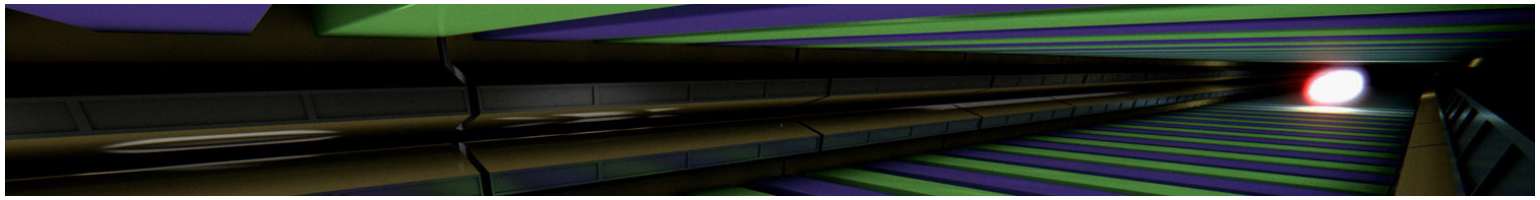
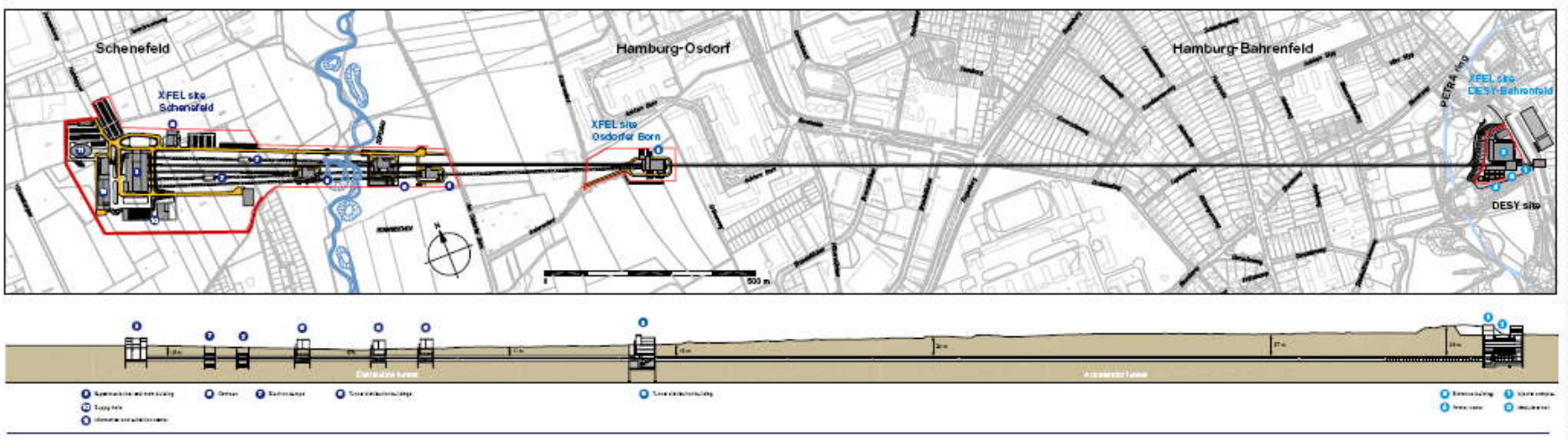


PES Using FELs: Time-Resolved Surface Stidies

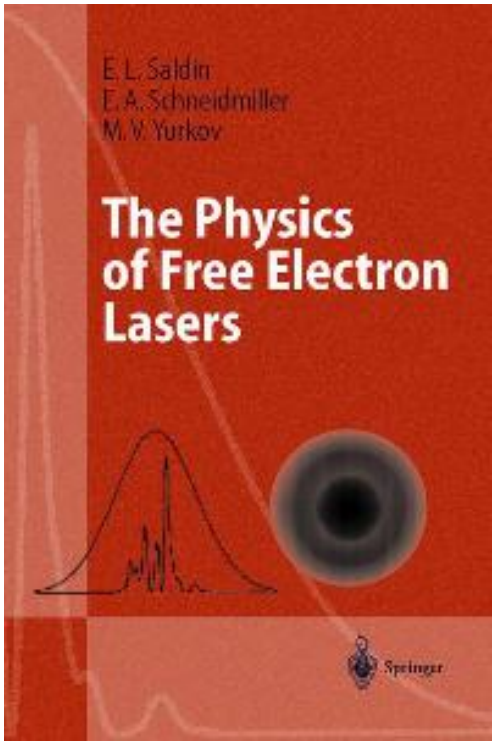
S.L. Molodtsov
European XFEL GmbH

X-Rays

New Generation Sources
Free Electron Lasers (FELs)

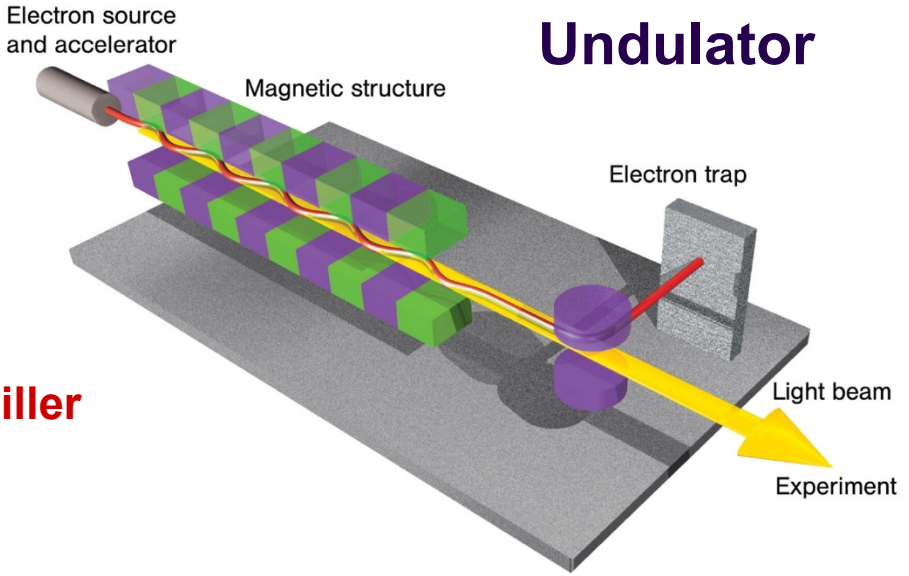


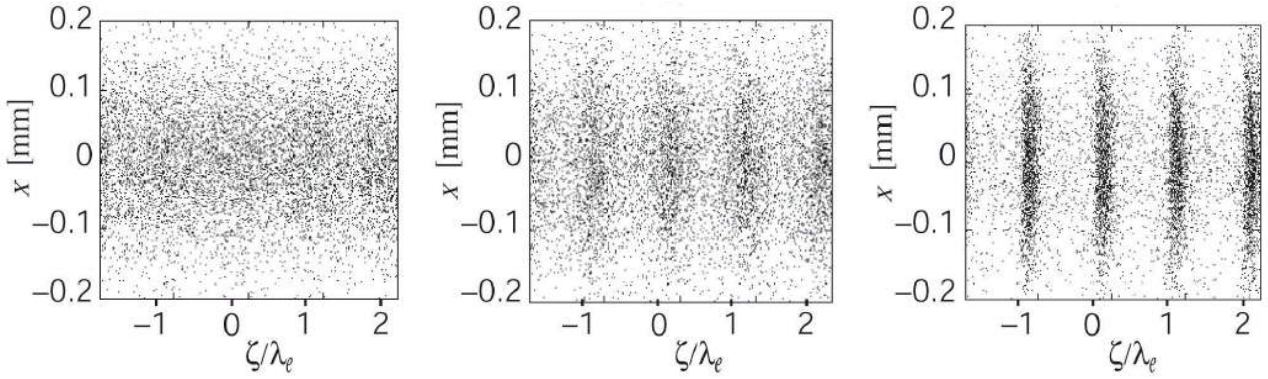
Basics of SASE FEL process



E.L. Saldin
E.A. Schneidmiller
M.V. Yurkov

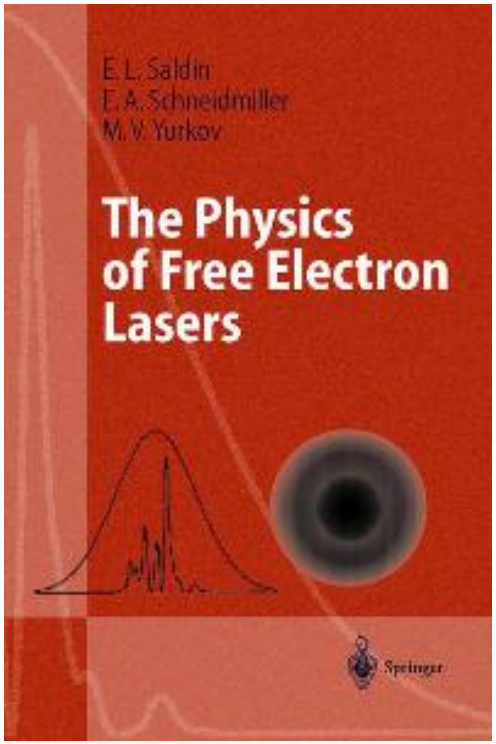
Undulator





simulations at the radiation wavelength (λ_e), ζ – distance inside the undulator

Basics of SASE FEL process



E.L. Saldin
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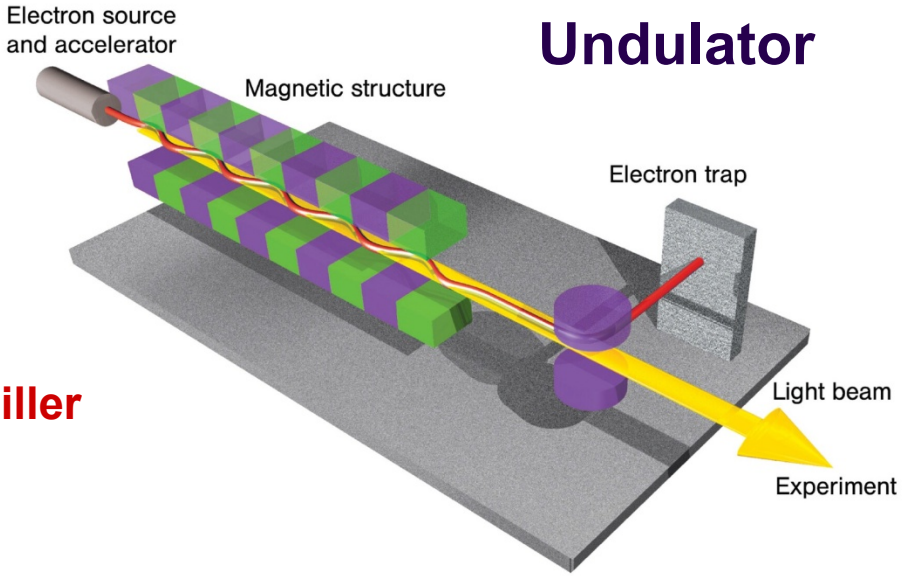
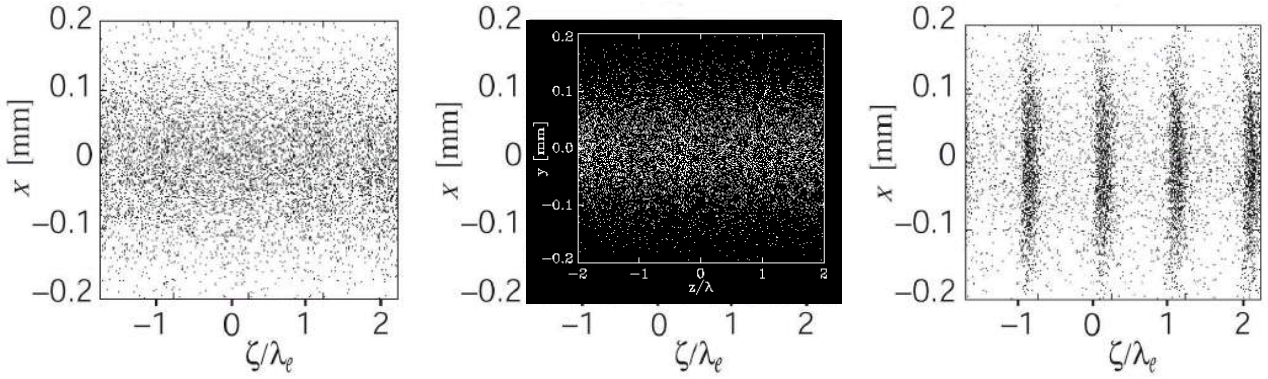
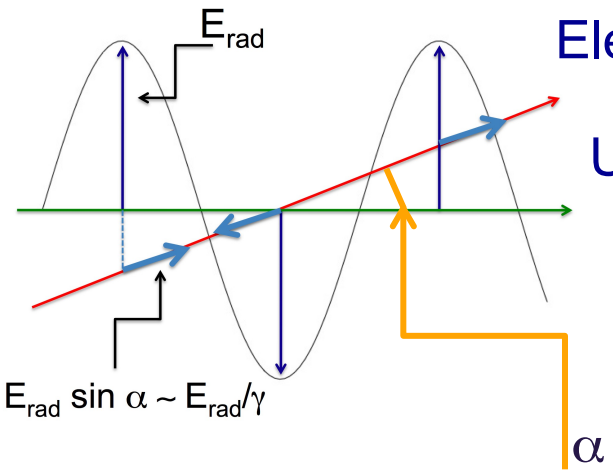
Undulator





