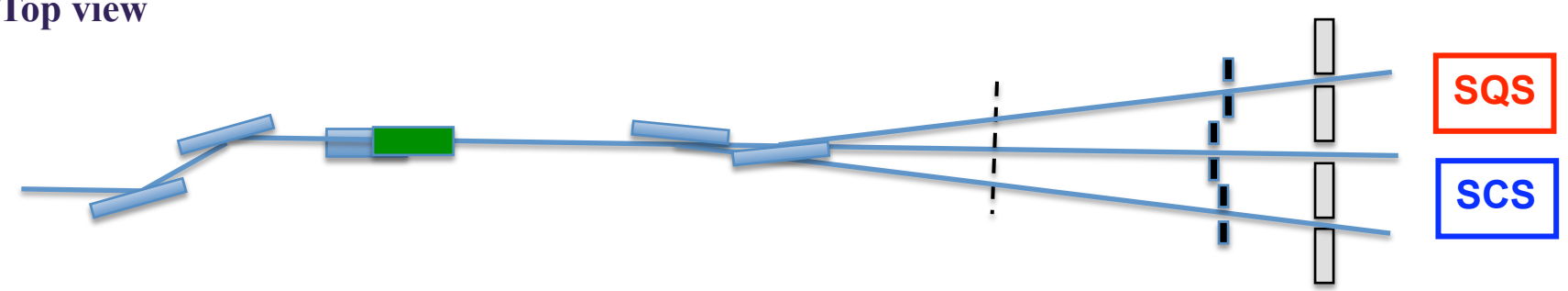
Soft X-Ray Monochromator (H. Sinn)

VLS (Variable Line Spacing) Grating

Side view



Top view



Wavelength regime:
0.5 – 3 keV (optimized)
0.25 – 0.5 keV (reduced)

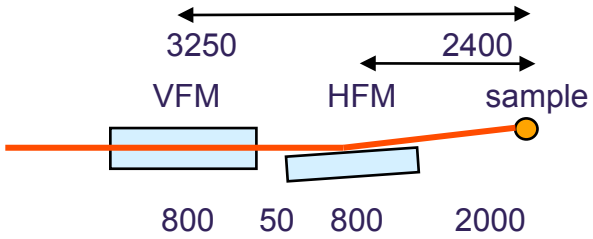
Spectral resolution:
$\lambda / \Delta\lambda \geq 10\,000$
(>30 000)

Temporal resolution:
$\Delta T \leq 100$ fs

European XFEL

Focusing Optics

1st port : Kirkpatrick-Baez system



KB-Mirror:

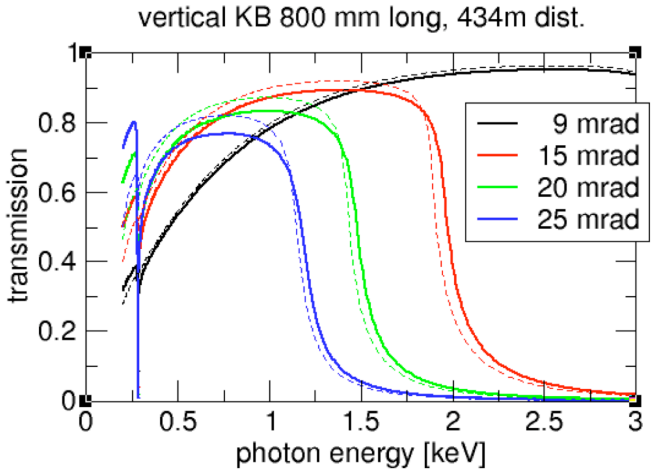
- small focus spot (1-10 μm)
- variable focus position (size)

