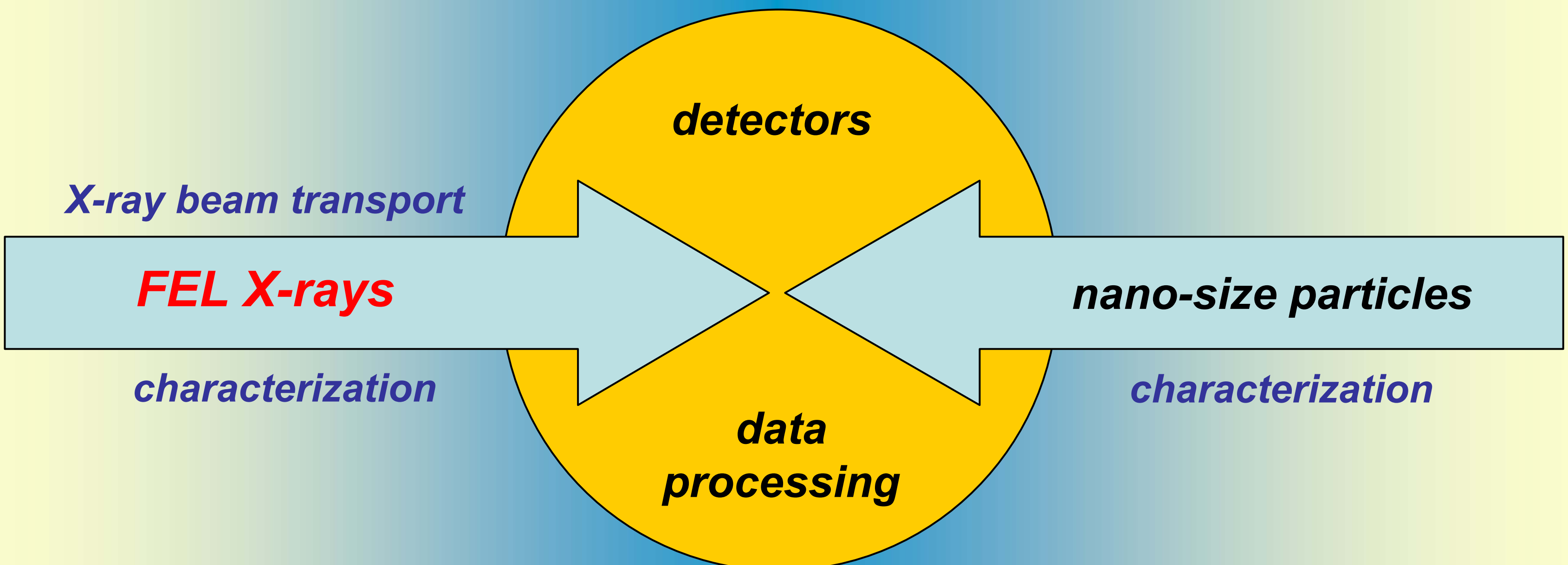
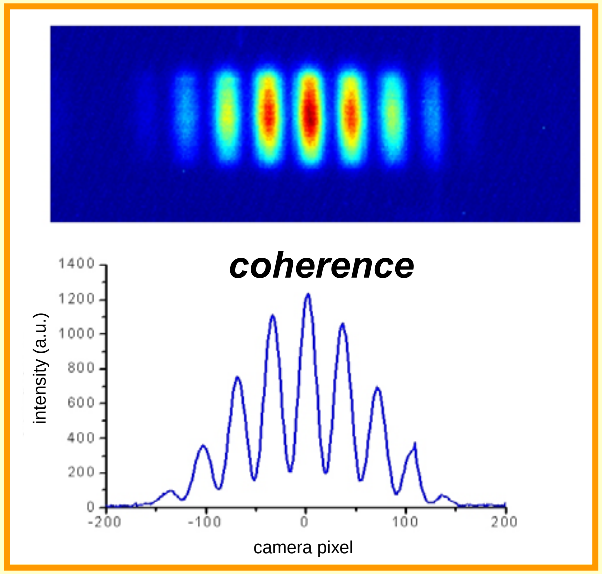
Science at

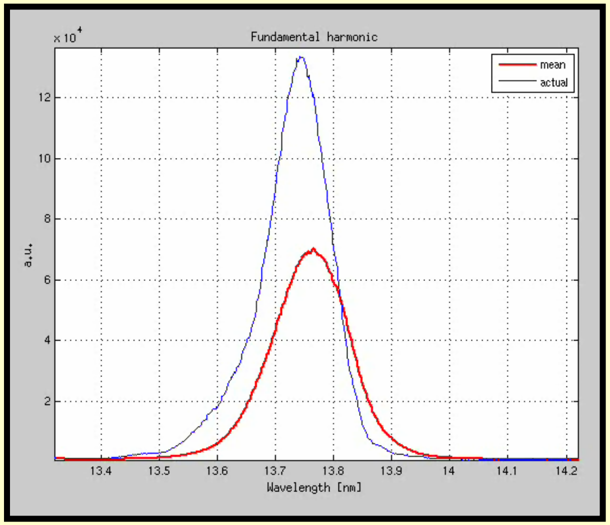
Single Pass X-ray FELs



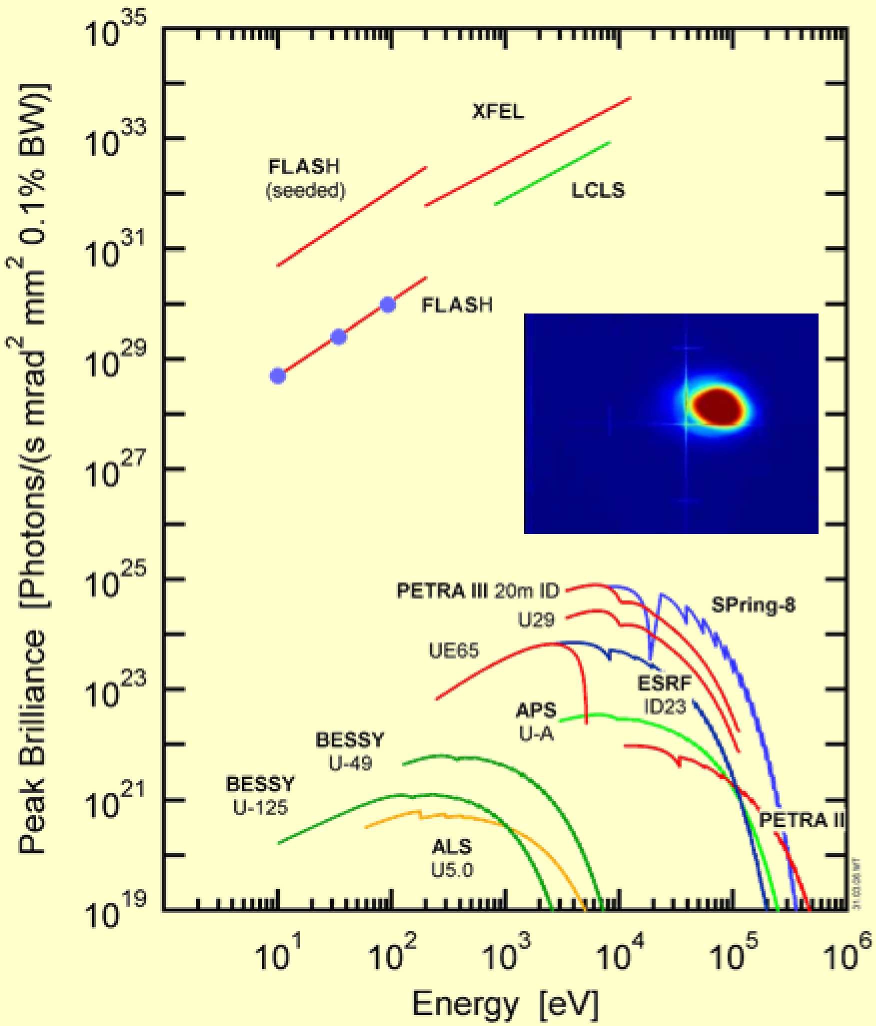
Jochen R. Schneider
DESY

SASE FEL: Shot by shot fluctuations



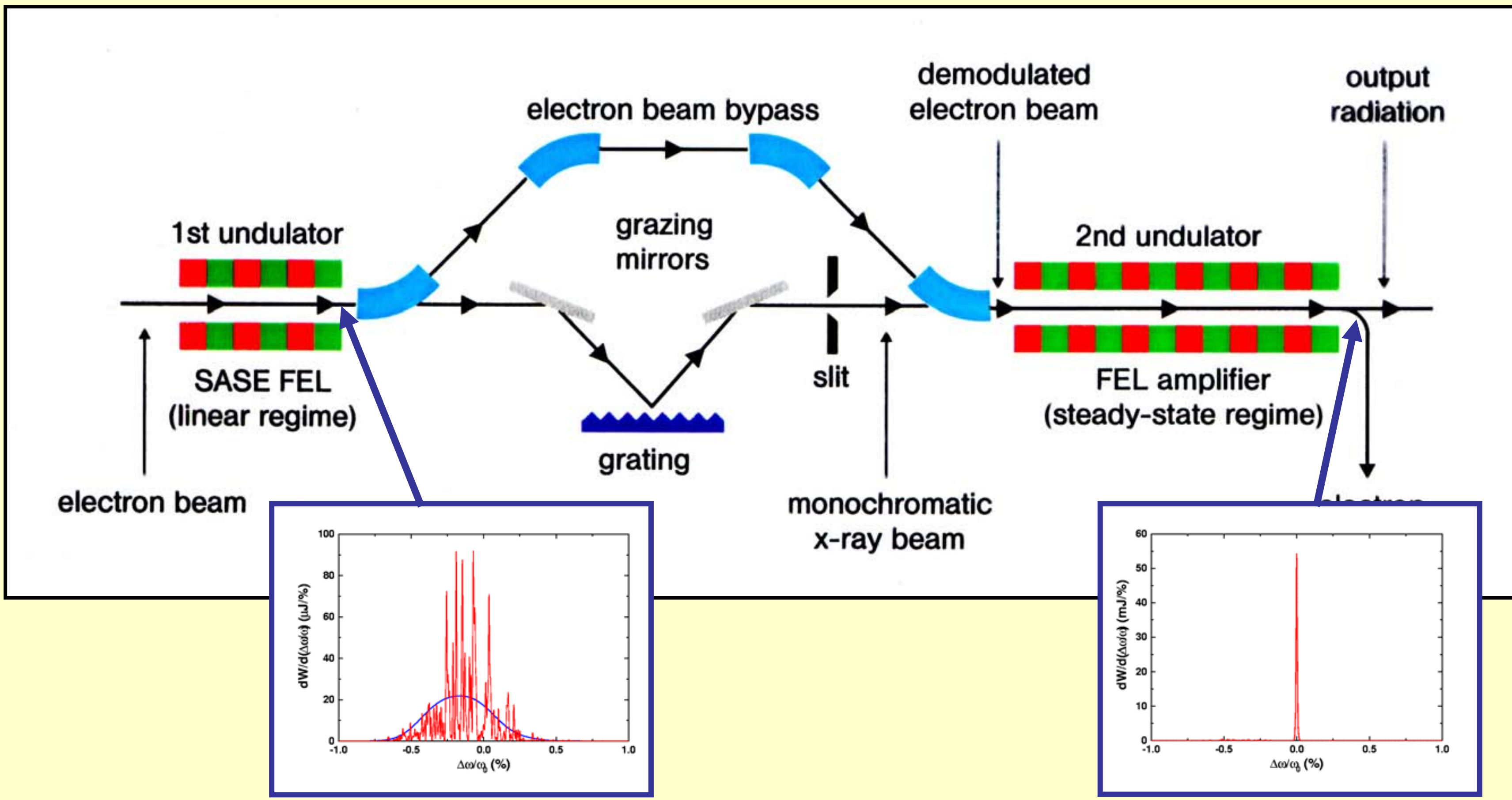


spectral distribution (13.7 nm, 90 eV)