simulations at the radiation wavelength (λ_e), ζ – distance inside the undulator

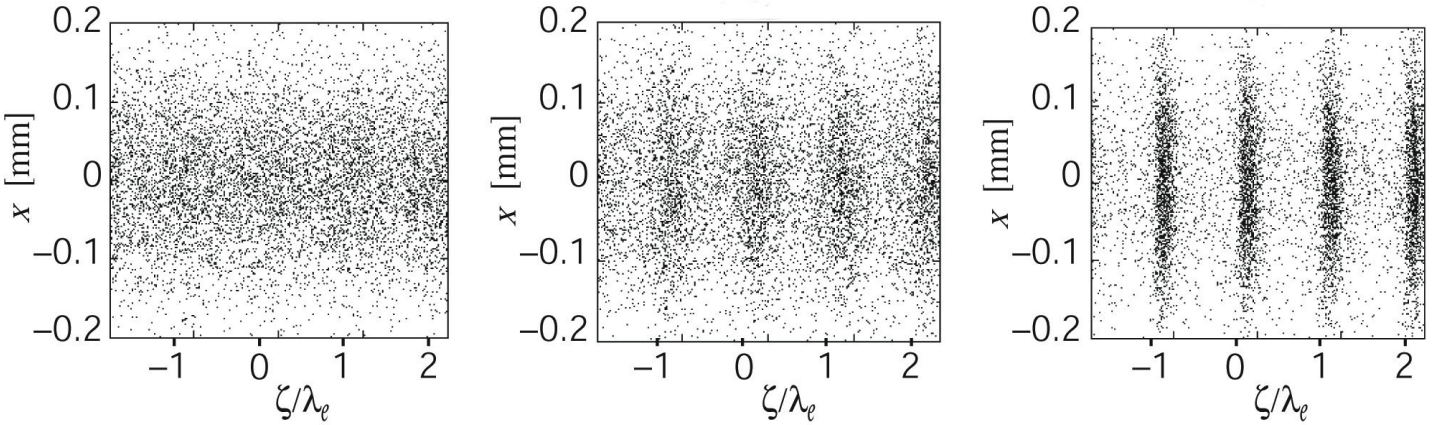
Origin of microbunching



Electron trajectory

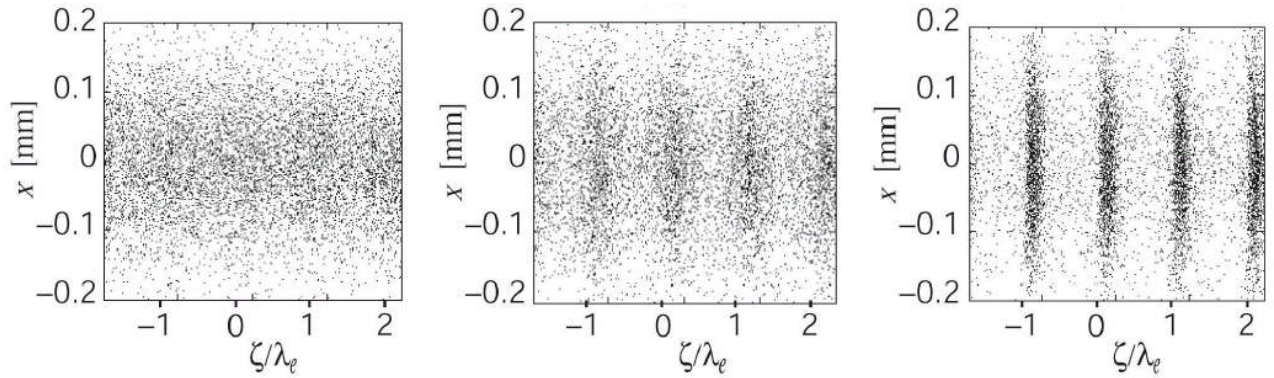
Undulator axis

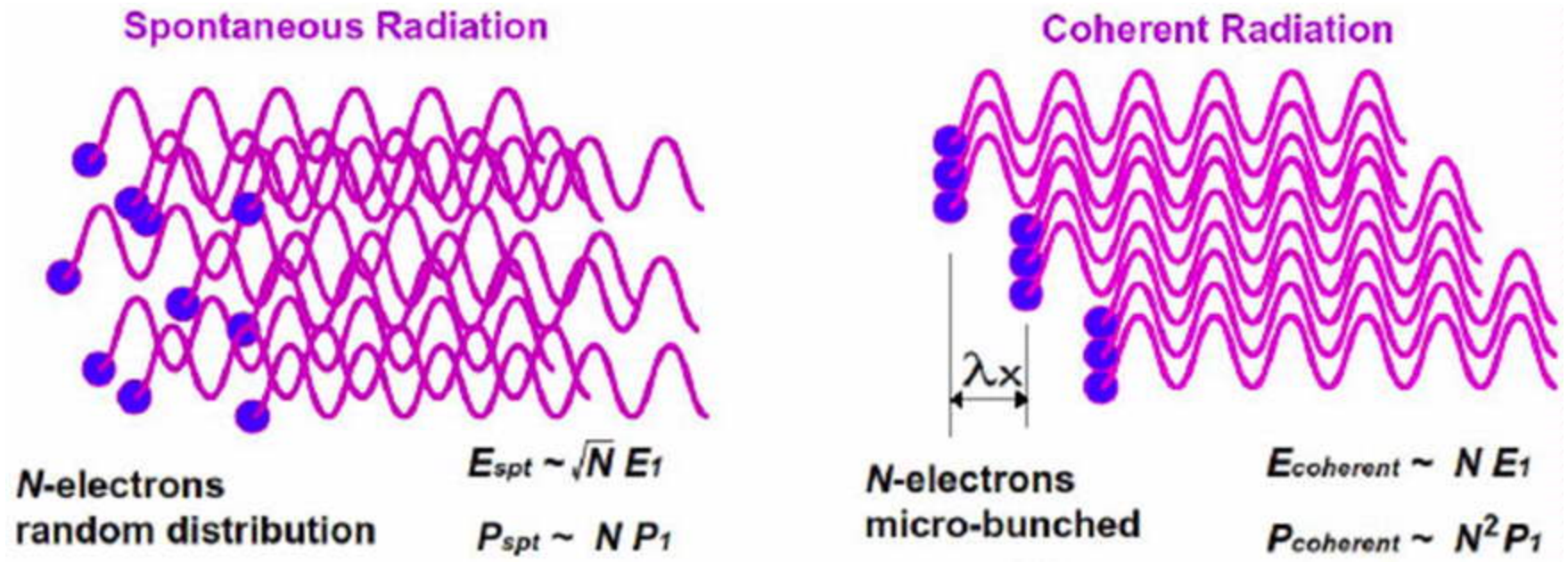
Radiation electric field has a small component parallel to electron velocity, which can accelerate or decelerate electrons



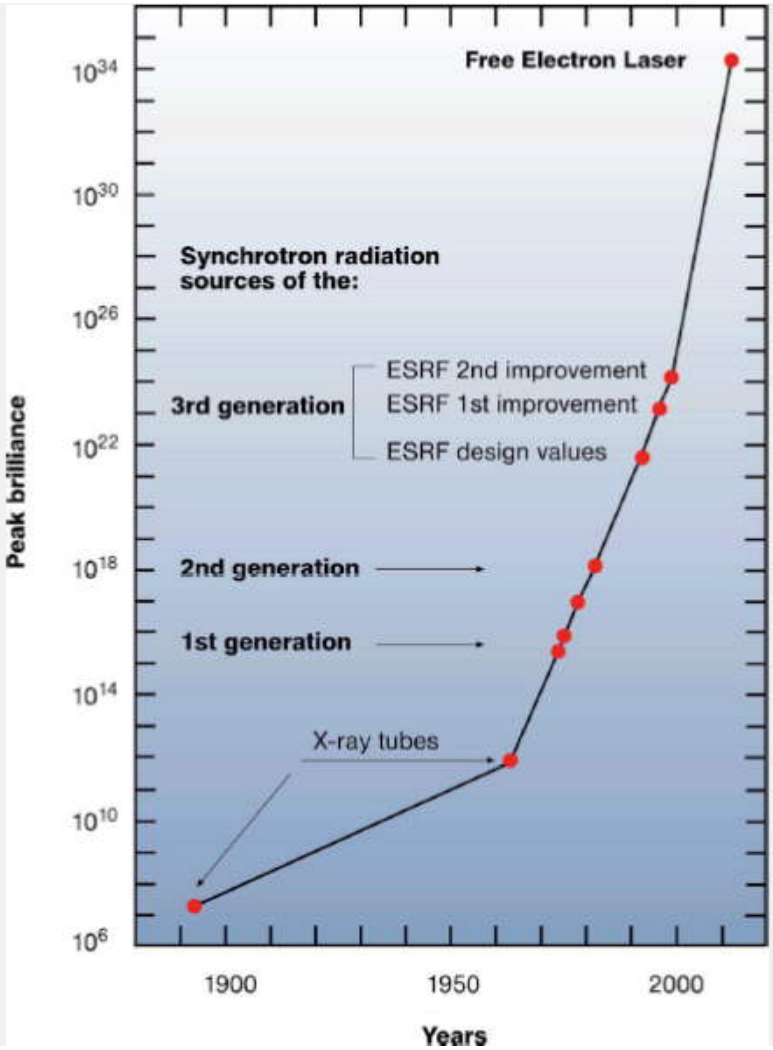
European XFEL

Spontaneous vs. coherent radiation in undulators





Peak brilliance of X-Ray sources vs. time



Free Electron Lasers:

-Based on Linear Accelerator

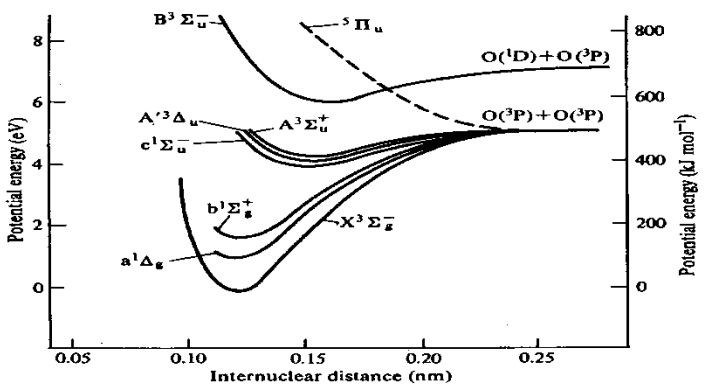
-Delivers ultrashort pulses

(100 fs = 0.1 ps= 10^{-13} s or less)

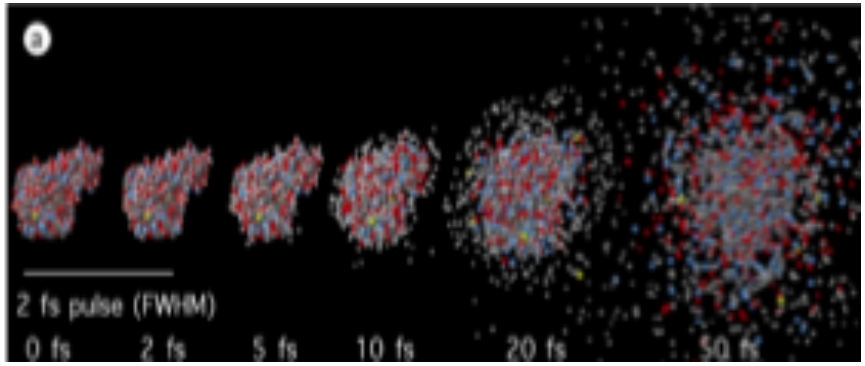
- (Transversely) Spatially coherent (laser-like) radiation

Wanted … More brilliant X-ray sources, with:

wavelength down to < 0.1 nm ==> *atomic-scale resolution*



ultrashort (<1 ps) pulses
==> *"molecular movies"*



ultra-high peak brightness,
transverse spatial coherence

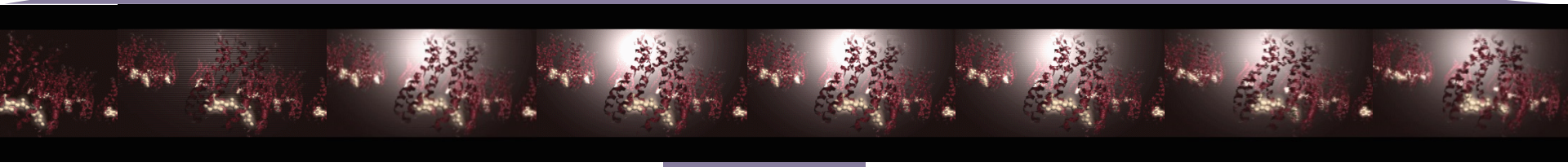
==> imaging of single nanoscale objects, possibly down to individual macromolecules (no crystals)

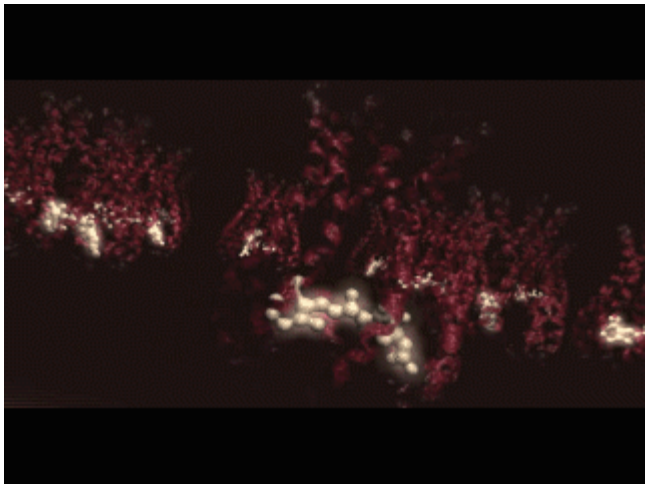
==> investigation of matter under extreme conditions…