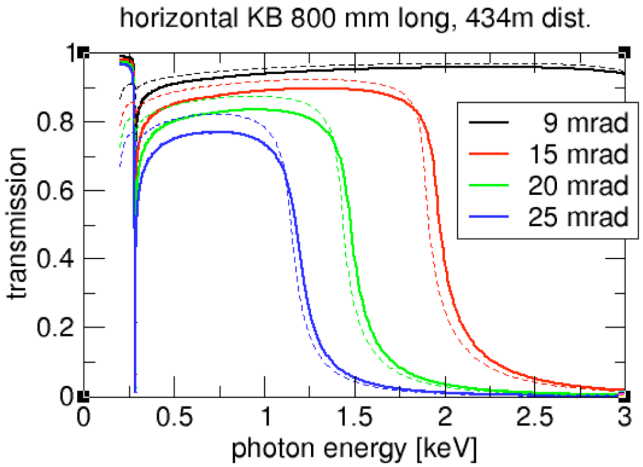
1) Standard operation mode (~15 mrad)

- maximal transmission: 500 – 2000 eV
- reduced transmission: 260 – 500 eV

2) High energy mode (9 mrad)

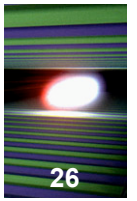
- maximal transmission: 2000 – 3000 eV





European XFEL

SQS end-station



Gas phase targets:

- Molecular beam (atoms & molecules)
  supersonic jet, effusive jet, cells

- Cluster beam (mass-selected)

- Nano-particles, Nano-crystals,
  bio-molecules
  (aerosols, liquid jet)

Particle analyzers:

- High-resolution TOFs

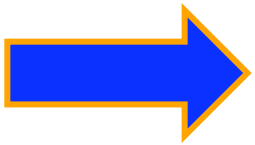
- High resolution X-ray spectrometer

- Magnetic Bottle Electron Spectrometer

- Velocity-Map-Imaging

- Reaction Microscope

- Thomson Parabola



- **AQS** (Atomic-like Quantum Systems) Chamber
- **NQS** (Nano-size Quantum Systems) Chamber