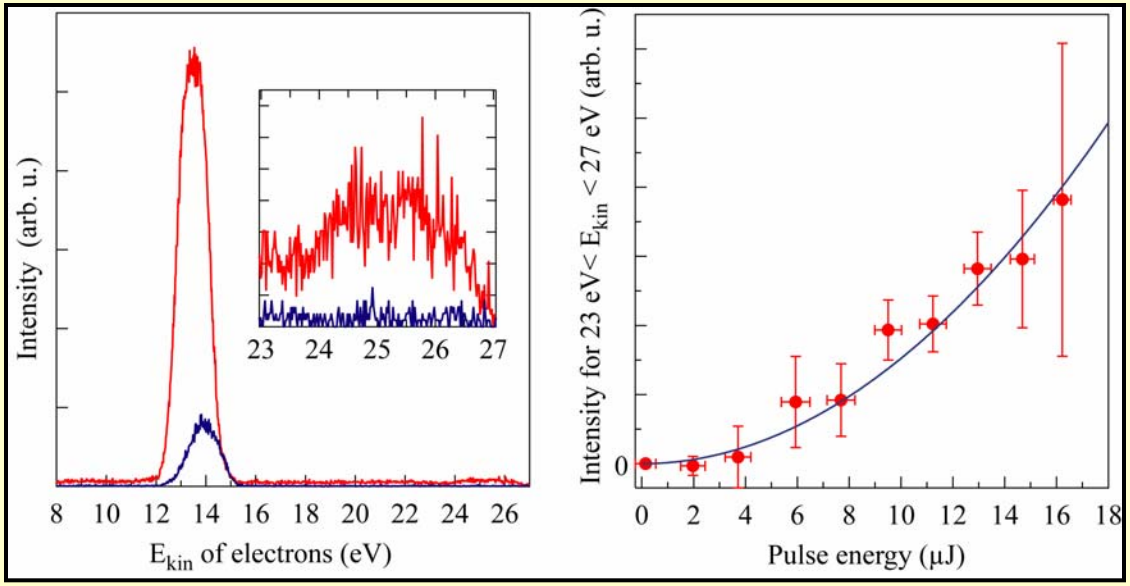


Improved beam properties by self-seeding

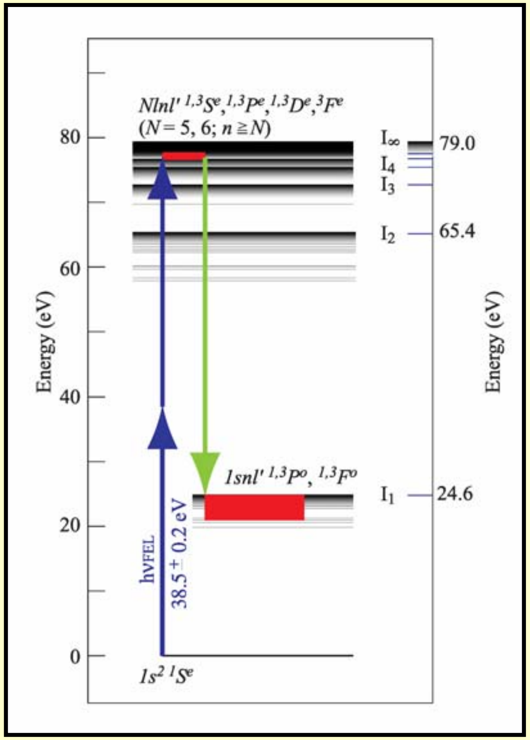
- *Transform-limited bandwidth*
- *Full longitudinal coherence*
- *Suppression of fluctuations*



Resonant two-photon absorption



$h\nu$ (FEL) = 38.5 eV



He^{+}: 24.587 eV
He^{2+}: 54.416 eV
He 1s – 2s: 19.8 eV

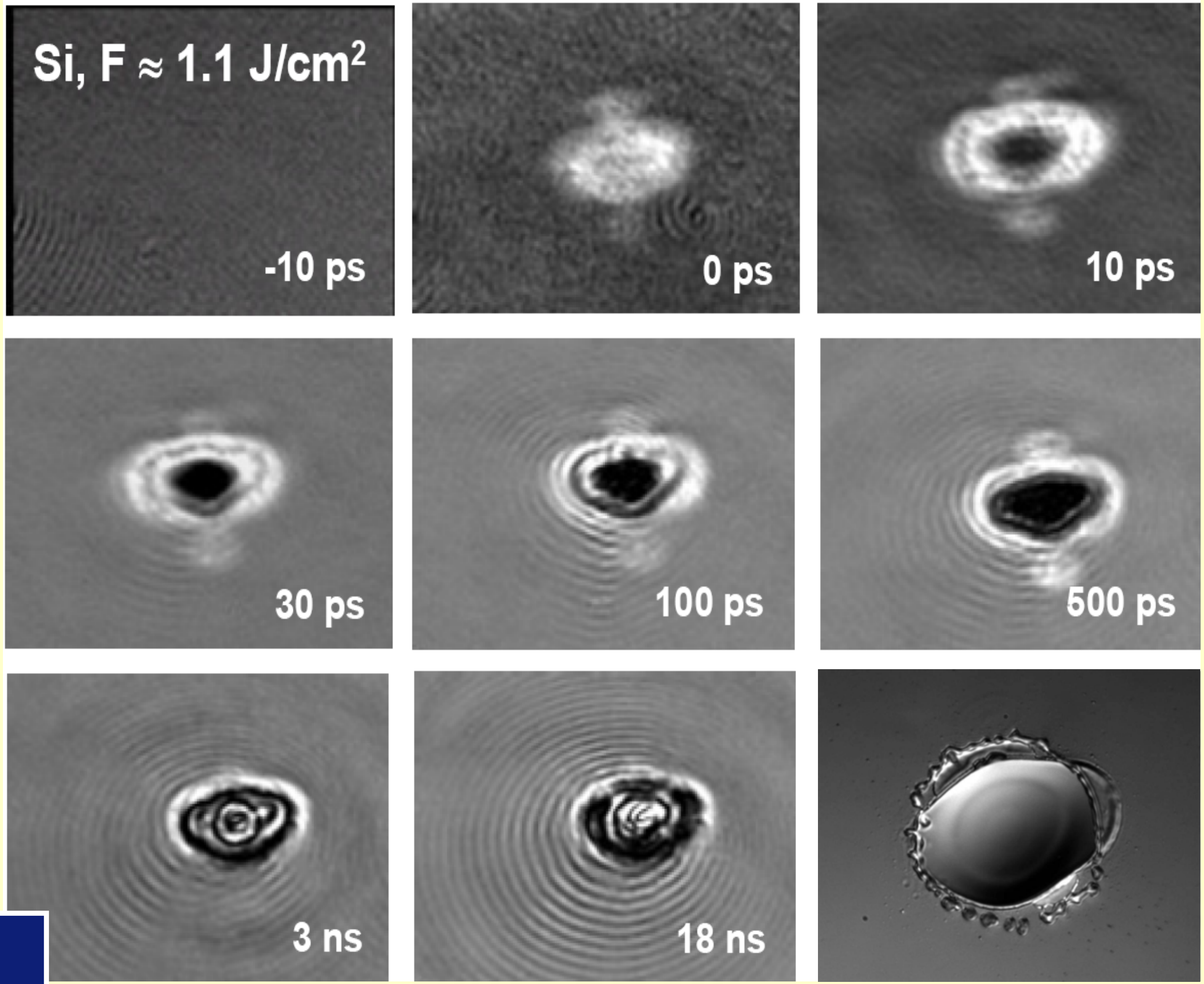
Evidence for non-sequential resonant two photon absorption

A. Föhlich, W. Wurth et al

Energy levels from: Zhen-sheng Yuan et al., Physical Review A **70**, 062706 (2004)