Making molecular movies

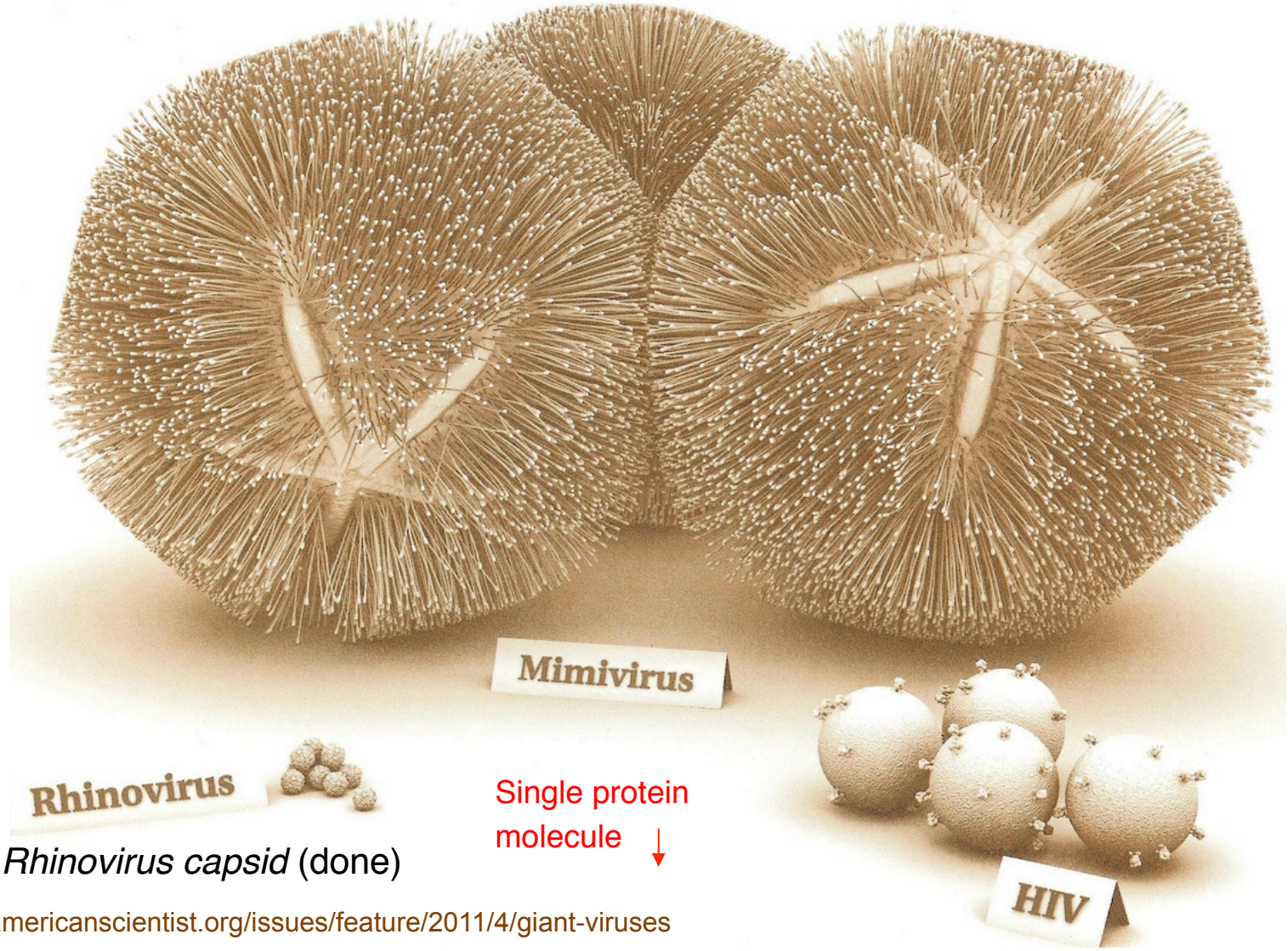
Eadward Muybridge
1892

European XFEL
2017





Tremendous variety of bio-objects to be studied



Rhinovirus capsid (done)

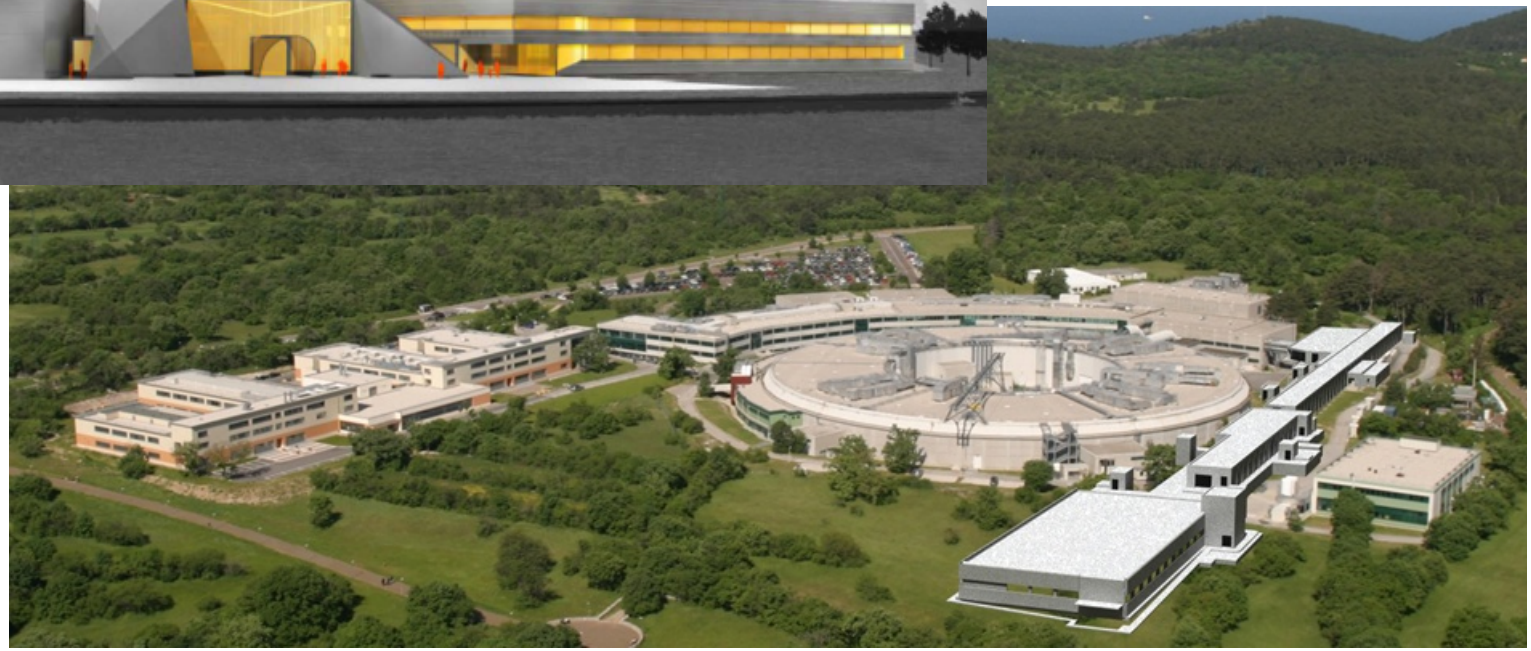
Single protein molecule ↓

http://www.americanscientist.org/issues/feature/2011/4/giant-viruses

Soft X-ray projects

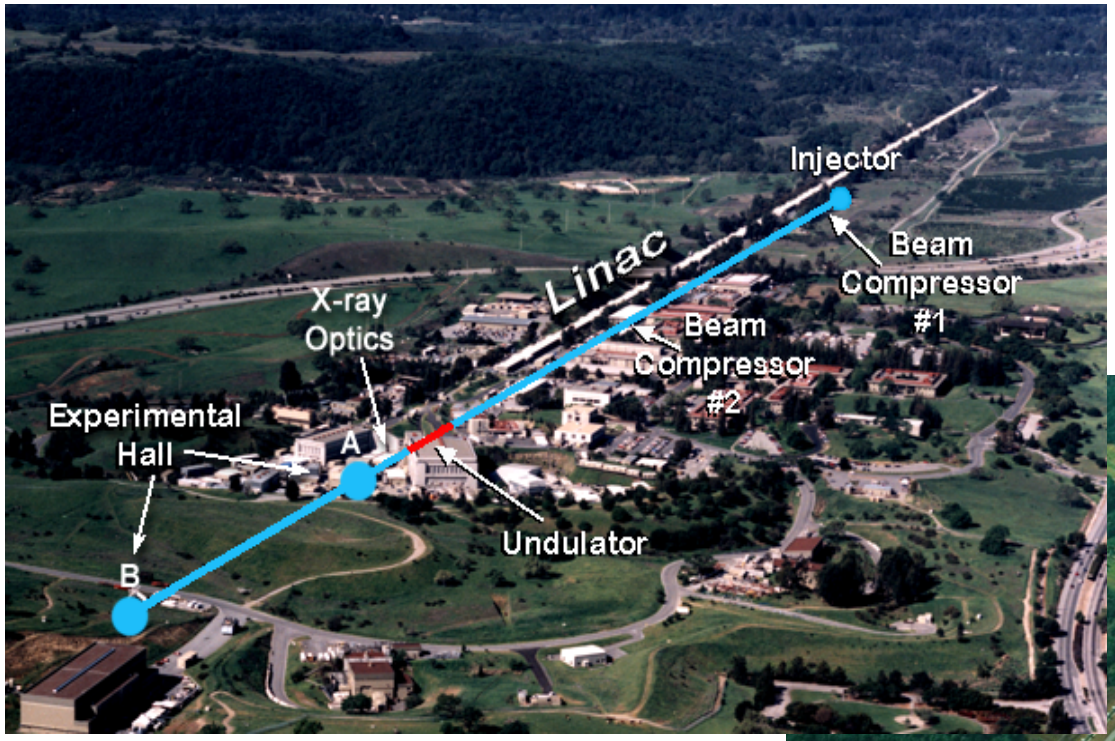
FLASH / DESY

FERMI / ELETTRA



European XFEL

Hard X-Ray FEL facilities



2011 - 60 p/s
SCSS
SPring-8 Compact
SASE Source

2009 -120 p/s
LCLS
LINAC COHERENT
LIGHT SOURCE

European XFEL

Hamburg, 30.11.2009: the European XFEL Convention Signing Ceremony

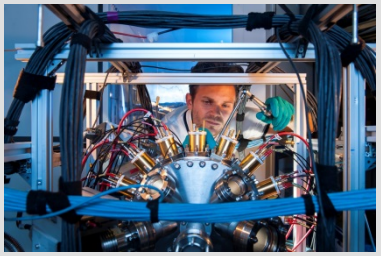
Total costs ≈1.500 MEUR

European XFEL

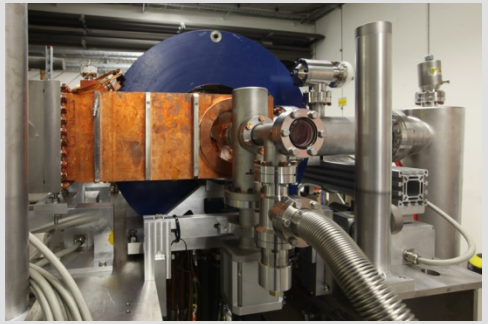
European XFEL - a leading new research facility

How it works – a closer look at the facility

Scientific instruments and instrumentation



Electron injector

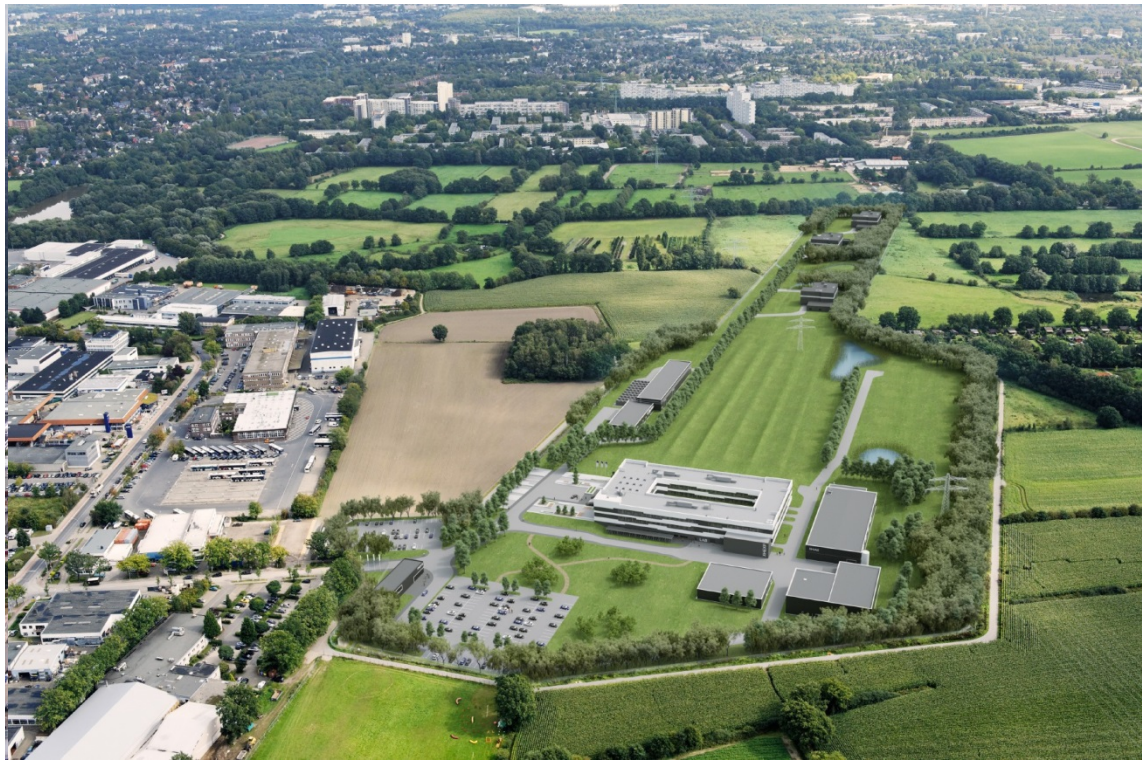


Undulator systems

Superconducting electron accelerator

European XFEL – a leading new research facility

The European XFEL is a research facility, now under construction, which will use high-energy X-ray light to help scientists better understand the nature of matter.