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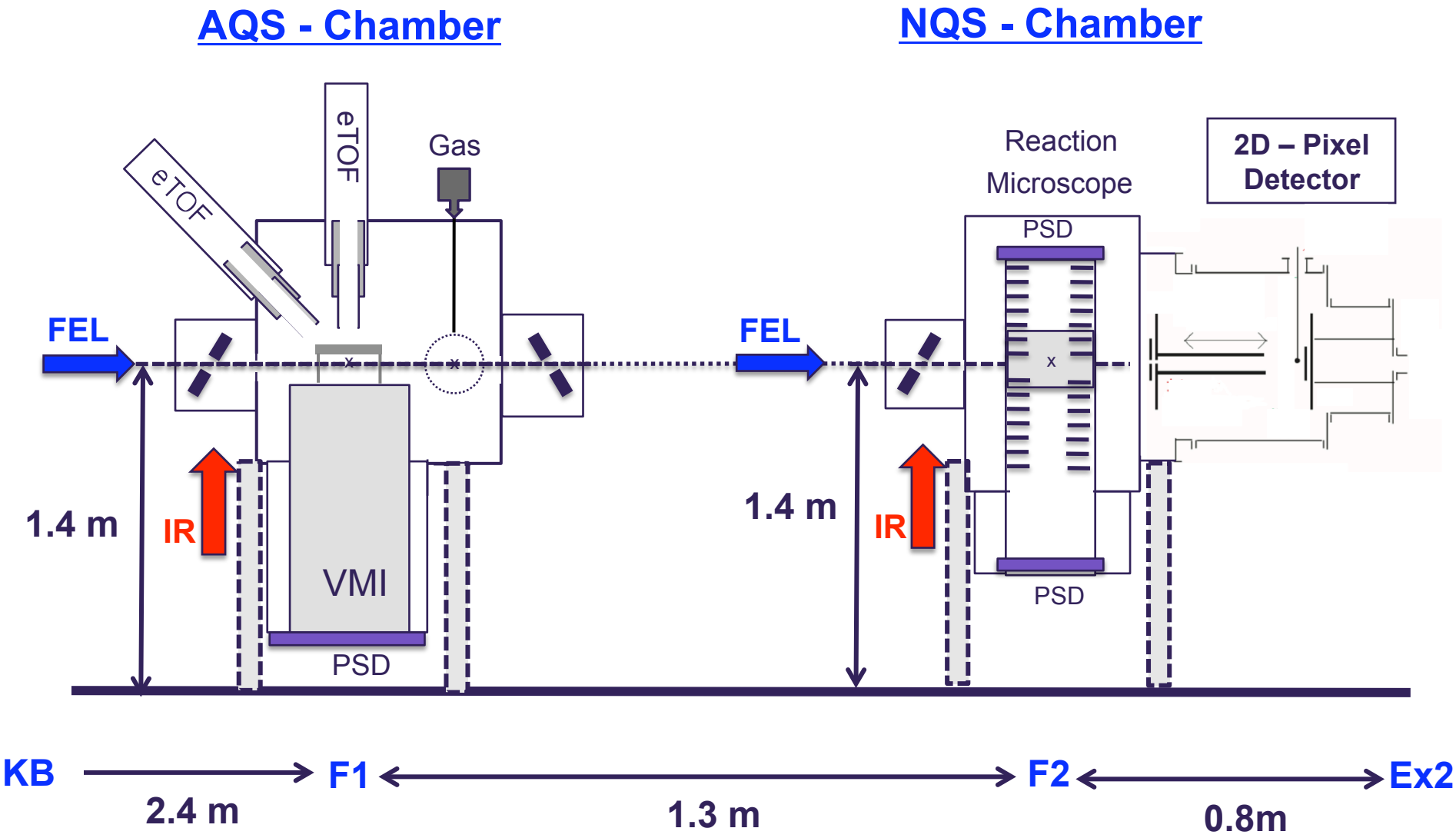
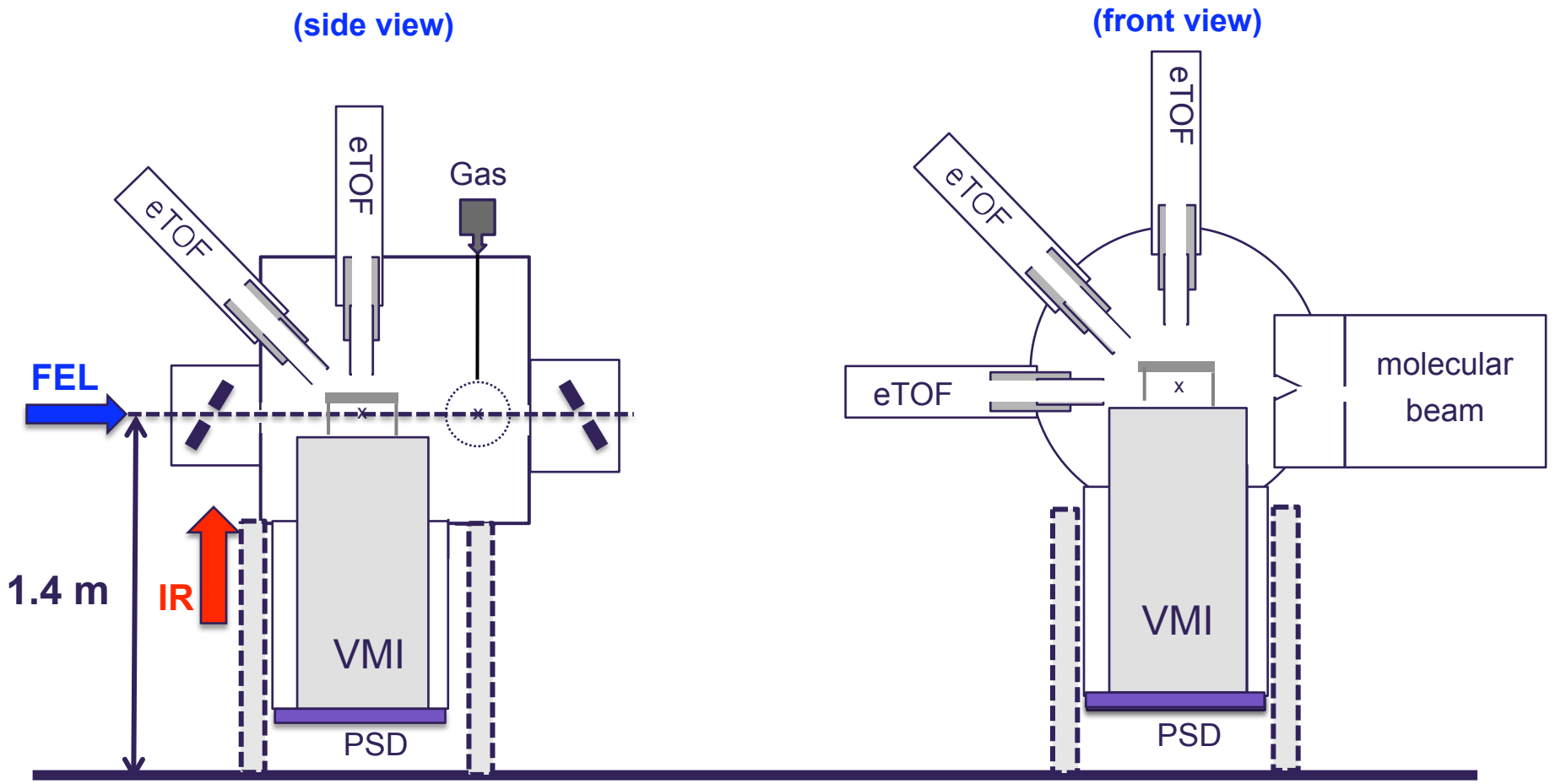
SQS end-station