Results: Transient Reflectivity

time resolved microscopy



UNIVERSITÄT
DUISBURG
ESSEN

K. Sokolowski-Tinten et al.

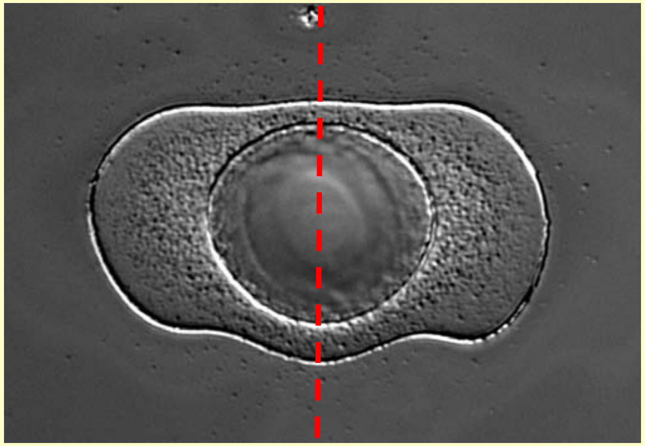
Results: surface morphology - GaAs

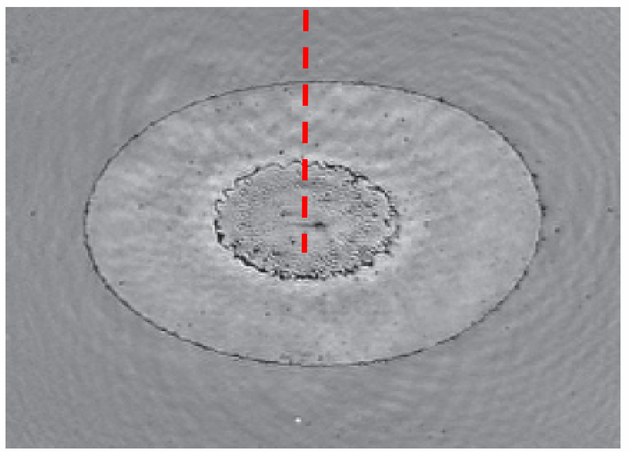
HELMHOLTZ GEMEINSCHAFT

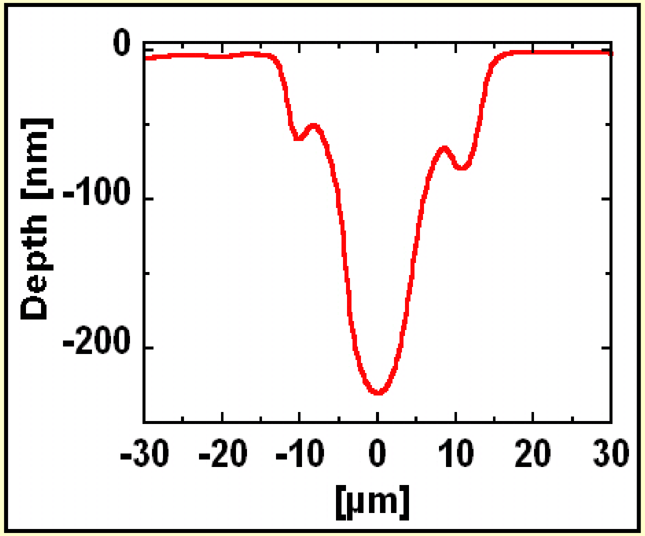
UNIVERSITÄT DUISBURG ESSEN

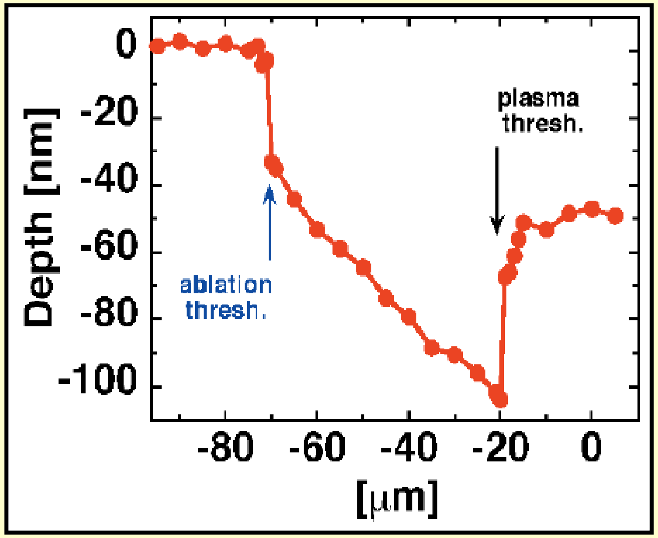
VUV-FEL

fs opt. laser



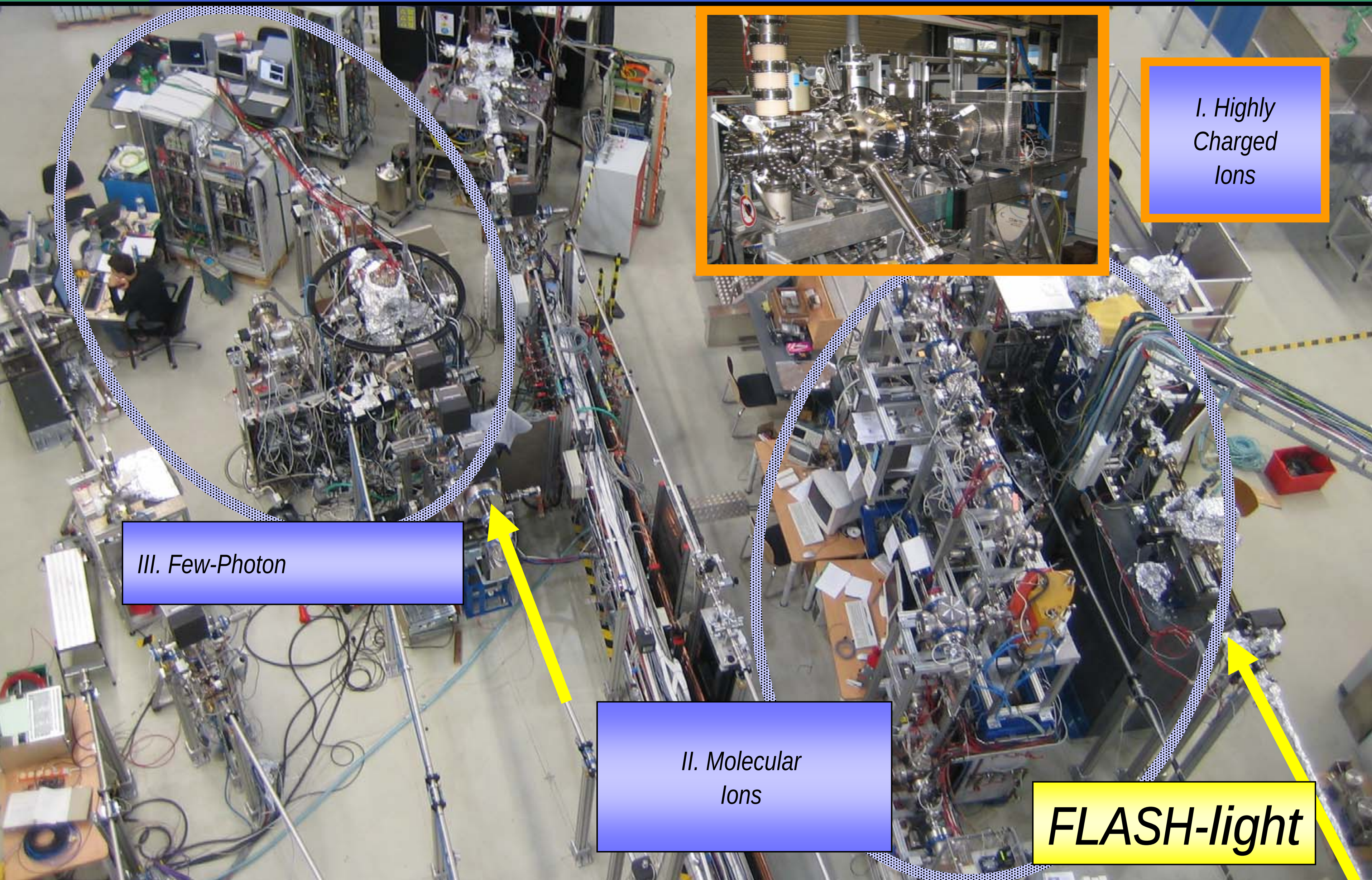






K. Sokolowski-Tinten et al.

MPI-K @ FLASH


I. Highly Charged Ions
II. Molecular Ions
III. Few-Photon
FLASH-light

Impact of studying highly charged ions

Highly charged ions (HCIs) play an essential role in high-temperature terrestrial plasmas, they are everywhere in the universe providing us with direct and unique information on the composition and state of matter of even the most distant known objects.

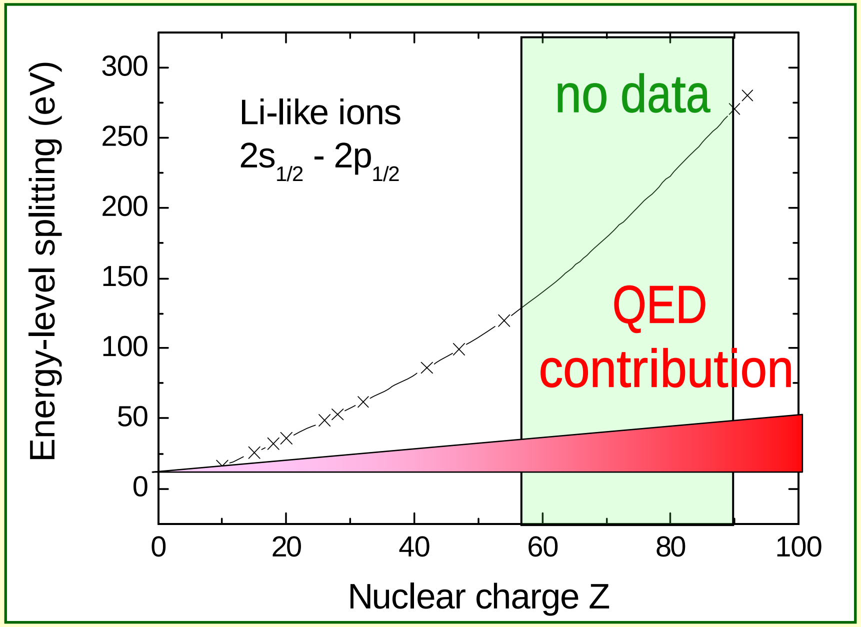
Besides their importance in plasma and astrophysics, HCI provide an ideal testing ground for forefront atomic structure theory.

The most important problem, is that leading one-photon exchange contributions from bound state quantum electro dynamics (QED) not only scale with about the fourth power of the nuclear charge Z, but moreover, cannot be calculated in a perturbative way since the expansion parameter $Z\alpha$, with α=1/137 being the fine-structure constant, approaches almost unity for uranium.

Epp, Crespo López-Urrutia, Brenner, Mäckel, Ullrich et al.

Highly charged ions: Testing QED

***Highly charged ions (HCIs)** play an essential role in high-temperature terrestrial plasmas, they are everywhere in the universe providing us with direct and unique information on the composition and state of matter of even the most distant known objects.*



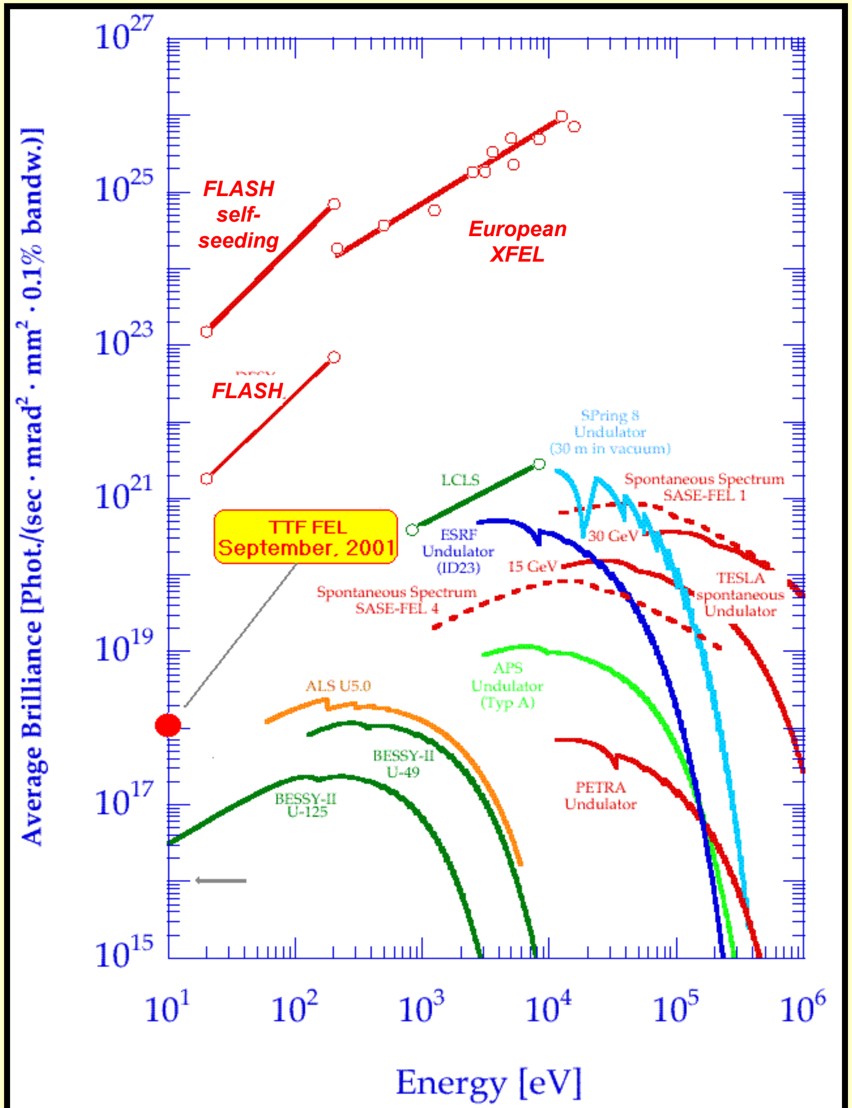
- ***typical present accuracy:*** $\Delta\lambda/\lambda = 10^{-3}$-$10^{-4}$