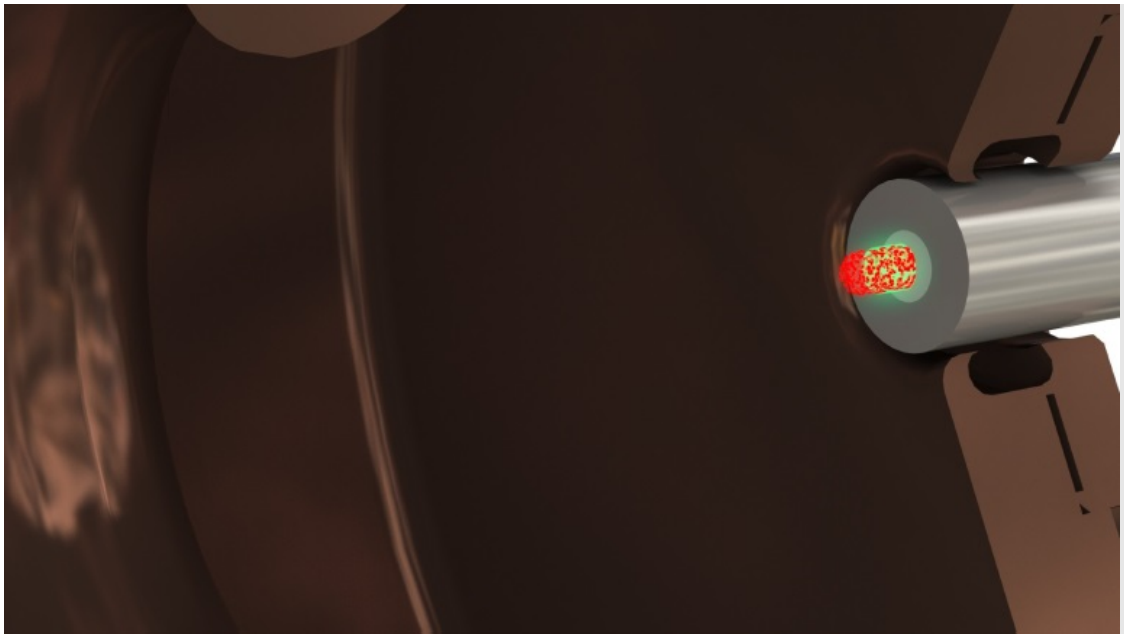
Site photo taken on 9 August 2013

Schenefeld & Hamburg, Germany

User facility with 260 staff (+ 230 from DESY)

2017: Start of user operation

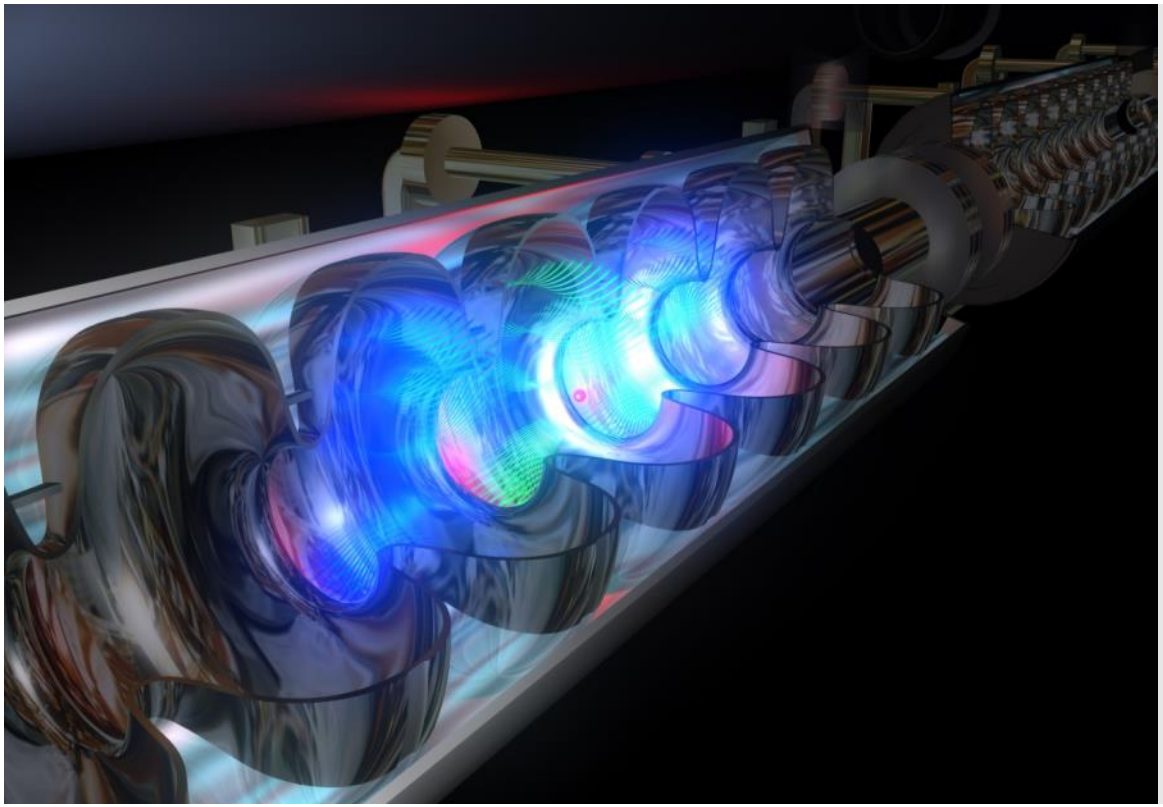
Injector: creating bunches of electrons



- Optical laser strikes Cs_2Te surface, releasing a cloud of electrons
- Electrons move into a magnetic field, shaping into a bunch
- Small accelerator module “fires” bunch into the main electron accelerator

European XFEL

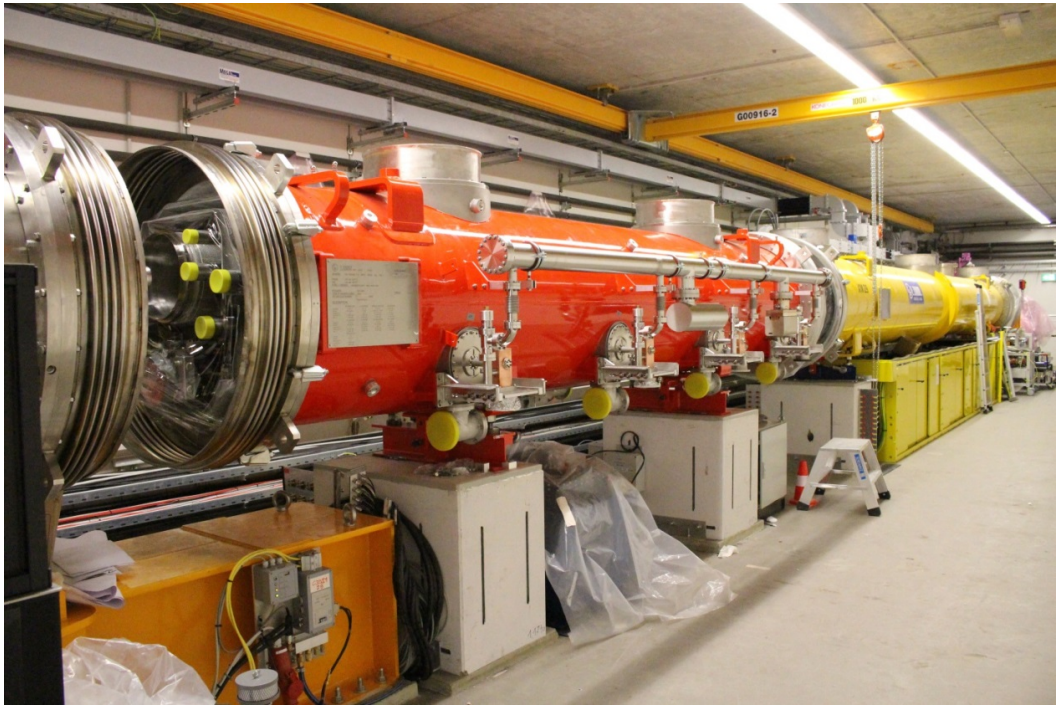
Accelerator: electrons at close to light speed

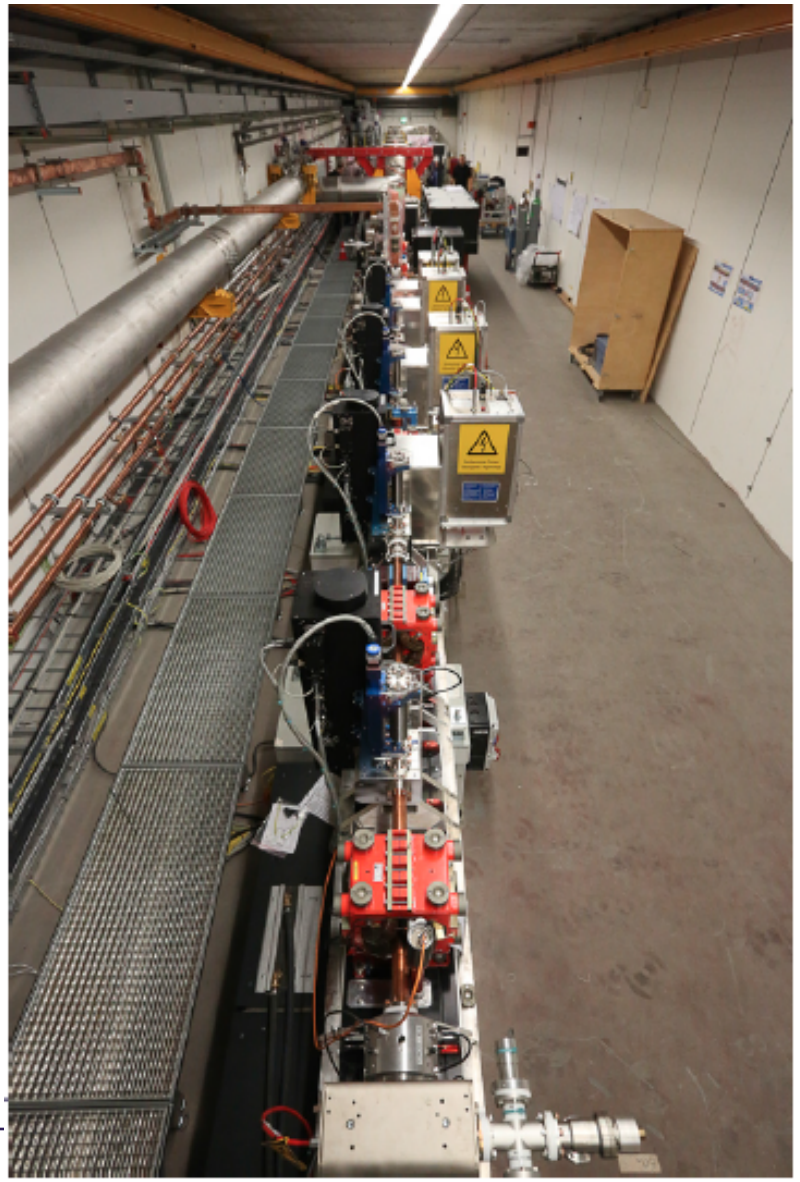


- 100 accelerator modules over 2 km bring the electron bunch to near light speed and high energies
- Superconducting niobium cavities powered by intense radio frequency accelerate electrons

First accelerated electron beam in the injector

- **Injector commissioning started**, injector tunnel closed, cool down to 2 K successful.
- First 130 MeV Electron beam on 18.12.2015!