European XFEL

SQS end-station

AQS - Chamber

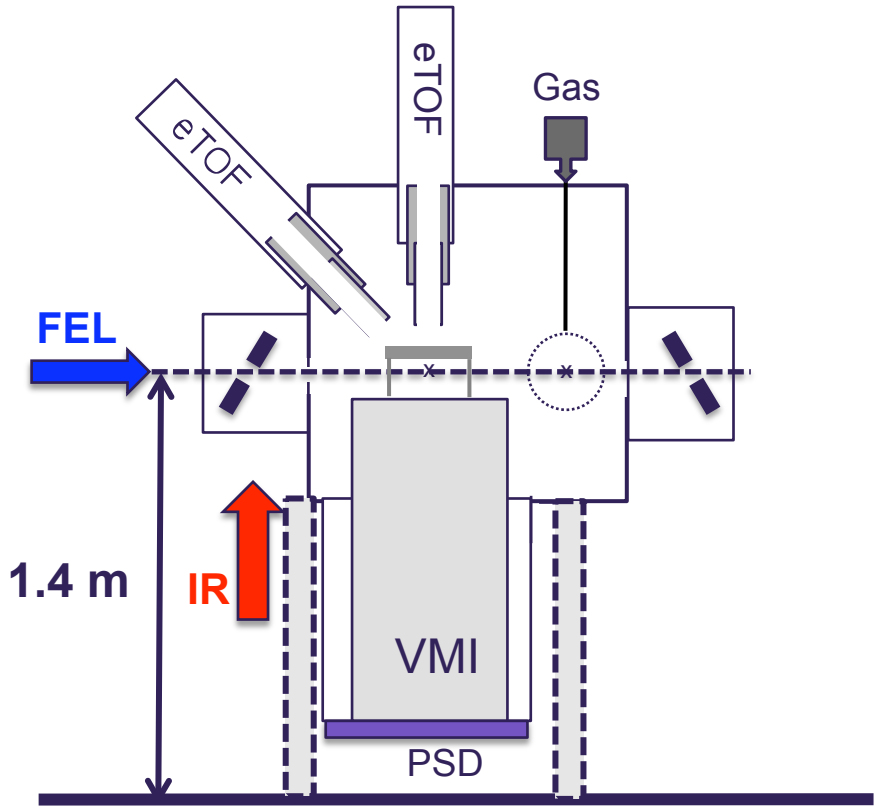


European XFEL

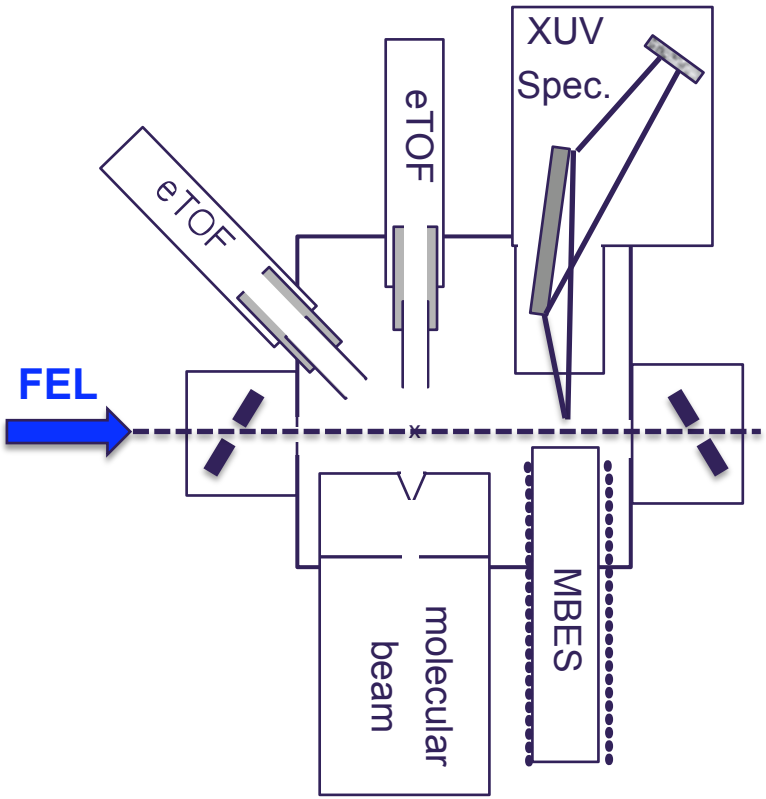
SQS end-station

AQS - Chamber

(side view)