- ***FLASH:*** $\Delta\lambda/\lambda = 10^{-5}$-$10^{-6}$

- ***high average brilliance needed***

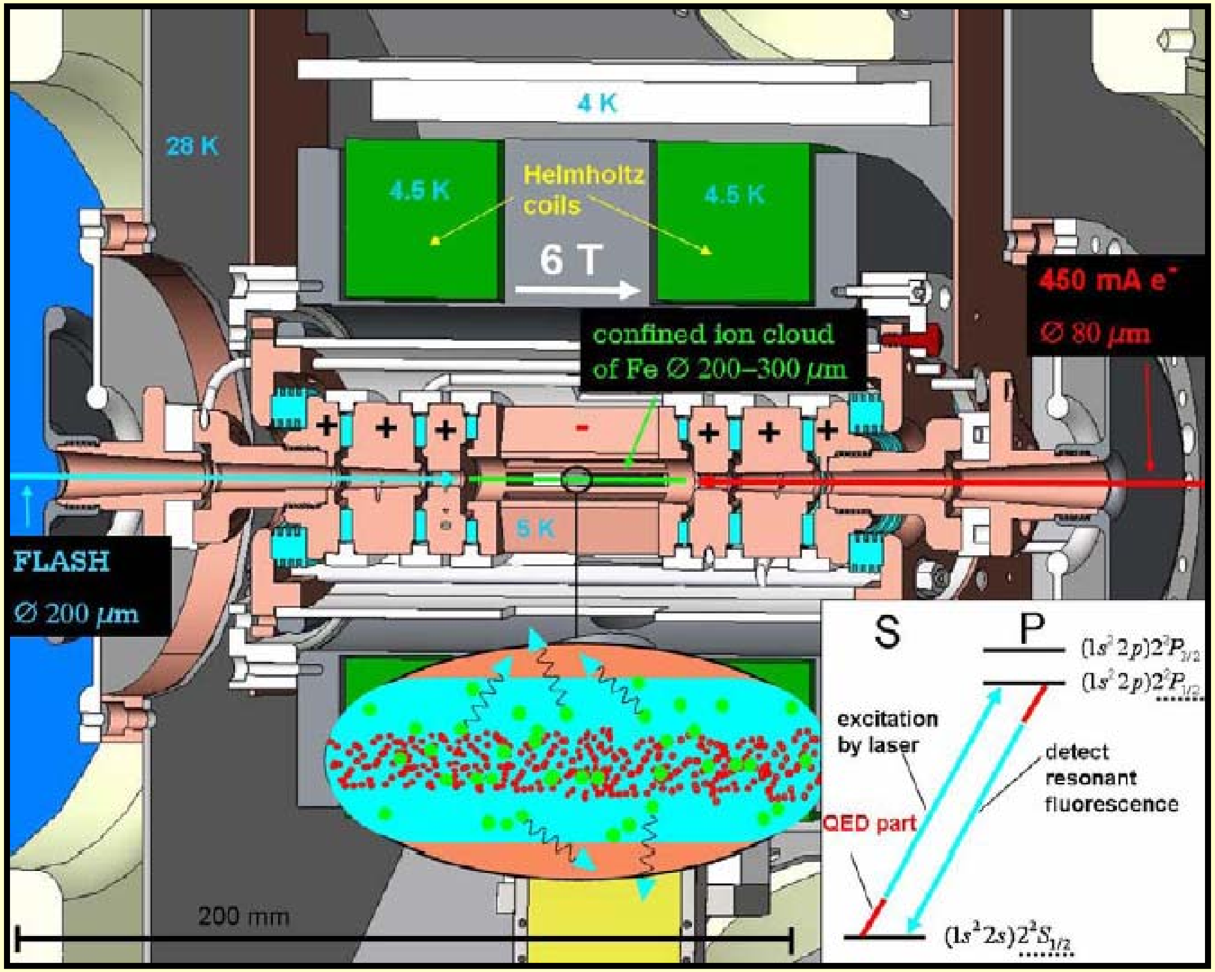
Epp, Crespo López-Urrutia, Brenner, Mäckel, Ullrich et al.

FEL average brilliance



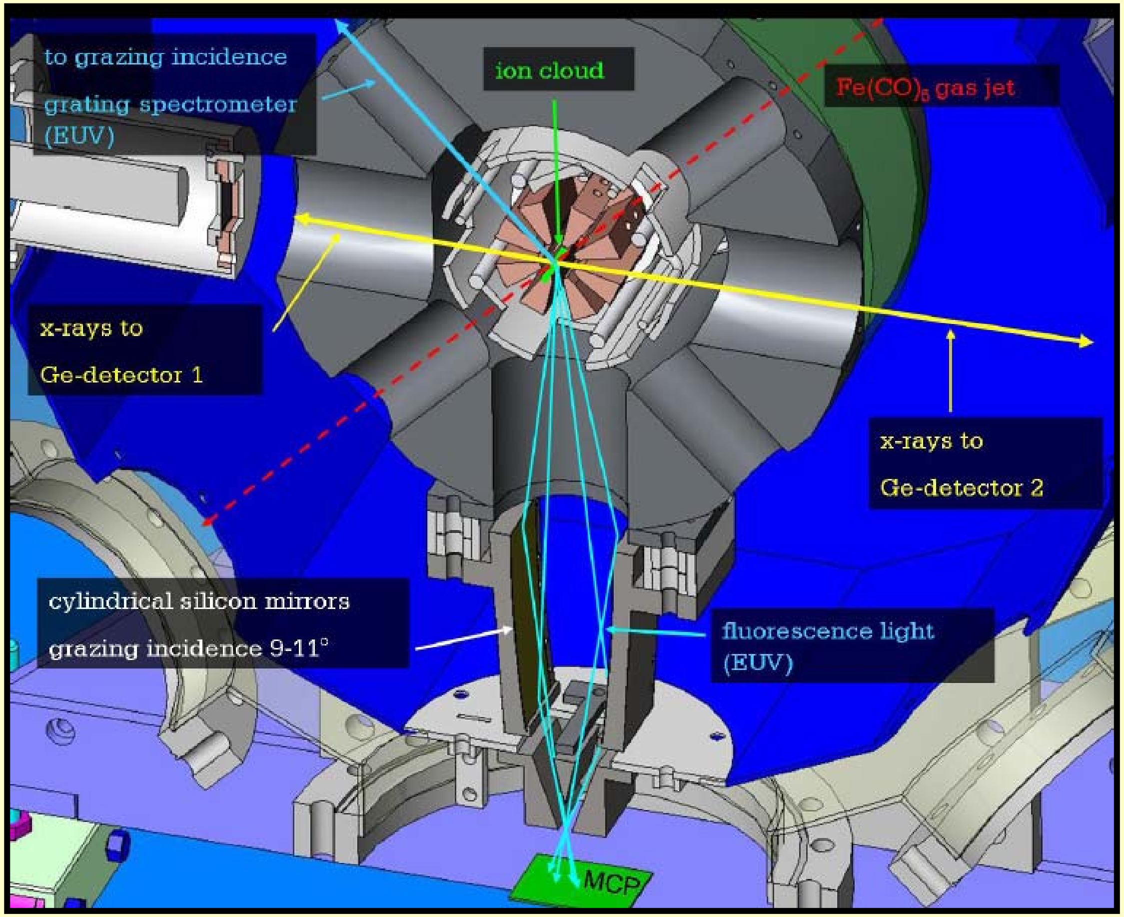
Max-Planck-Institut für Kernphysik

Electron beam ion trap (EBIT)



Epp, Crespo López-Urrutia, Brenner, Mäckel, Ullrich et al.

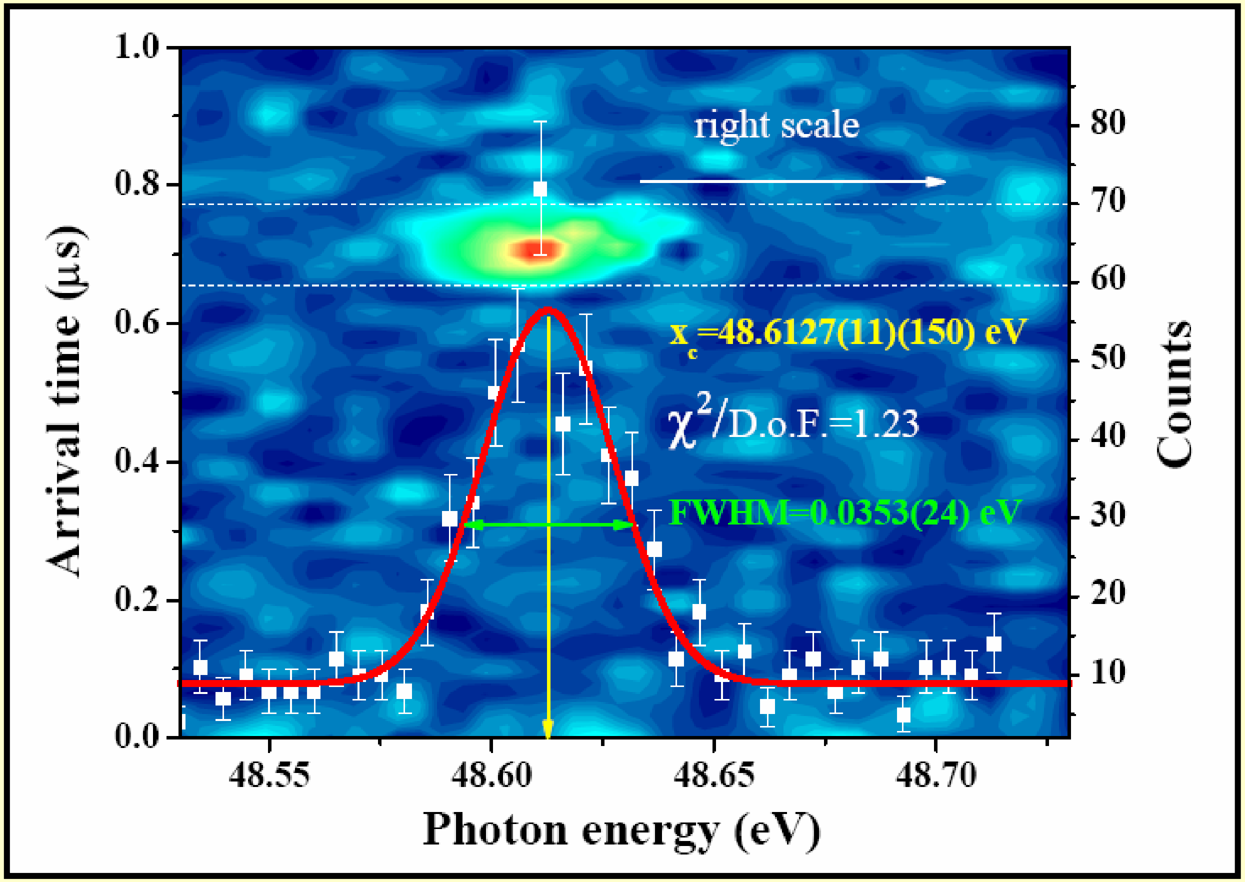
EBIT trap region



Transverse cross section of the EBIT trap region illustrating the various ports dedicated to X-ray detection with two Ge-detectors as well as the grazing incidence flat-grating spectrometer for the VUV and the atomic beam injection

Epp, Crespo López-Urrutia, Brenner, Mäckel, Ullrich et al.

2 $^2S_{1/2}$ to 2 $^2P_{1/2}$ line of Li-like Fe^{23+} at 48 eV



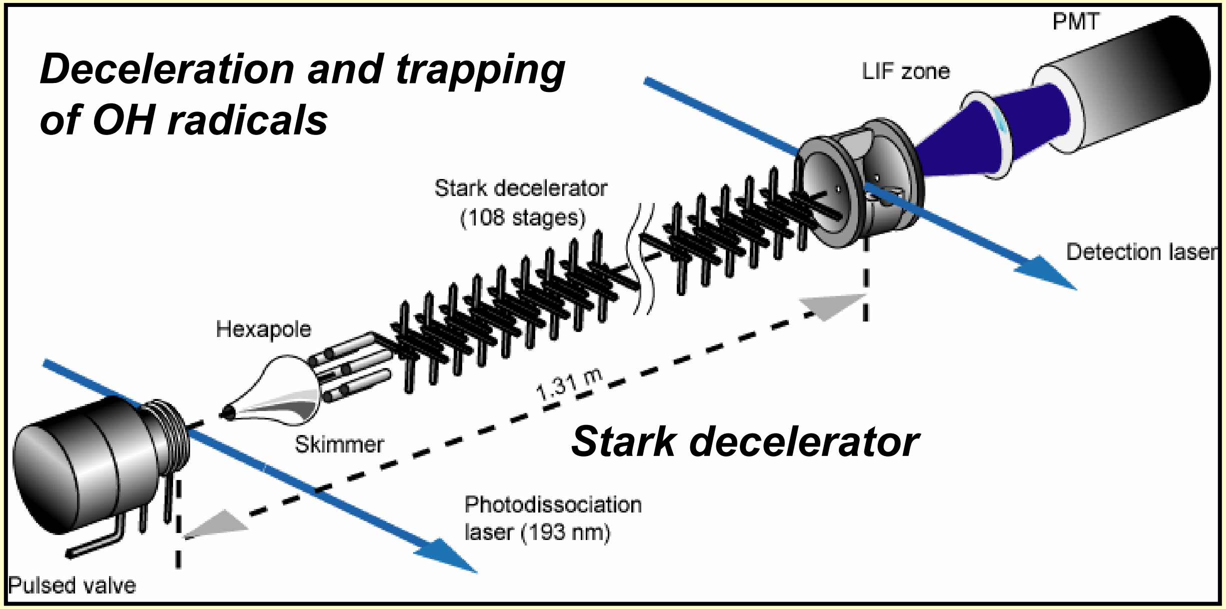
Δt=1987 sec

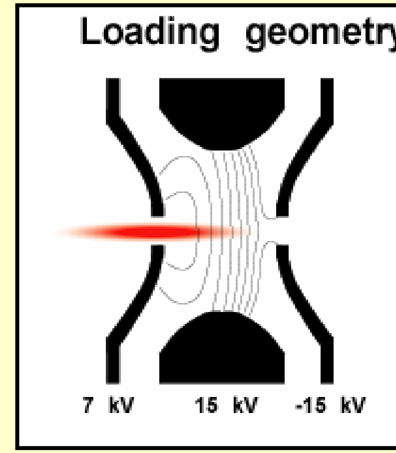
2D plot of the fluorescence signal as a function of the photon arrival time relative to the FEL pulse.