European XFEL

Testing accelerator modules prior to installation

European XFEL

Accelerator module test facility

European XFEL

Construction site DESY-Bahrenfeld

European XFEL

Injector complex DESY-Bahrenfeld

European XFEL

Power RF – Installation check

European XFEL

Construction site Osdorfer Born

European XFEL

Tunnel branch Osdorfer Born (2017)

European XFEL

35 segments of SASE1 Undulator rolled in

Roll-in of SASE3 starting, see presentation by Joachim Pflüger

European XFEL

Aligning the undulators

European XFEL

Optical elements of the SASE1 beamline

European XFEL

Photon diagnostics for the SASE1 beamline

European XFEL

SASE3 hutches coming up

European XFEL

Moving to Schenefeld campus in June 2016

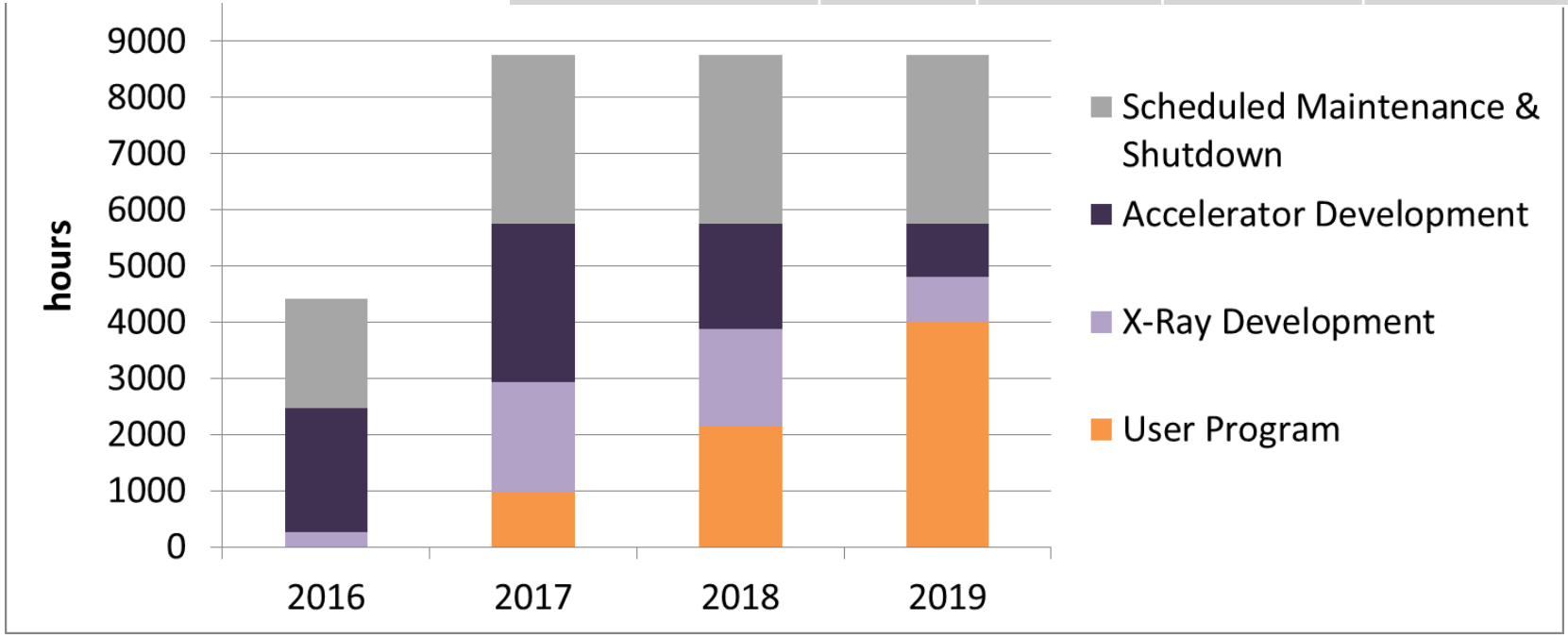
Availability of user time (accelerator)

(DRAFT – these numbers require further definition)

ASSUMPTION

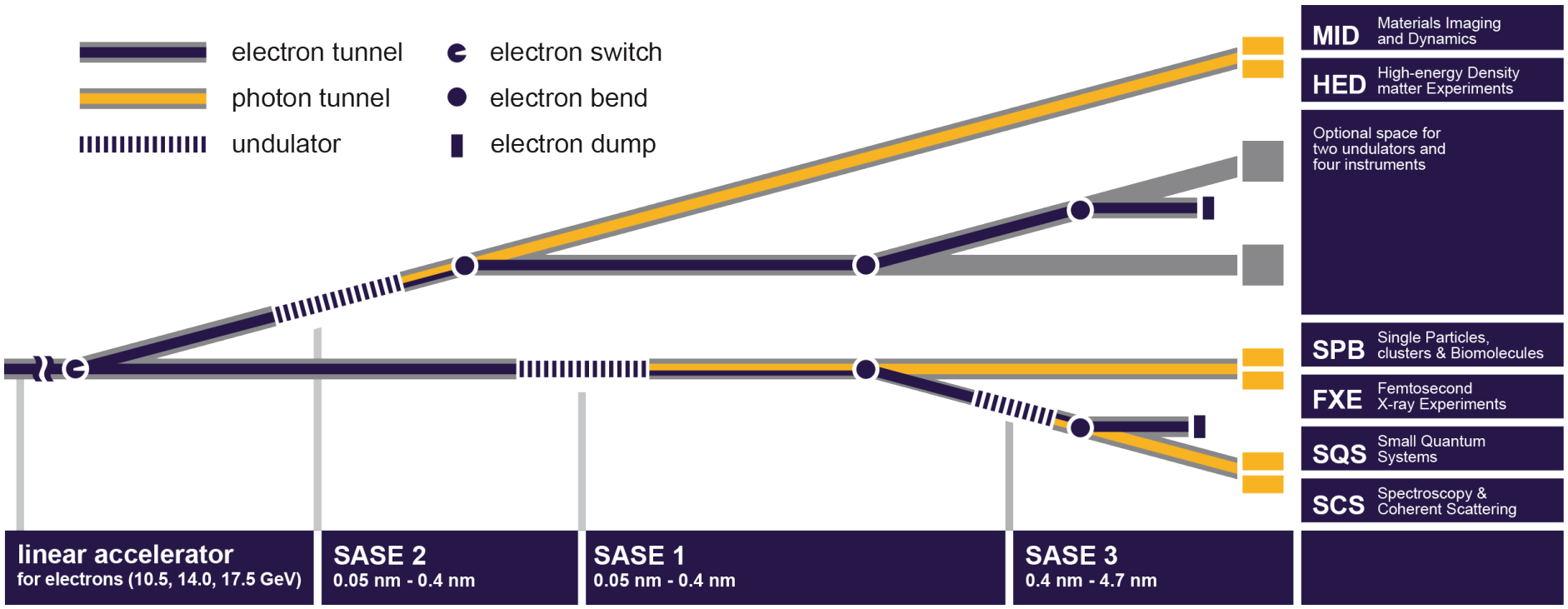
- First lasing Dec 2016

hrs	2016	2017	2018	>2018
Accelerator	~2500	5600	5600	5600
X-ray delivery	<200	2800	3900	4800
Users time	0	1000	2000	4000



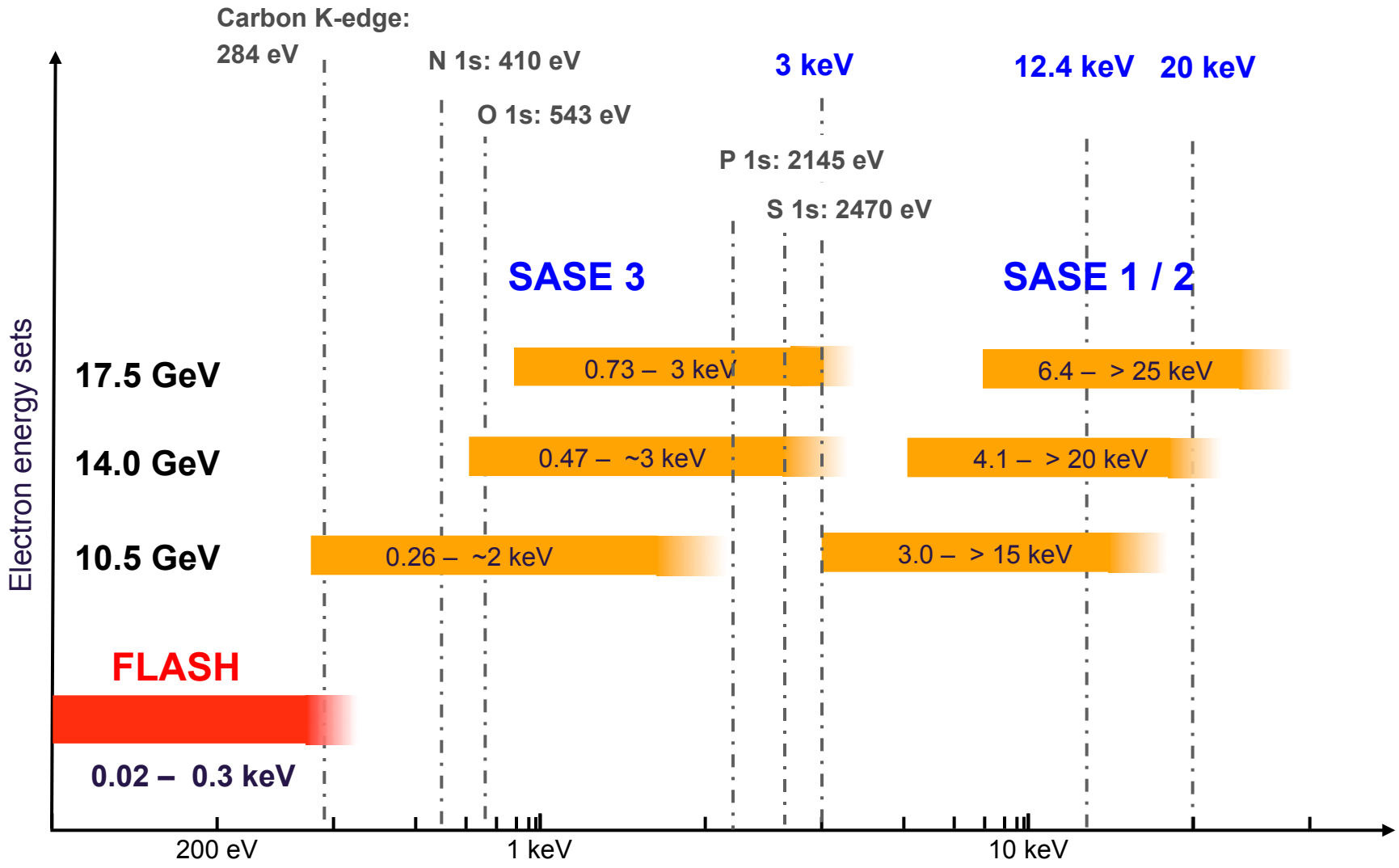
European XFEL

Beamline layout & experiment stations



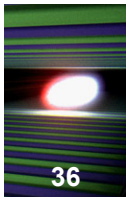
European XFEL

Photon energy ranges



European XFEL

Scientific instruments



Hard X-rays

SPB: Single Particles, Clusters, and Biomolecules

- Will determine the structure of single particles, such as atomic clusters, viruses, and biomolecules

MID: Materials Imaging and Dynamics

- Will be able to image and analyze nano-sized devices and materials used in engineering

FXE: Femtosecond X-Ray Experiments

- Will investigate chemical reactions at the atomic scale in short time scales—molecular movies

HED: High Energy Density Physics

- Will look into some of the most extreme states of matter in the universe, such as the conditions at the center of planets

Soft X-rays

SQS: Small Quantum Systems

- Will examine the quantum mechanical properties of atoms and molecules.

SCS: Spectroscopy and Coherent Scattering

- Will determine the structure and properties of large, complex molecules and nano-sized structures.

General Soft X-Ray radiation parameters

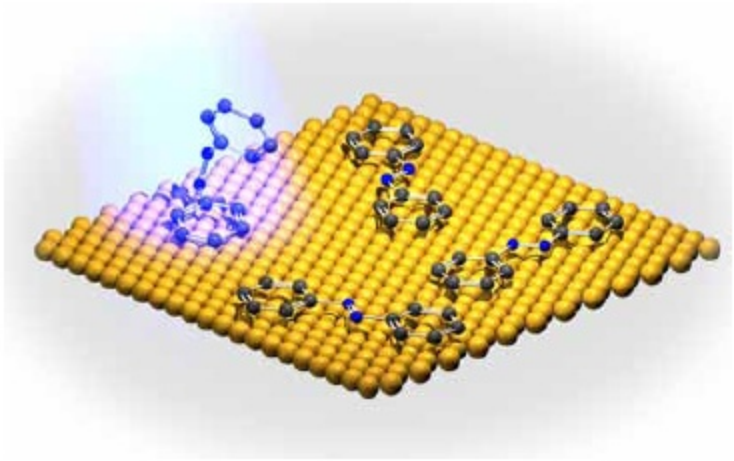
Pulse widths	**2 – 100 fs**	**Coherence time**	0.3 – 1.8 fs
Pulse energy	**0.2 – 11.0 mJ**	**Bandwidth**	0.25 – 0.7 %
Peak power	50 – 120 GW	**Number of photons**	**0.1 – 2 x 10^{14}**
Average power	3 – 300 W	**Average flux of photons**	0.3 – 5.4 x 10^{18}
Beam size	40 – 80 μm	**Average brilliance**	0.03 – 2.6 x 10^{24}
Rep. rate	**10 Hz (2700 pulses in bunch train) = 27.000 pulses/s**		

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

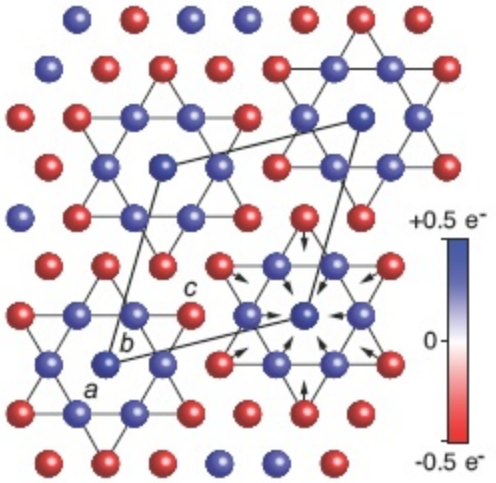
Science
@
SCS Scientific Instrument
(trXPS and trARPES)
Spin-resolved photoemission (?)