(top view)



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

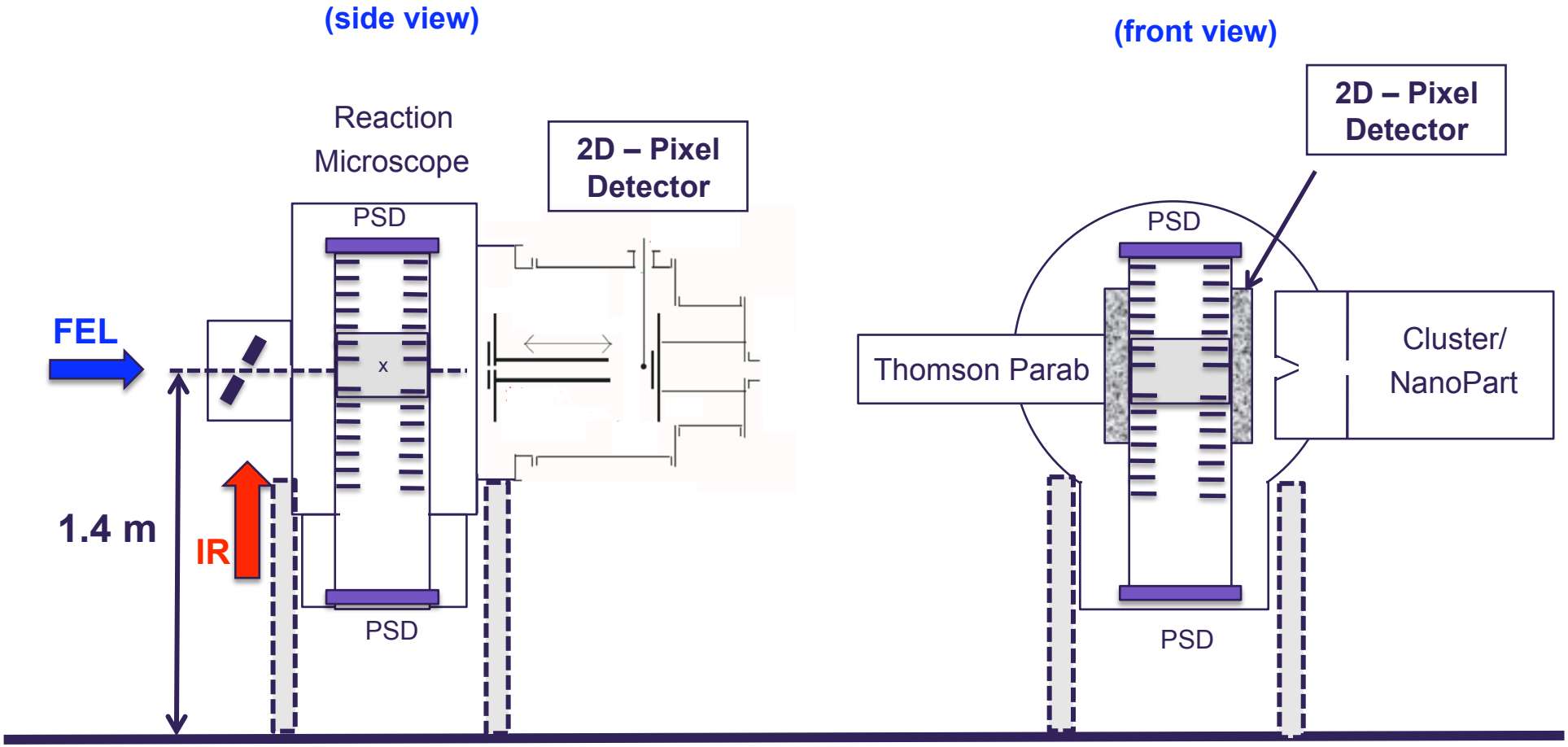
4. **XUV fluorescence spectrometer**
   - high spectral resolution
   - **2D - CCD**