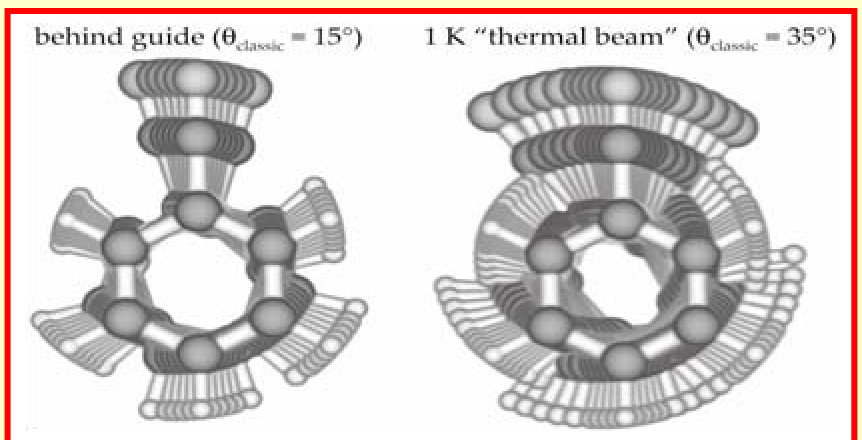
Inset: Projection of the 2D representation onto the energy axis yielding the number of photons (white squares) per 5 meV photon energy interval as a function of photon energy

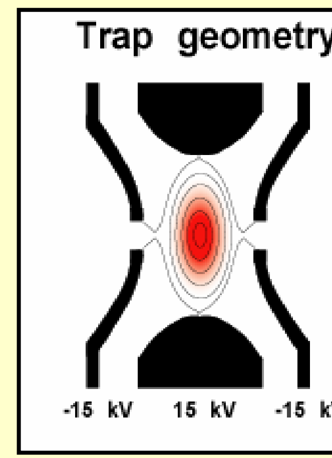
Epp, Crespo López-Urrutia, Brenner, Mäckel, Ullrich et al.

Producing samples of trapped cold molecules









Nature 406 (2000) 491

10^4-10^5 oriented molecules in a volume of 2x2x25 mm^3

Trapped cold molecules

The merging of molecular beam methods and accelerator physics methods has yielded new tools to produce samples of state-selected and spatially oriented, ground-state molecules at mK temperatures.

- ***ND_3 molecules and OH radicals have been trapped at densities of 10^7-10^8/cm3 and at temperatures of 1-50 mK.***
- ***An AC electric trap for ground-state molecules has been demonstrated.***
- ***Trapped molecules have been used to measure the lifetime of metastable states. Decelerated beams have been used for high-resolution spectroscopy. Near-threshold inelastic scattering experiments using molecular beams with a tunable velocity have been demonstrated.***

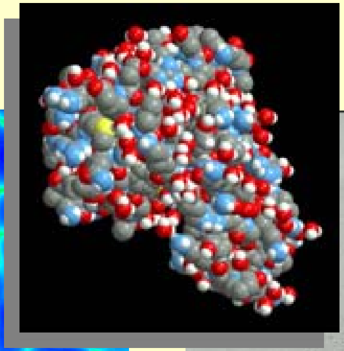
G. Meijer et al

Fritz-Haber-Institut der Max-Planck-Gesellschaft

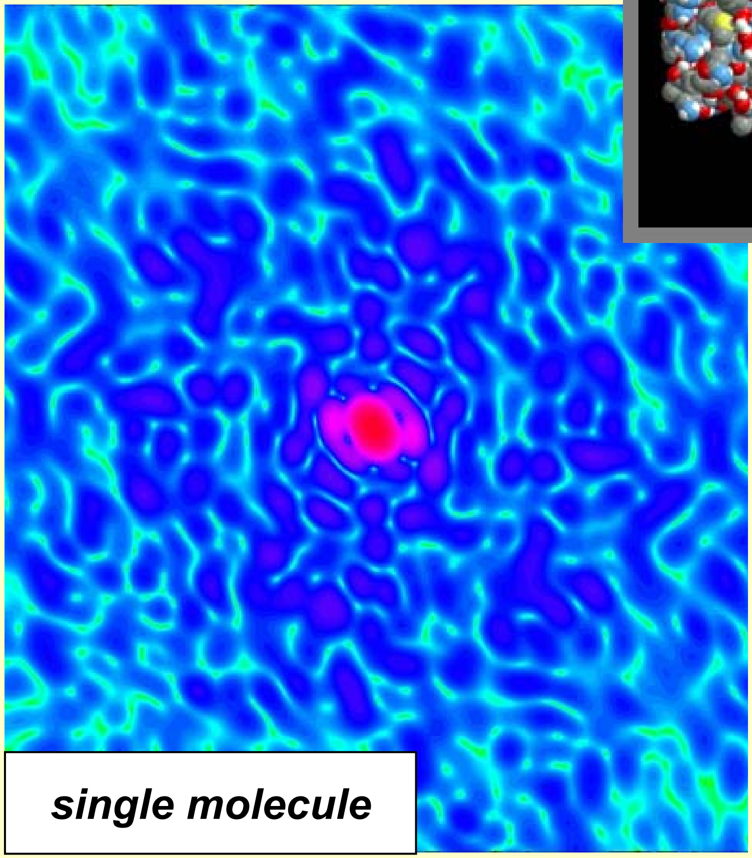
Reviews: ***Int. Rev. Phys. Chem. 22 (2003) 73***
Adv. in At., Mol., and Opt. Phys. 52 (2005) 209
Ann. Rev. Phys. Chem. 57 (2006) 159
Phys. Chem. Chem. Phys. 8 (2006) 2666

Imaging of a single bio-molecule

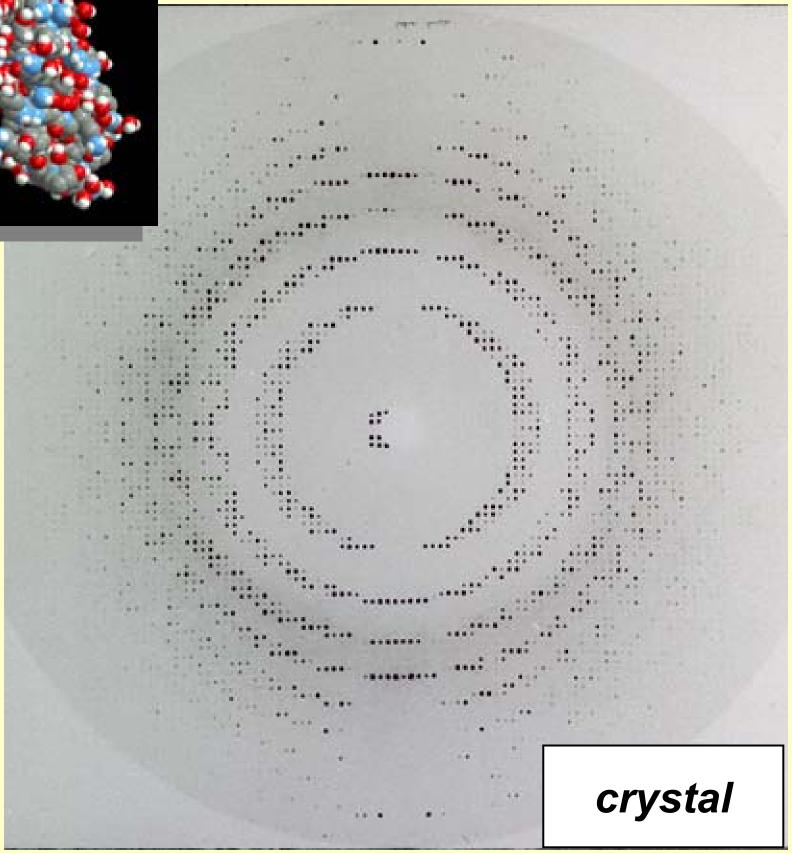
with atomic resolution



Lysozym



single molecule

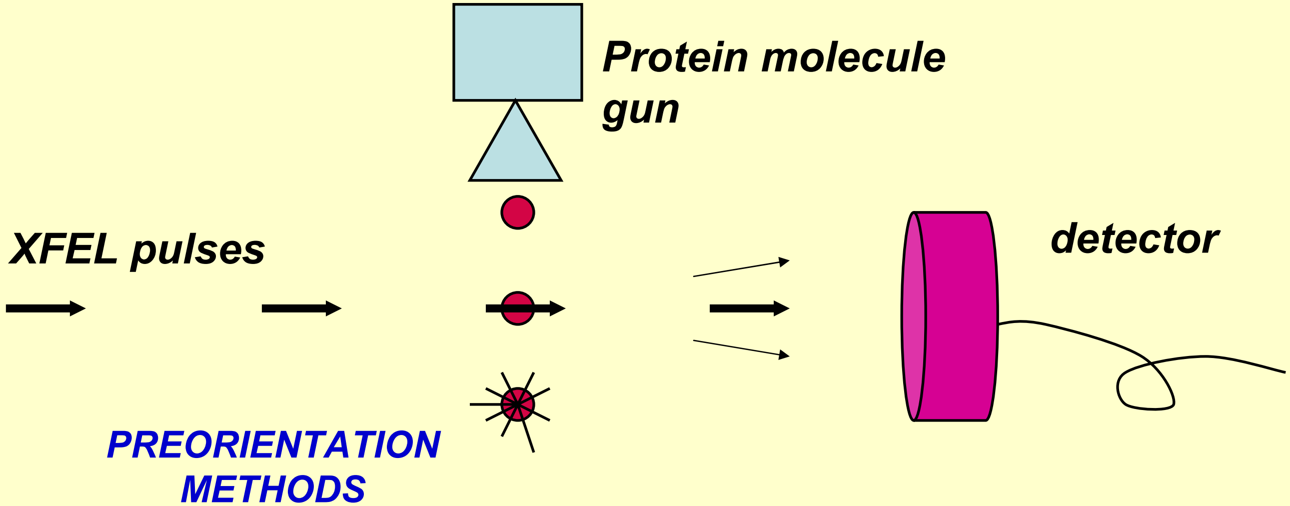


crystal

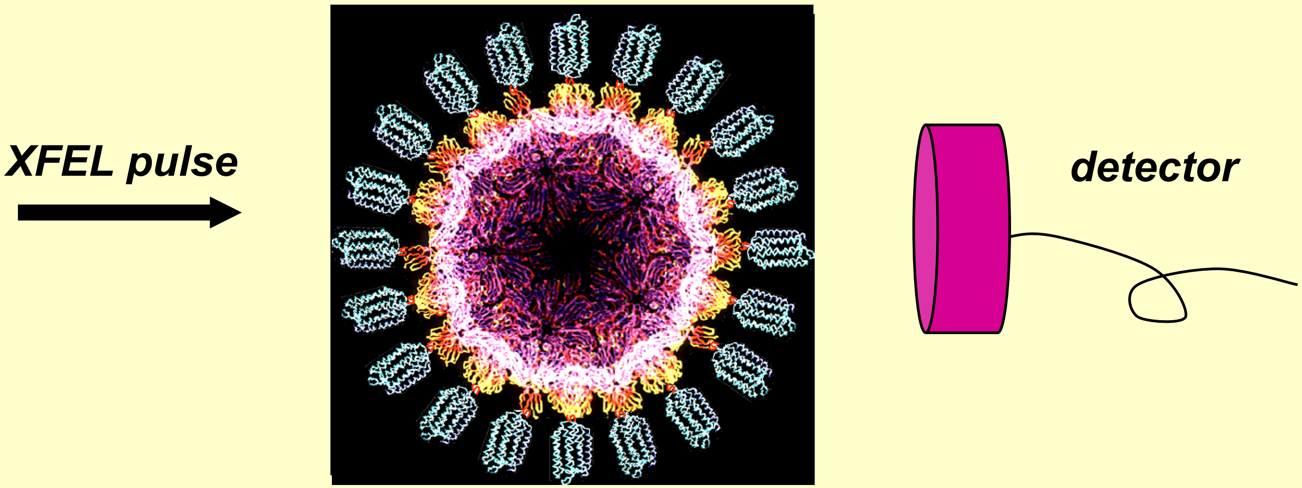
Oversampling: J. Miao, K.O. Hodgson and D. Sayre, *PNAS* 98 (2001) 6641-6645