Photoemission at FELs: Motivation

Surface chemical reactions

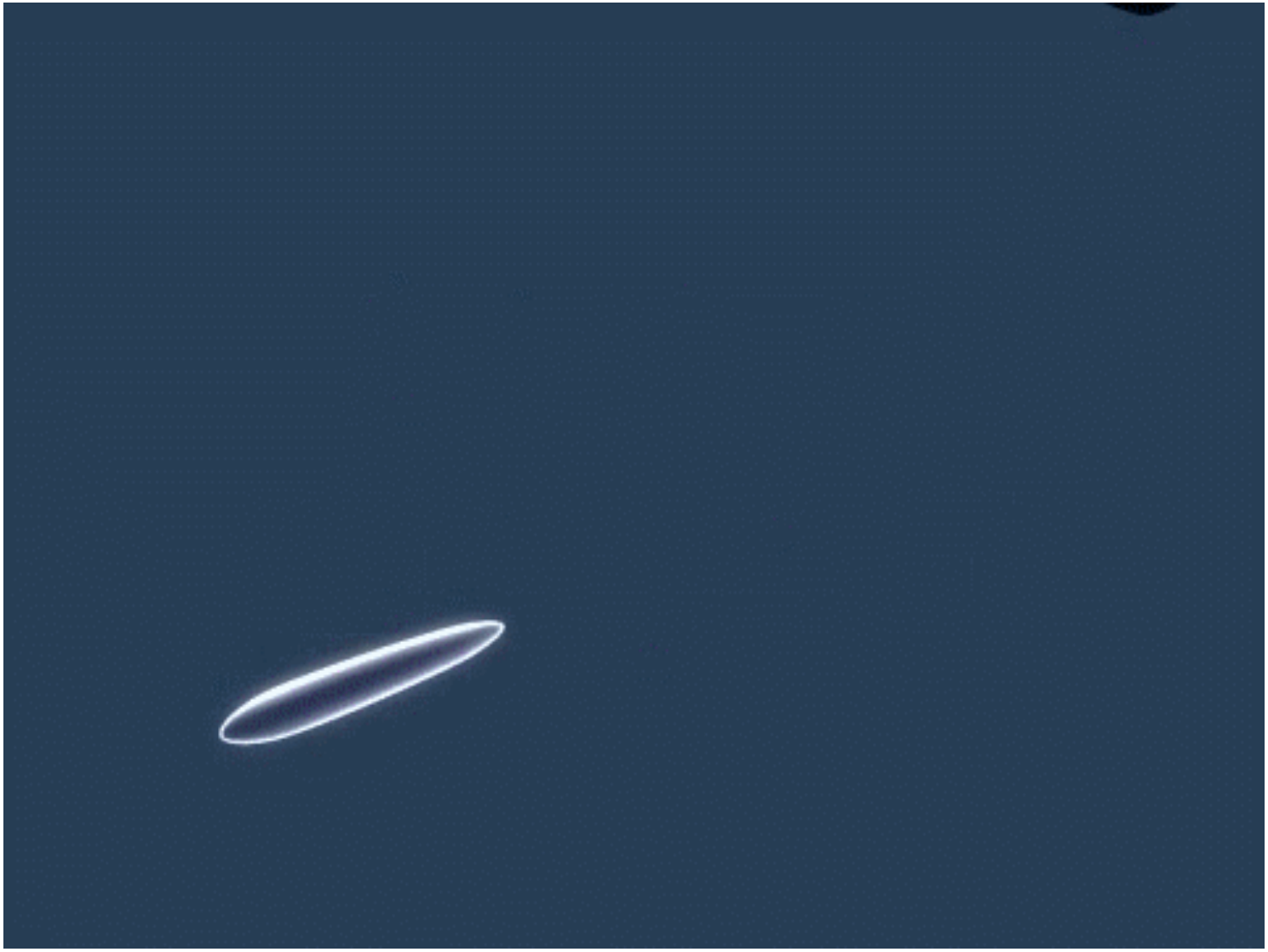


Charge order dynamics



Time scale: 10 fs - 1 μs, reversible processes are preferable

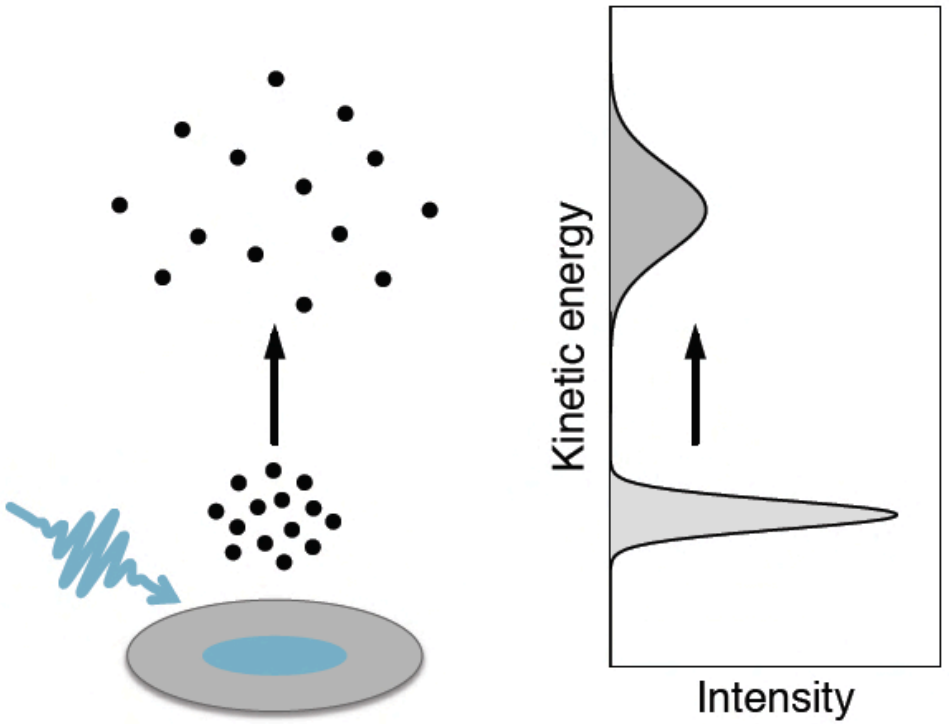
Pump-probe experiments at XFELs



European XFEL

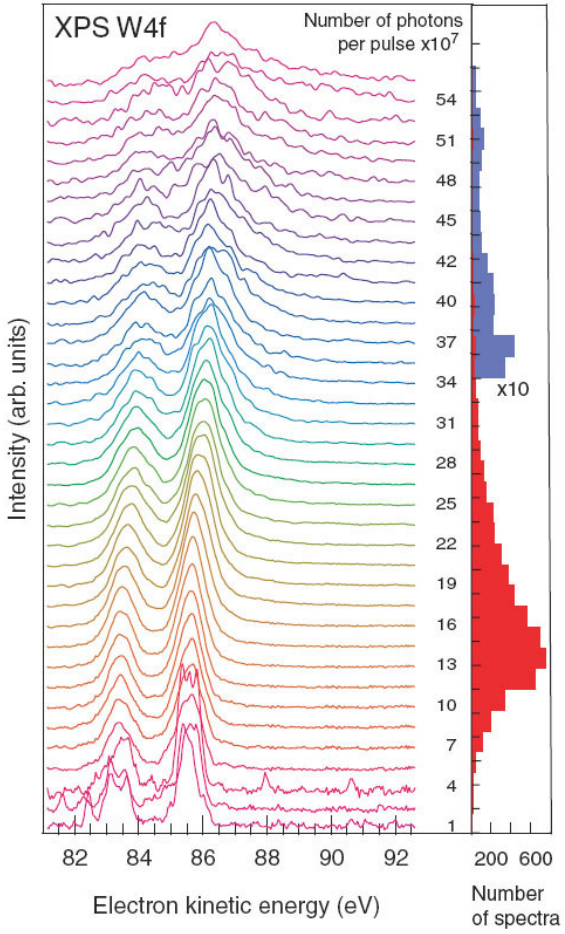
Problems to be solved (Kai Rossnagel)

Challenge I:
Vacuum space-charge effects

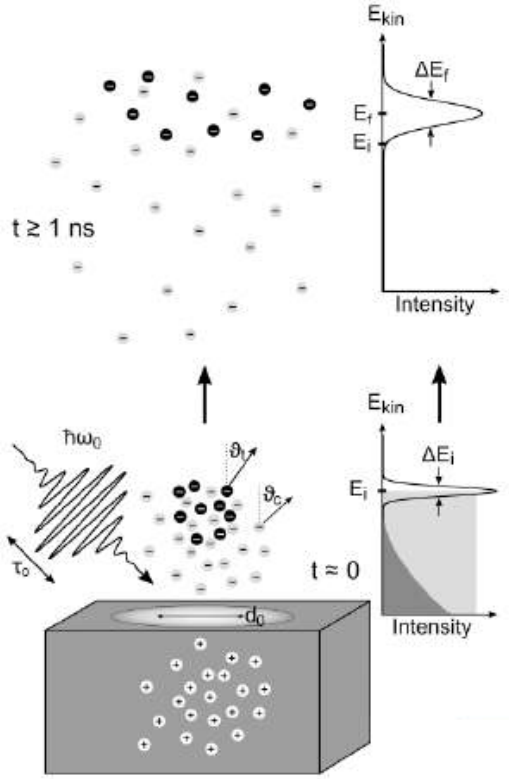


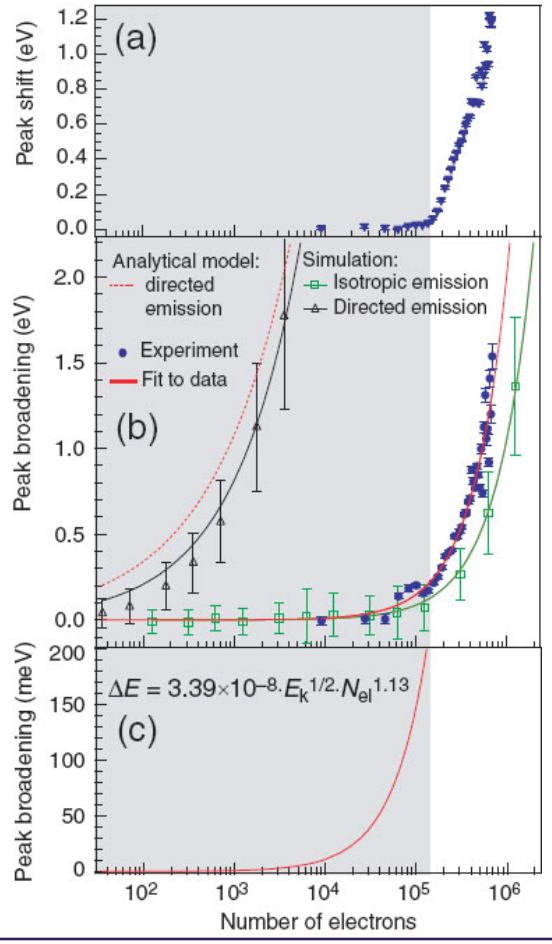
Core-level X-ray photoemission spectroscopy (XPS)

Core-level PE was proven to be extremely useful tool for time-resolved studies of, e.g. chemical interactions at FLASH and LCLS (W. Wurth, L. Kipp, A. Nilsson).



space charge (1mm spot)
> 10^8 phot/pulse
> 10^4 el/pulse

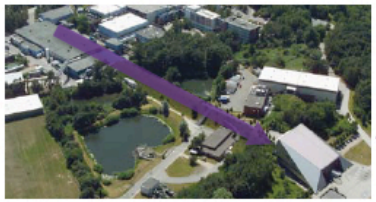


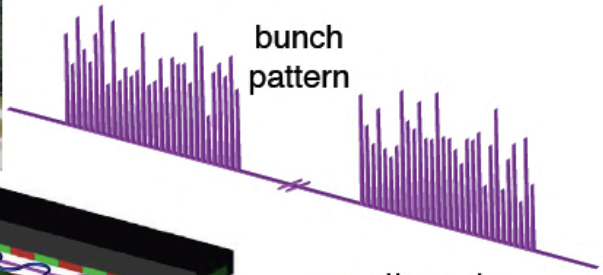


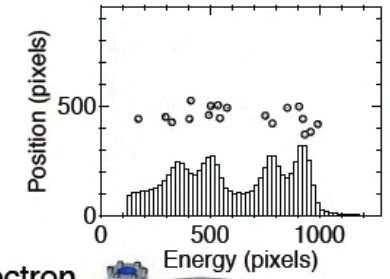
European XFEL

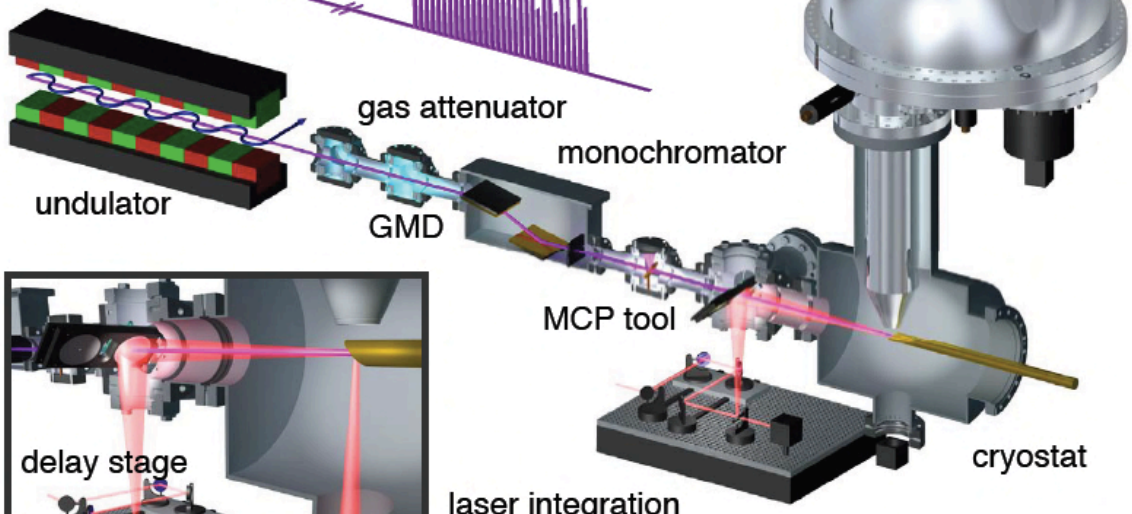
Problems to be solved

Challenge II: FEL fluctuations









NJP **14**, 013062 (2012)