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

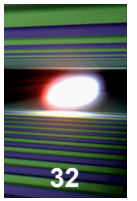
European XFEL

SQS end-station

NQS - Chamber



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 pn-CCD**

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

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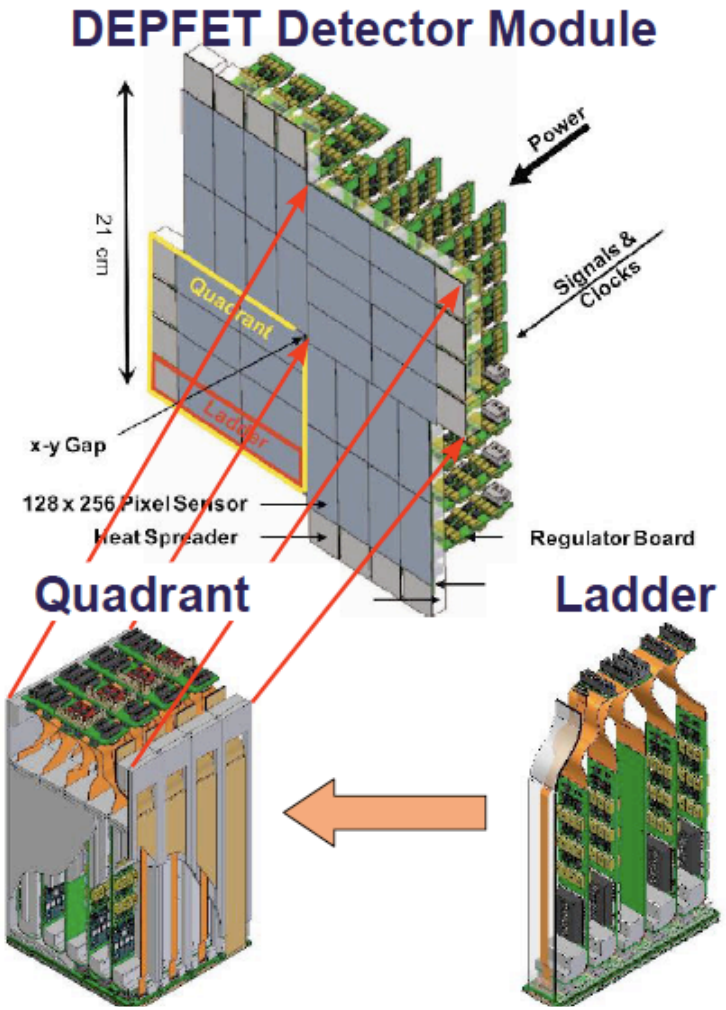
DSSC 1 M Pixel Detector Module (M. Kuster)