Determination of 3D structure will require multiple samples and multiple orientations

Serial method



Parallel method



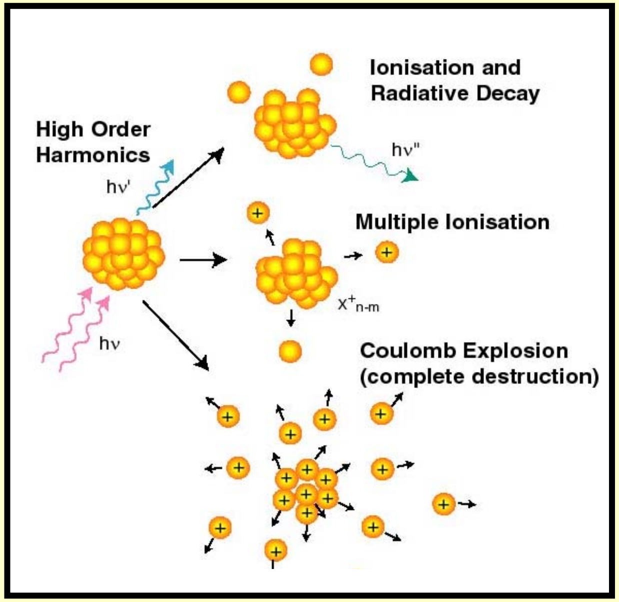
Protein molecules arranged in a regular nanocluster

courtesy J. Hajdu

Interaction of intense soft X-rays with atomic and molecular clusters

T. Möller, C. Bostedt, E. Eremina, M. Hoener, H. Thomas (TU-Berlin)
T. Fennel, K.-H. Meiwes-Broer (Universität Rostock)
E. Plönjes, M. Kuhlmann, H. Wabnitz (DESY)
T. Laarman (MBI-Berlin)
A.Rubens B. de Castro (LNLS, Campinas Brasil)

Goal: ***Understanding the interaction of high intensity, short-wavelength, short-pulse radiation with matter which is essential for future FEL experiments.***

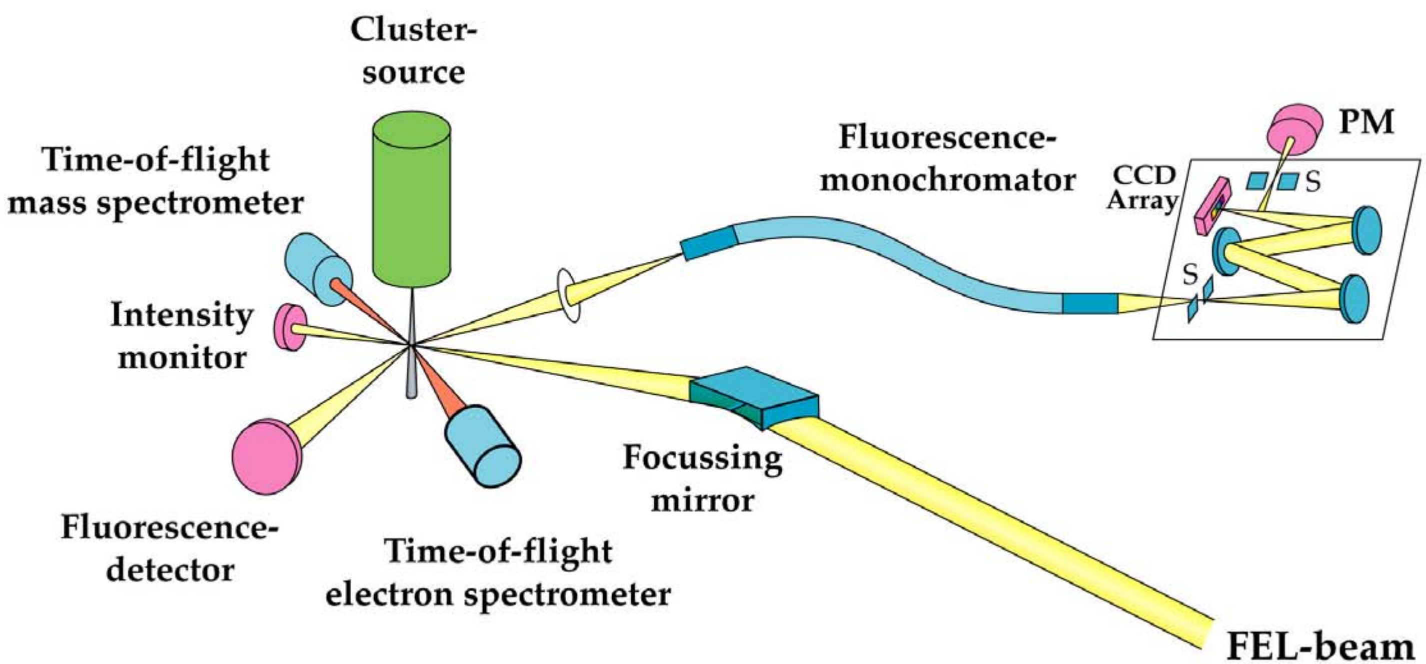


Example: Photo dissociation

Questions asked:

- *which multi-photon processes are observed*
- *cross sections (surface, bulk)*
- *which ions are prepared (charge state, electronically excited states)*
- *life time of intermediate states*
- *high-order harmonic generation*

First FEL Cluster Experiment at 100 nm



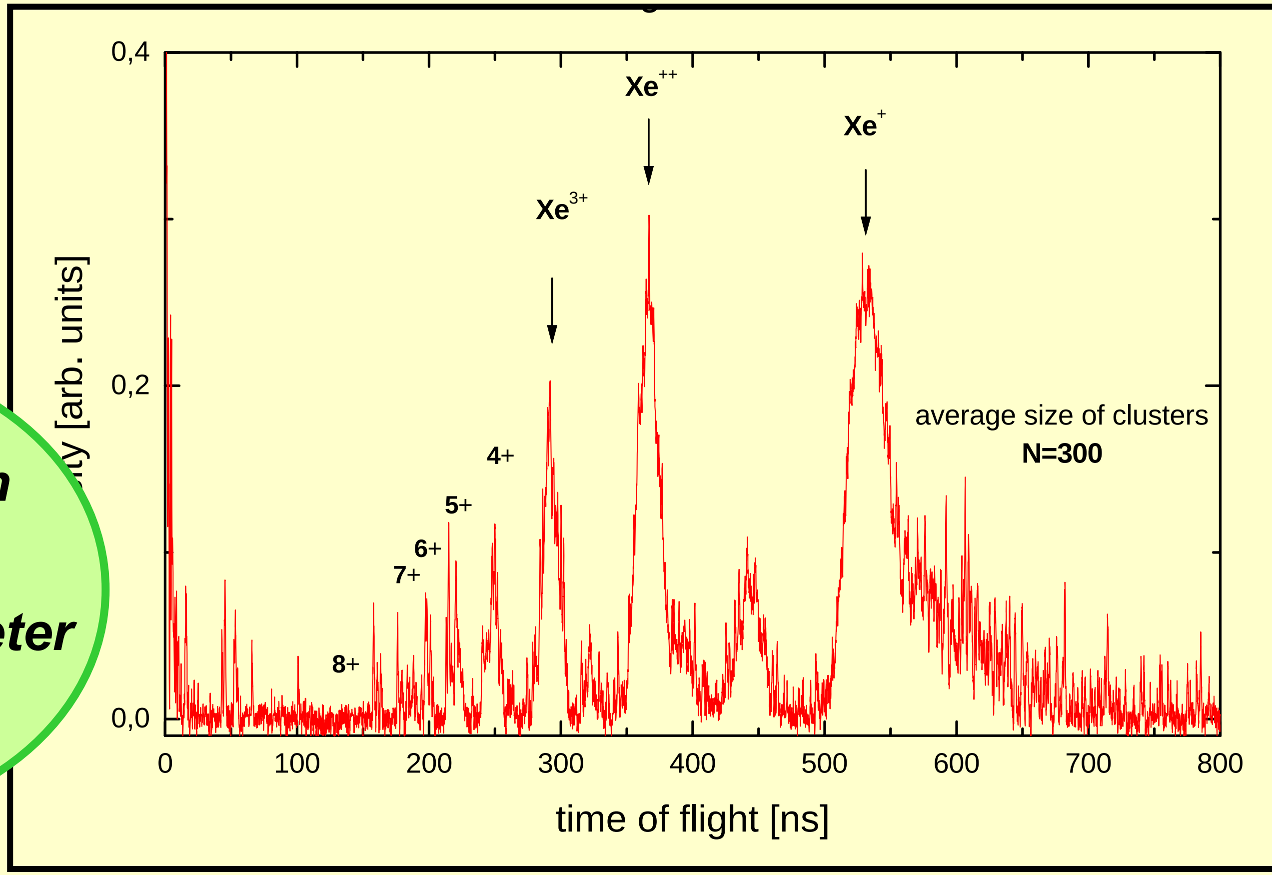
H. Wabnitz et al., Nature 420, 482 (2002)