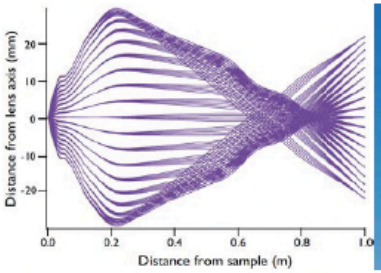
with W. Wurth (Hamburg)

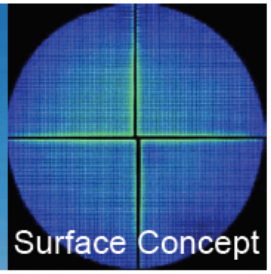
bmb+f Großgeräte der physikalischen Grundlagenforschung

Problems to be solved

Challenge III: Low FEL repetition rates

Angle imaging + TOF spectroscopy + multi-hit detection





Space-charge limit: $I_0 \approx 10^4 \frac{\mathrm{e}^-}{\mathrm{pulse}}$

Energy window: $\frac{\Delta E}{E} \approx 0.01$

Angular acceptance: $\frac{\Delta\Omega}{2\pi} \approx 0.034$

Electron counts per photon pulse:

$$I_0 \times \frac{\Delta E}{E} \times \frac{\Delta\Omega}{2\pi} \approx 3.4 \frac{\mathrm{e}^-}{\mathrm{pulse}}$$

1 *T*-TaSe2: trXPS using FLASH

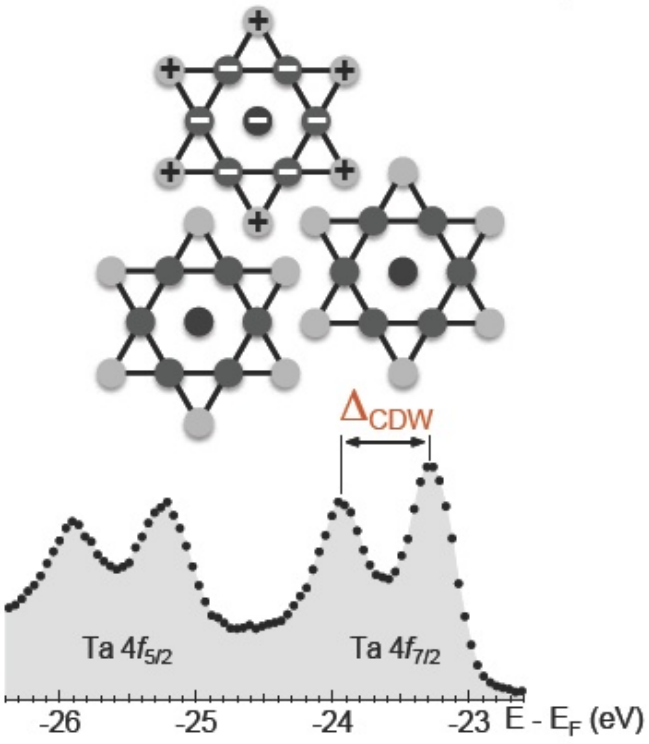
PRL **105**, 187401 (2010)

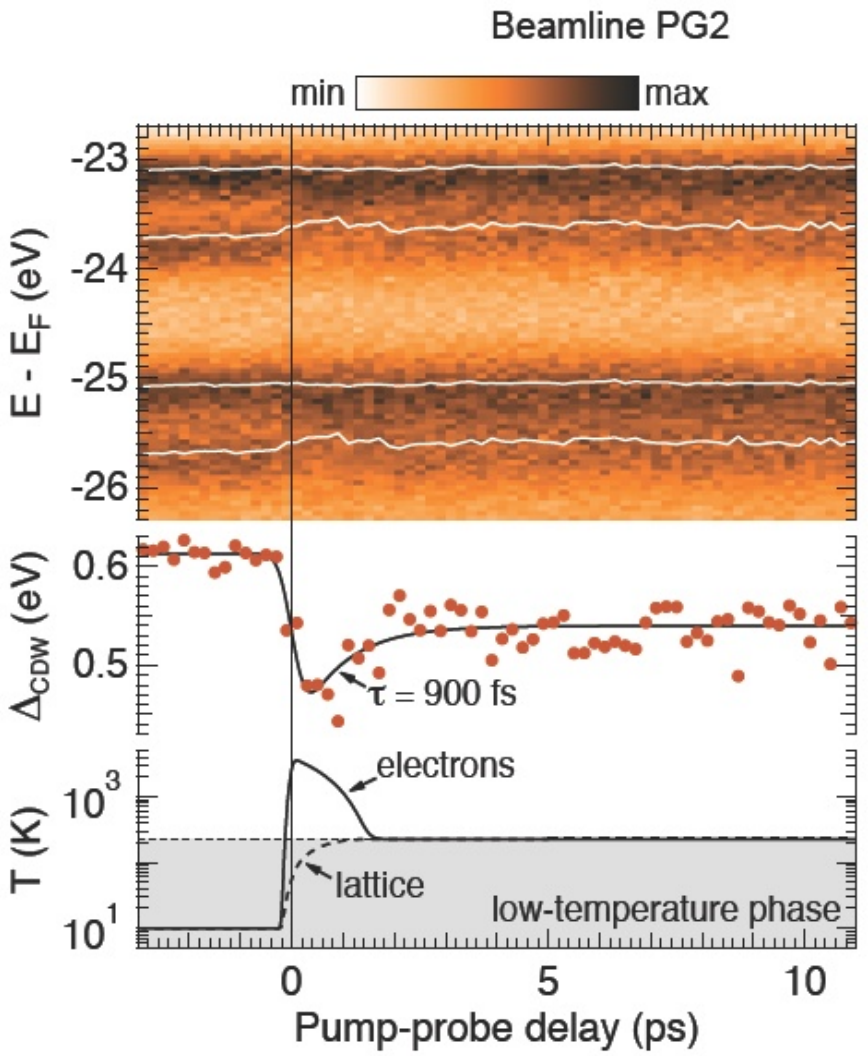
$T = 10$ K

$h\nu_{pump} = 1.55$ eV. $h\nu_{probe} = 156$ eV

$\Delta E \approx 300$ meV. $\Delta t \approx 700$ fs

$F = 1.8$ mJ/cm^2





Angle-resolved photoemission (ARPES)

In contrast, angle(spin)-resolved photoemission (ARPES) that for crystalline species is the only tool providing direct information on

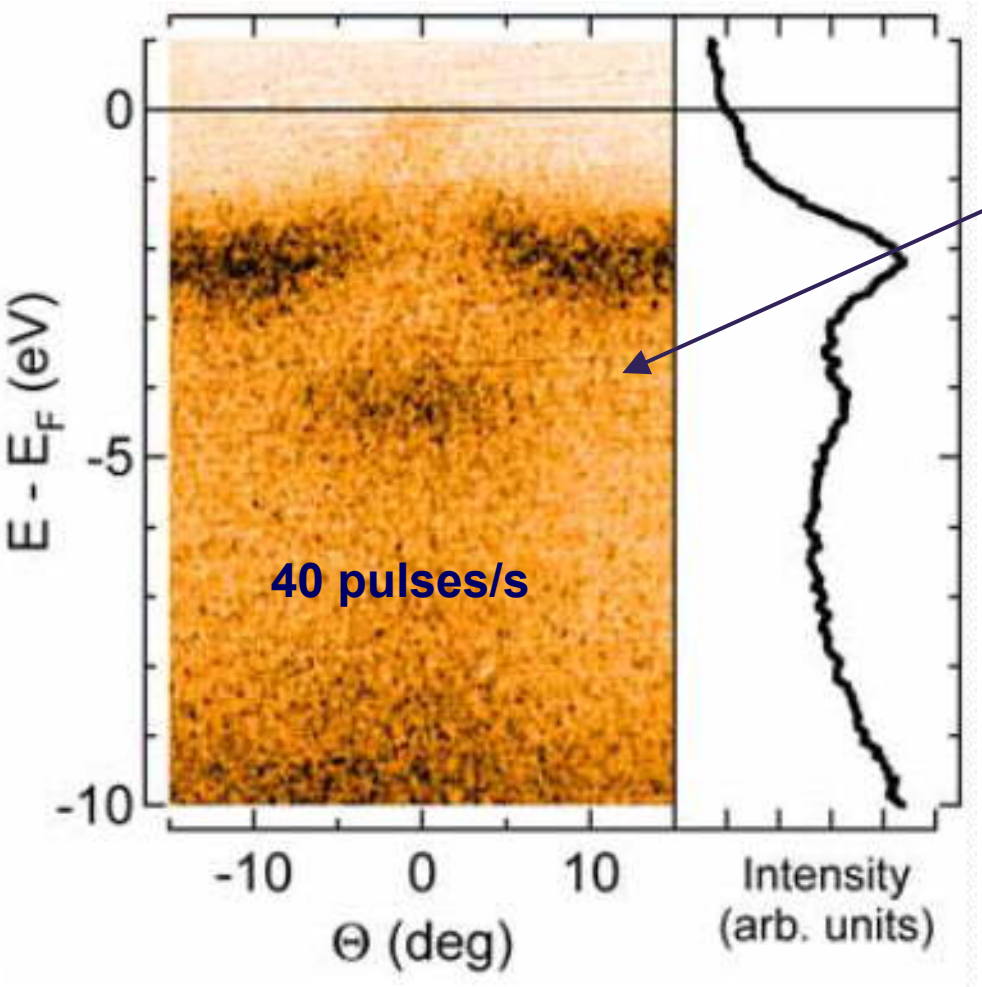
- single-particle excitations (simple *s*- and *p*-like systems) and
- electron interactions (correlated *d*- and *f*-systems)

is not straightforward at the existing low repetition rate FELs!

Reason: too less “allowed” excited electrons per second to acquire reasonable statistics

*Note: ARPES signal is 100-1000 lower than XPS one

ARPES at XFELs with low repetition rate



What you get at non-superconducting XFEL facilities (60 - 100 Hz rep. rate)

Why angle-resolved photoemission?

On the other hand, particularly temperature dependent electron dynamics that causes transitions between

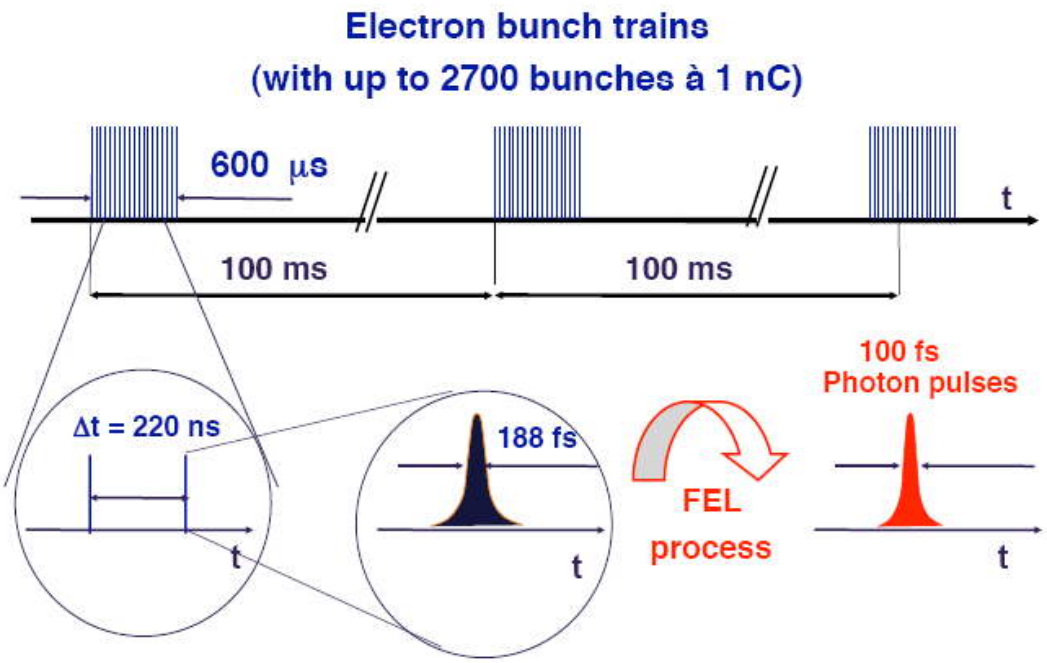
supercondcting, magnetic and
Kondo (heavy fermion) properties