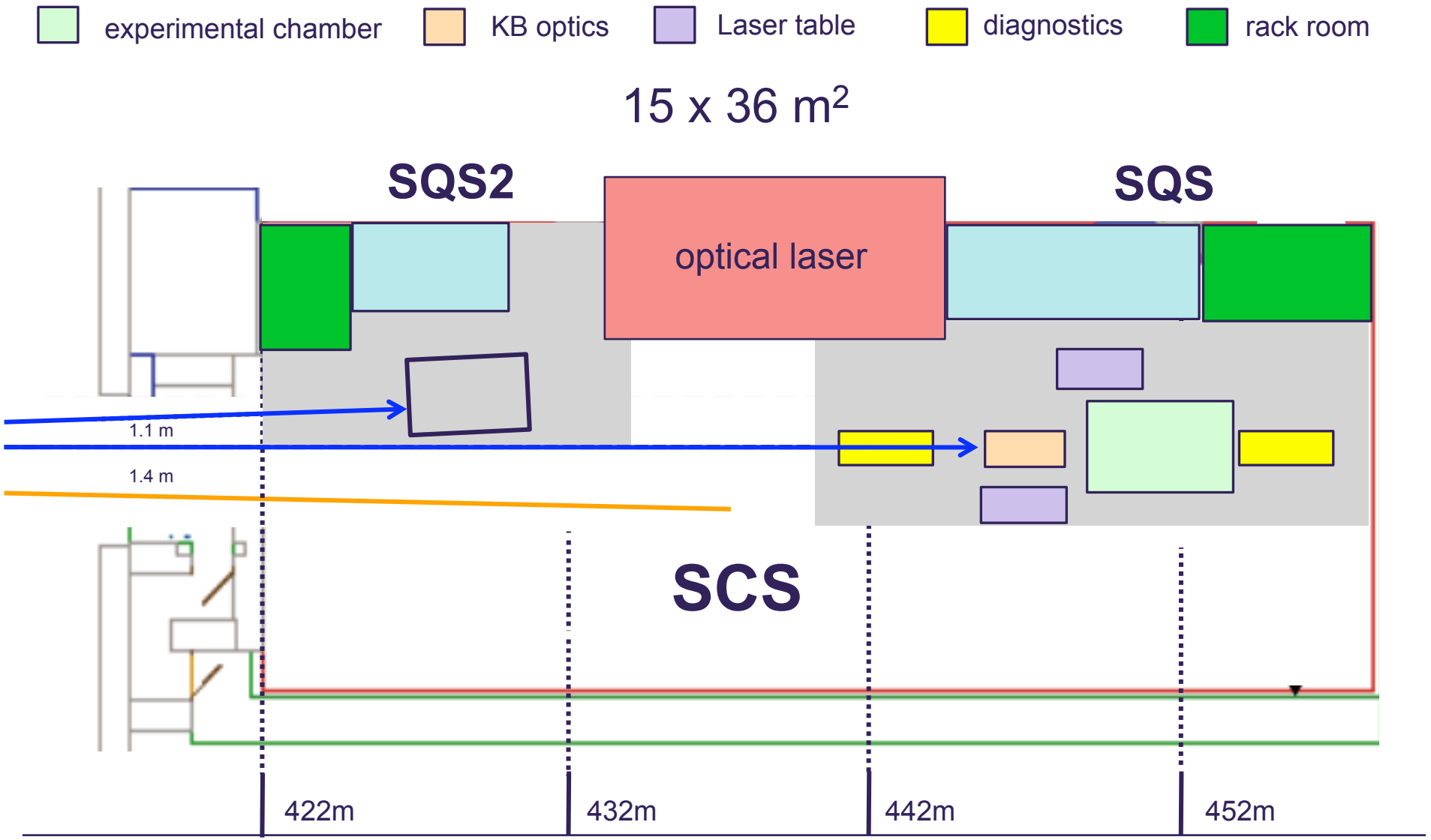


Key Detector Parameters

- Goal: Single photon sensitivity
  5 σ @1 keV and 4.5 MHz
- Energy range
  0.5 – 25 keV
  (0.5 – 4 keV optimized for)
- Dynamic range/pixel/pulse
  > 6000 photons @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
- 8 ladders built on quadrant
- 4 quadrants = 1k x 1k detector

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

Floor plan (SASE3)