Single shot time-of-flight spectrum

H. Wabnitz et al., Nature 420, 482 (2002)

$Ip_{Xe} = 12.1$ eV

$E_{phot} = 12.8$ eV

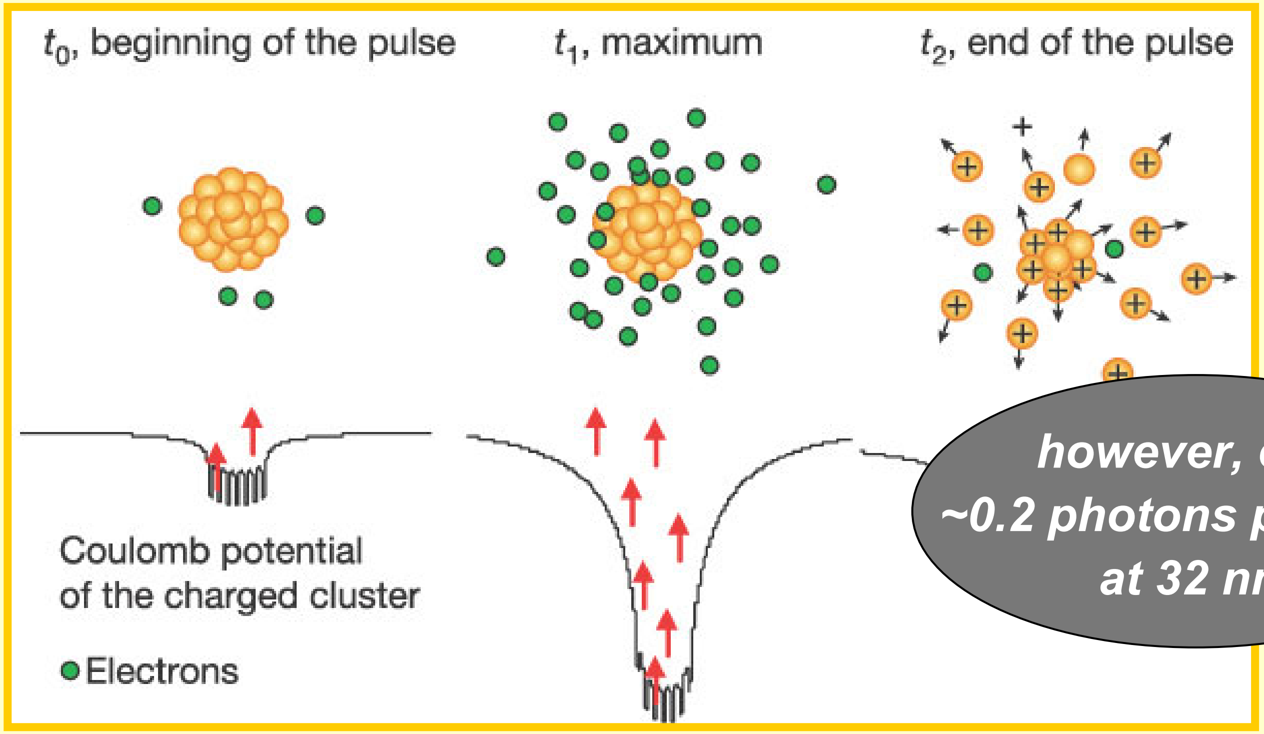


10^{13} photons in ~50 fsec in a 20 µm diameter focal spot

Coulomb explosion of Xenon clusters with ~ 300 atoms

Coulomb explosion of clusters

multi-photon absorption at 100 nm



however, only ~0.2 photons per atom at 32 nm

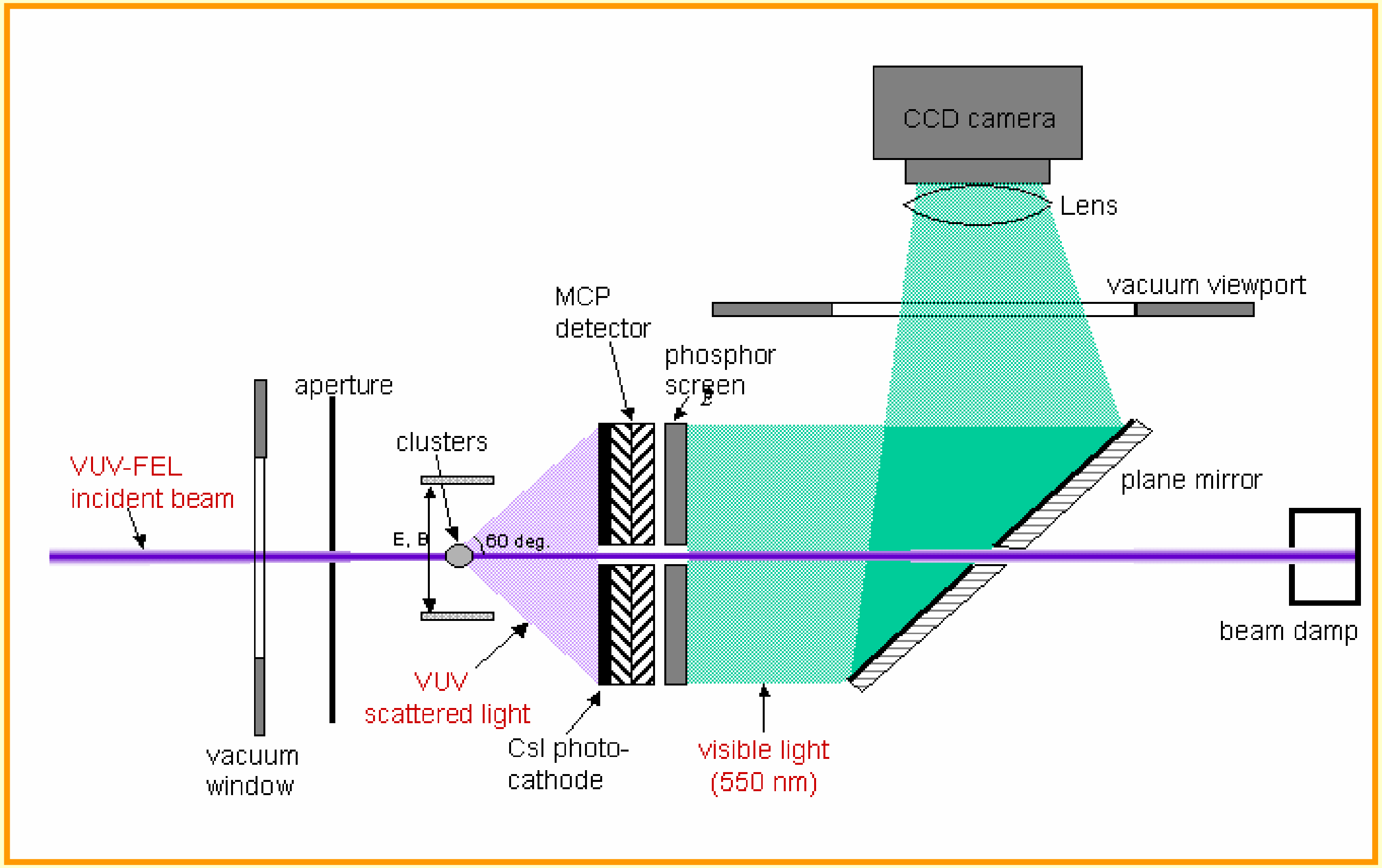
Absorption of ~40 photons per atom

Plasma absorption and thermionic effects are considered the dominant processes like for IR and visible light.

Th. Moeller et al.

Imaging of nano-particles in the gas phase by single shot diffraction

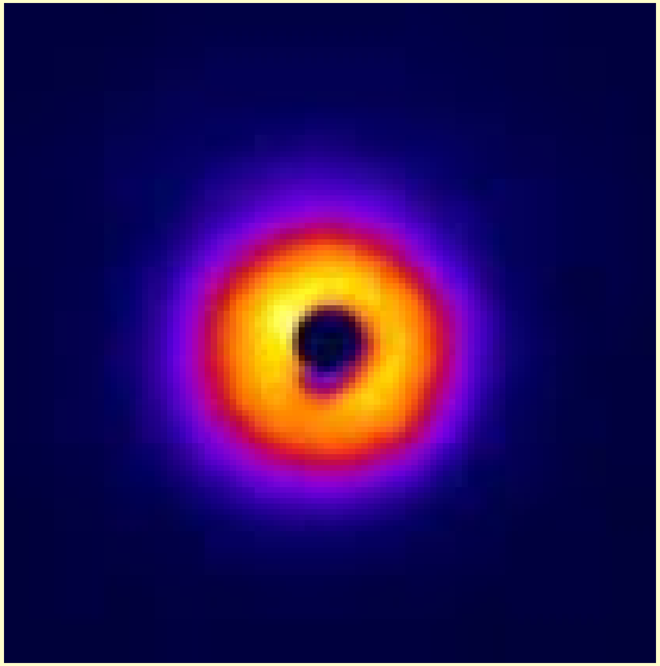
From time of flight mass spectra one concludes that the ions ejected from the cluster move with about 104 m/s, i.e. ions move ~ 3 Å in 30 fs and clusters stay essentially intact during exposure time.

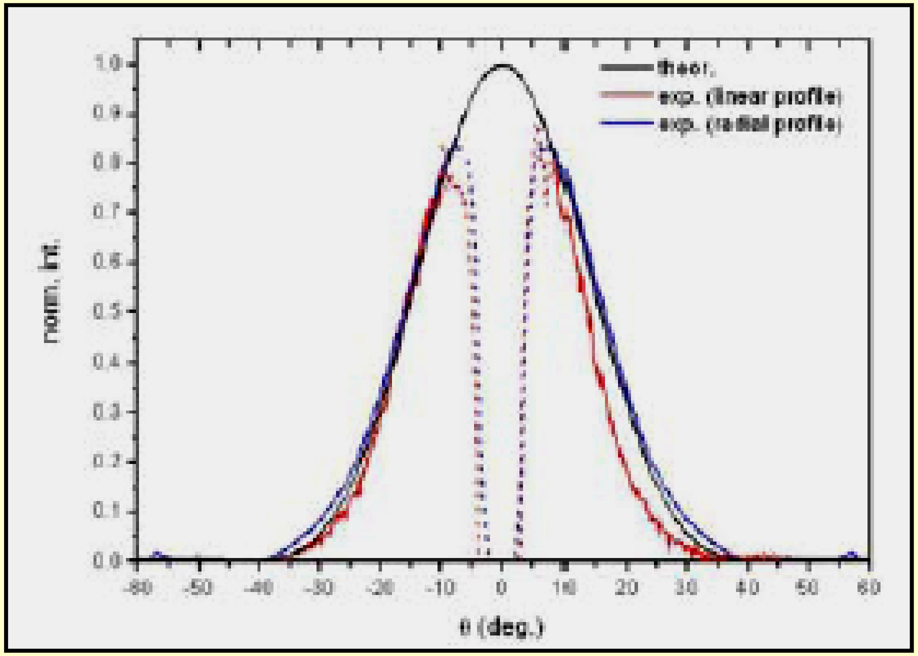


T. Möller et al.

Imaging of nano-particles in the gas phase by single shot diffraction

From the width of the intensity distribution of the scattered light the cluster radius is determined to range between 15 – 60 nm with an error of less than 10 nm. For the lowest nozzle temperatures the radius of the clusters is about two times larger than predicted by thermodynamic scaling laws.

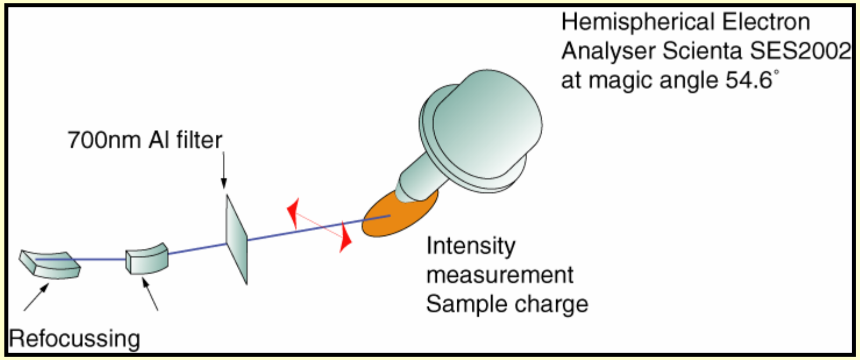




The intensity of the FEL beam was sufficient to record scattering patterns when the FEL beam was attenuated to 1%. Therefore time resolved studies with pump and probe techniques making use of the first and the third harmonic of the FEL will be possible.