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

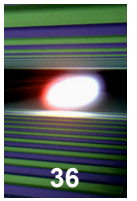
SQS Specific

- 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

European XFEL

Diagnostics (J. Grünert)



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

single shot / "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

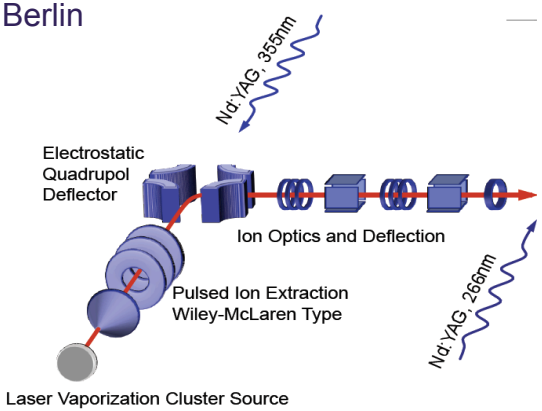
   YAG screens

European XFEL

Add-on Equipment

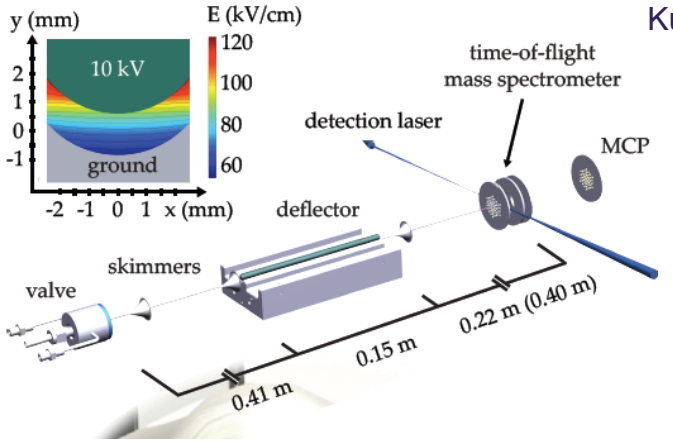
1) Mass selected Cluster Source

Meiwes-Broer, U Rostock
Möller, TU Berlin



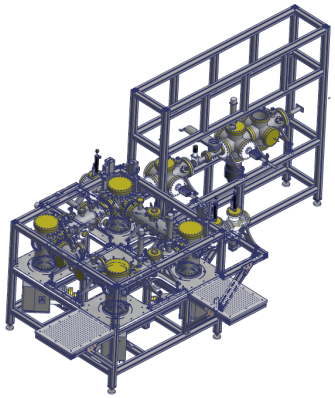
2) State-, size, and isomer-selected samples of polar molecules and clusters

Küpper FU Berlin



3) Ion storage ring

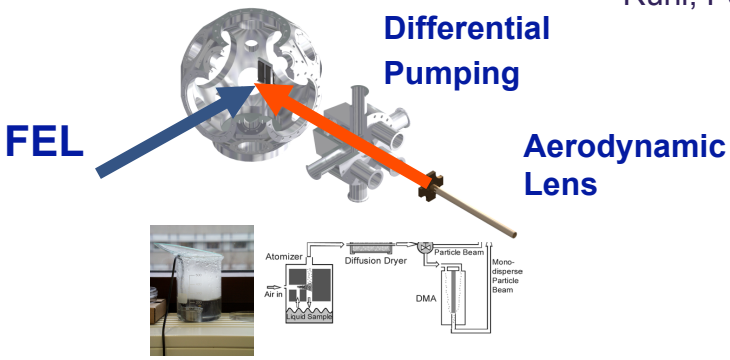
Pedersen (Aarhus)
Wolf (MPI Heidelberg)
Crespo (MPI Heidelberg)



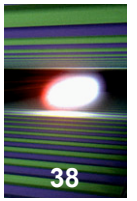
2.7 x 4.4 m²

4) Production of Nano-Particle beam

Rühl, FU Berlin



Timeline



SQS Instrument

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

Conceptual Design Report	April 2011
Technical Design Report	October 2012

SCS Instrument

Conceptual Design Report	Spring 2012
Technical Design Report	Spring 2013

Installation in experimental hall	mid 2014
Ready for beam	mid 2015

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!