Möller et al

Single Shot Photoemission

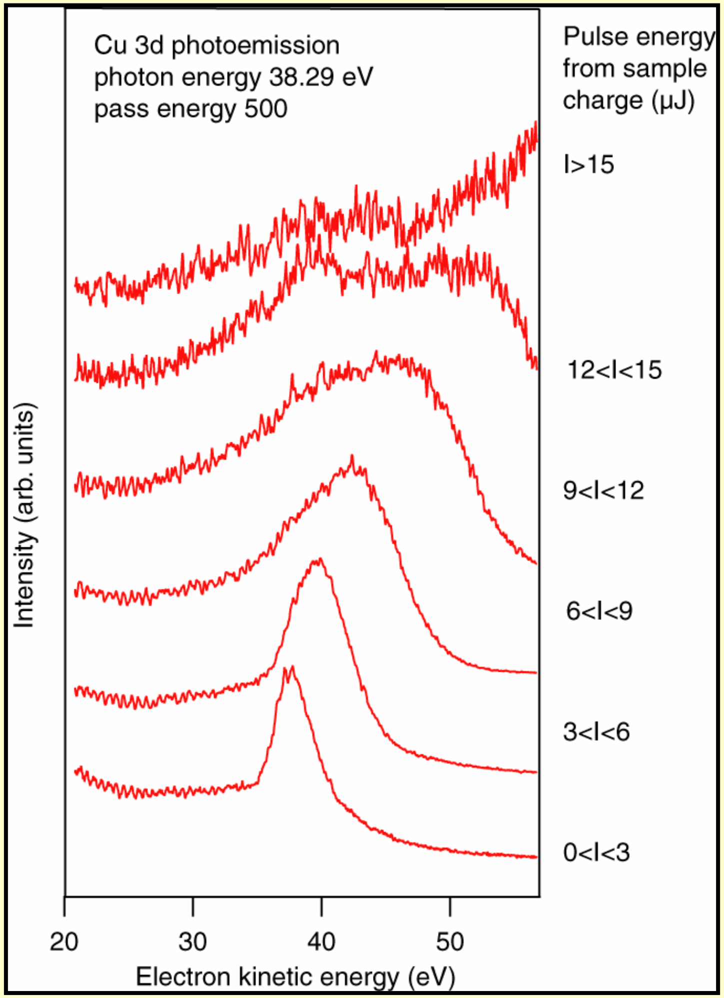


Towards single shot time resolved pump–probe spectroscopy for non-reversible dynamics.

At high peak brilliance space charge limitations.

Towards novel spectroscopic tools:

Resonant inelastic X–ray scattering (RIXS) of excited, non–equilibrium states.



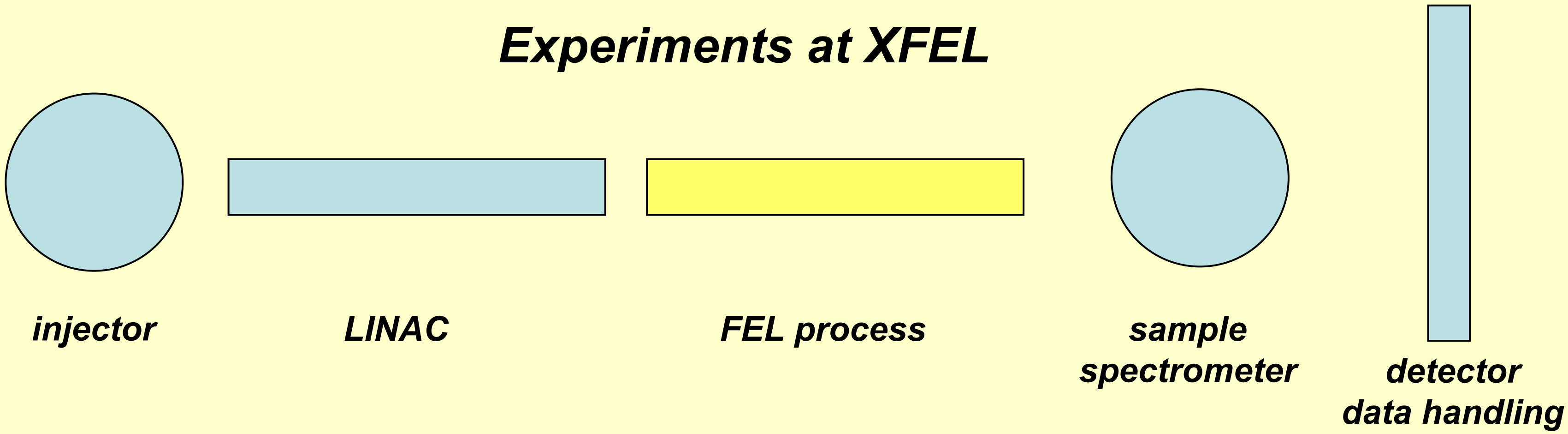
Cu subshell photoionization cross section at 38.29 eV:
3d: 9.934 Mb/atom 4s: 0.041 Mb/atom

UH

A. Pietzsch, A. Föhlisch, M. Nagasono, W. Wurth

Challenges for Science at FEL Facilities

Experiments at XFEL



FLASH

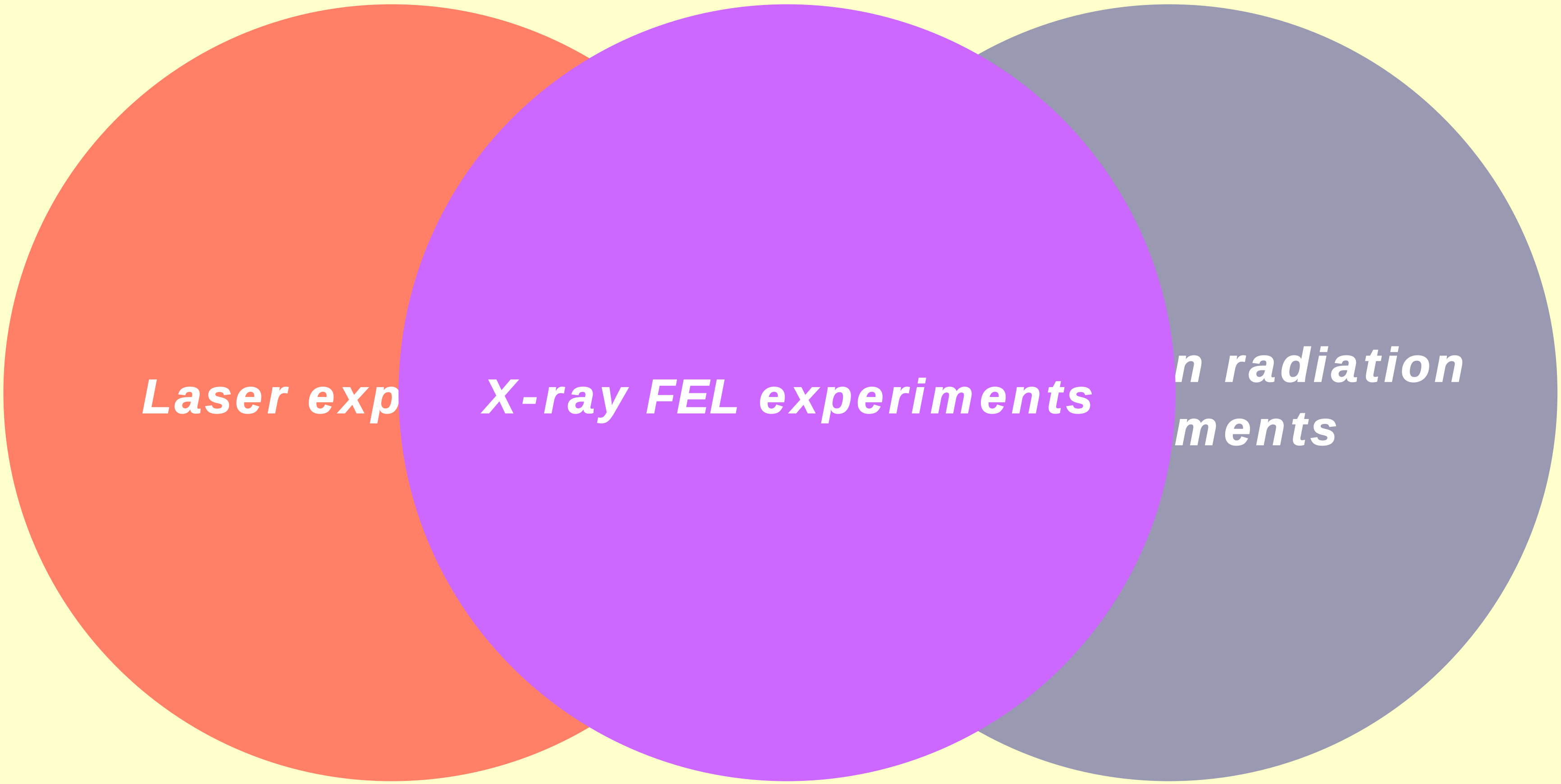
LCLS

SCSS

European XFEL

- *FEL process: pulse shaping*
- *e- and photon beam diagnostics, synchronization*
- *mechanical stability (10 fs ↔ 3 μm)*
- *interaction of FEL beam with matter*
- *sample preparation*
- *sample environment (pump lasers, synchronization)*
- *detector development*
- *data processing and analysis*

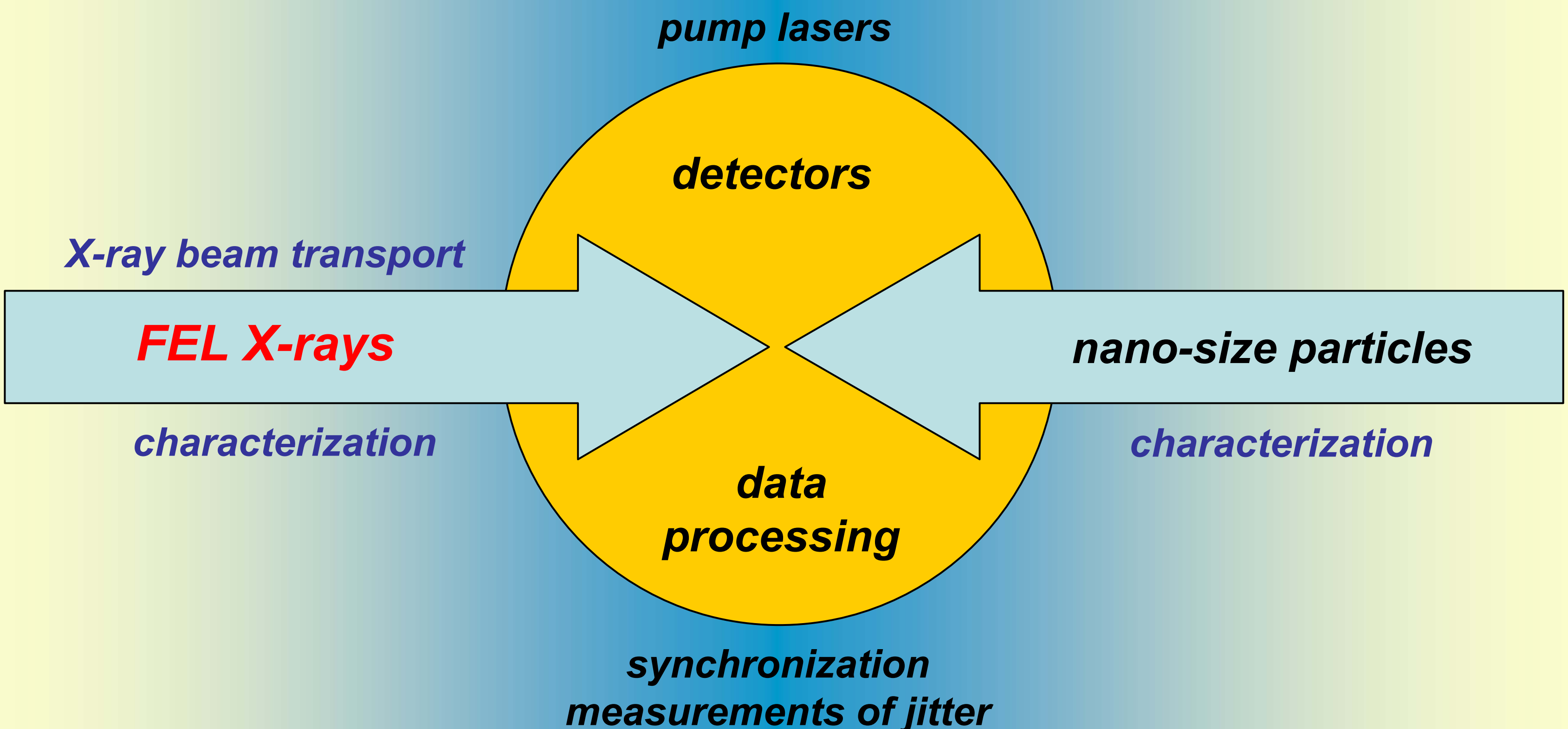
New experimental domain



Accelerator Science & Particle Physics methodology

Science at

Single Pass X-ray FELs



Jochen.Schneider@desy.de