in correlated systems is dreamed to be studied, since it allows

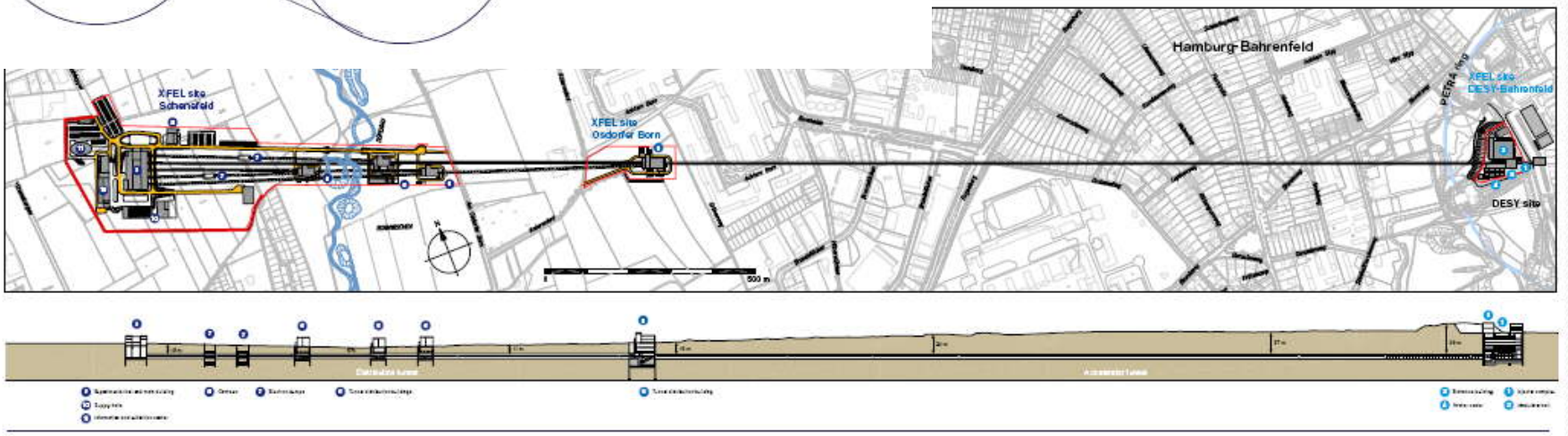
- understanding of underlying mechanisms of the phenomena
- switching from one behavior to another
- engineering of novel materials with well-defined properties

European XFEL

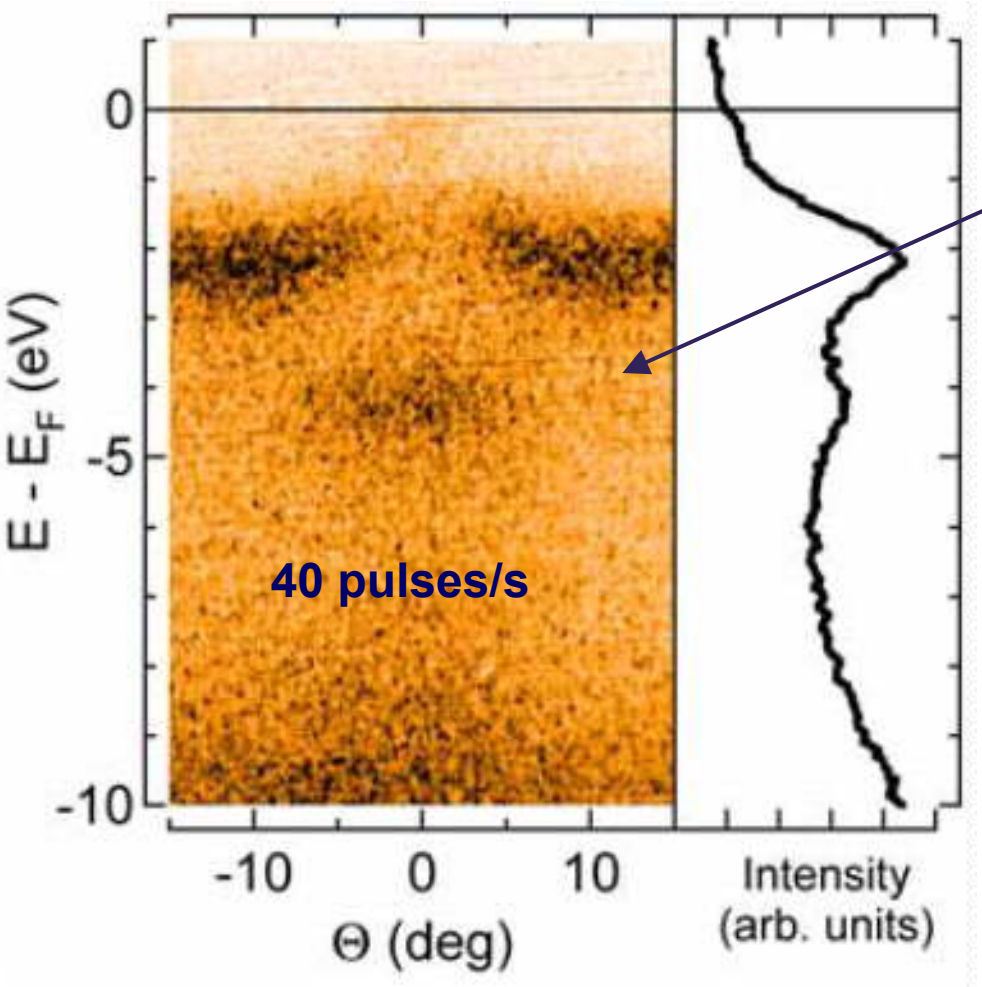
European XFEL: Time structure



Superconducting LINAC technology provides 27.000 light pulses/s in burst-like structure. It makes XFEL.EU attractive for photon-hungry experiments.



ARPES at European XFEL



What you get at non-superconducting XFEL facilities (60 - 100 Hz rep. rate)

Due to unique rep. rate photoemission response at the European XFEL is about 10^3 higher (statistics) → strong case for ARPES:

- two-color exp. (unfilled states)
- pump-probe (electron dynamics)

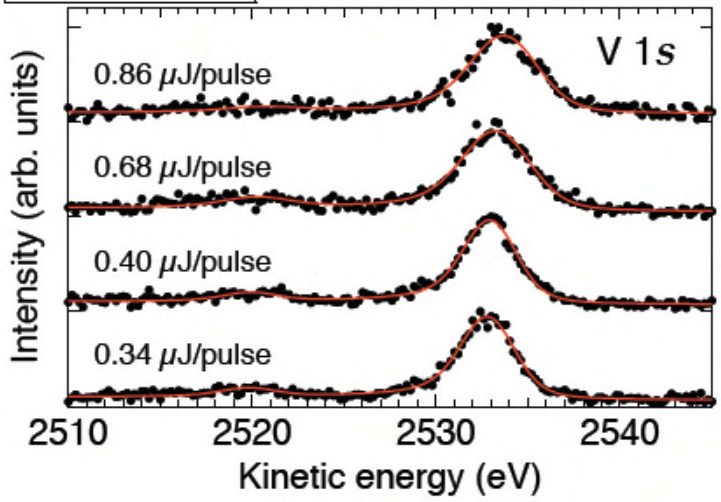
V 1s in VO2, SACLA (Japan)

NJP 16, 123045 (2014)

$h\nu = 7937\,\mathrm{eV}$

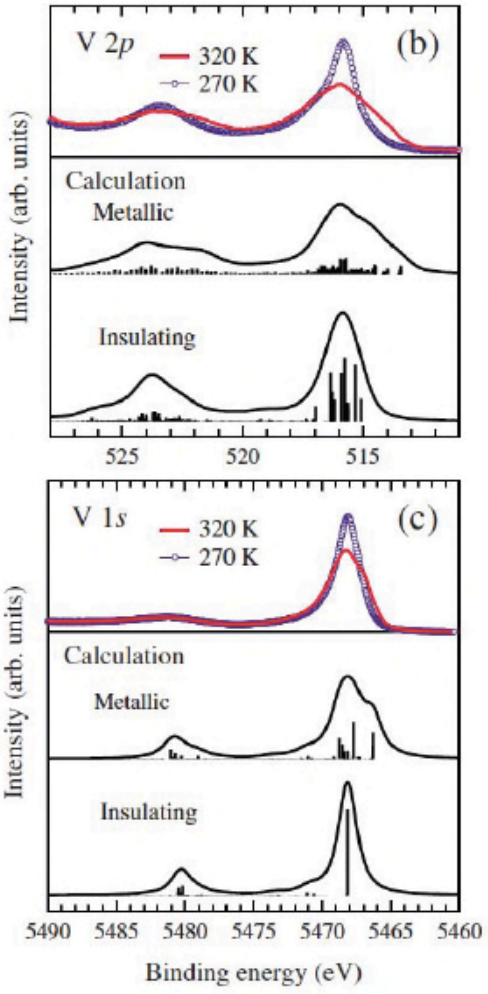
$\Delta E \approx 250\,\mathrm{meV}$

$h\nu = 8\,\mathrm{keV}$. $\Delta E \approx 1\,\mathrm{eV}$



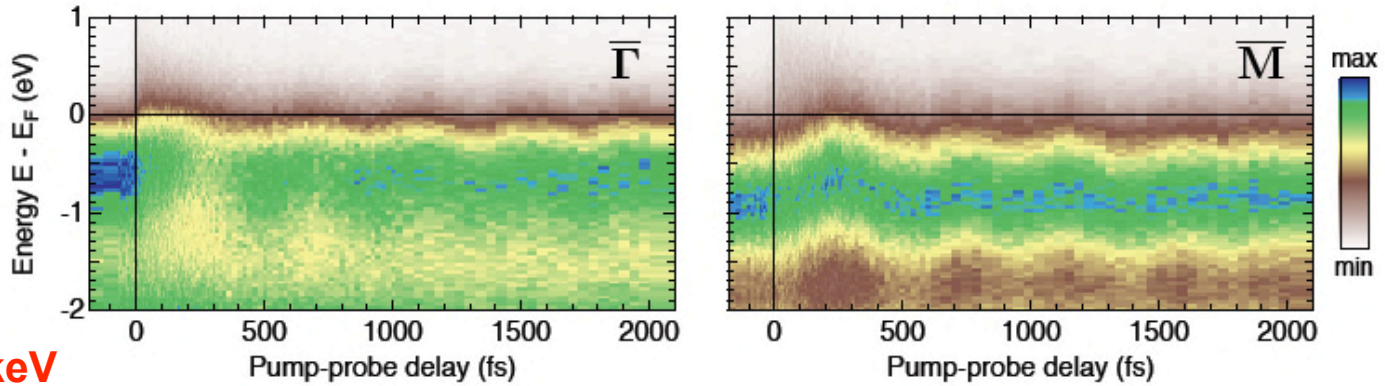
20 min at 20 Hz

Eguchi *et al.*, PRB **78**, 075115 (2008)



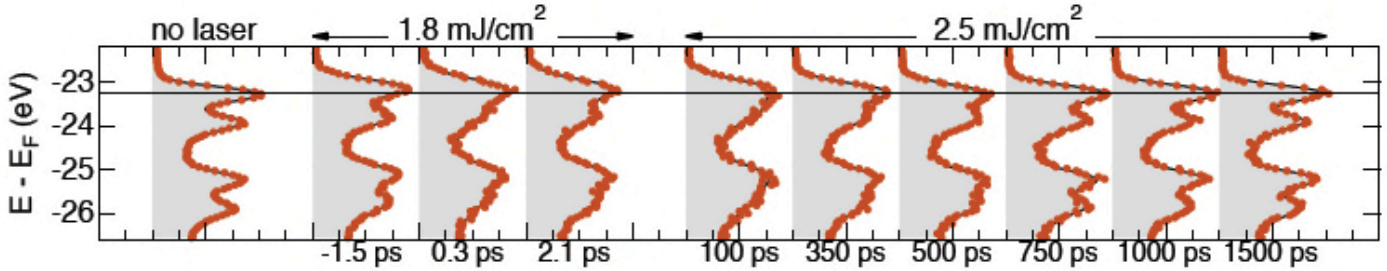
Combined probing of electronic & lattice order (Kai Rossnagel)

Spectral gaps
trARPES

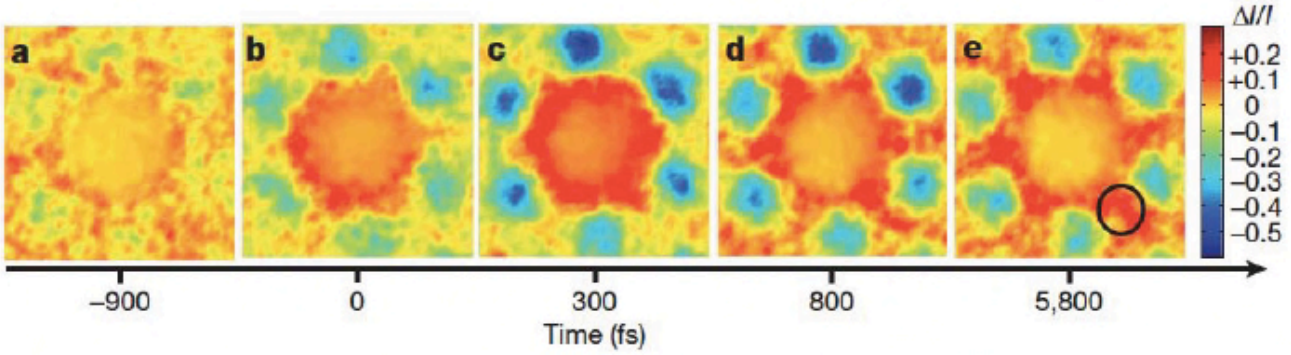


$h\nu_{probe}$ ≈ 0.1–2(> 5) keV

Charge
density wave
trXPS



Periodic
lattice distortion
UED
trXPD



Participants of the TR-XPES User Consortium (W. Wurth)

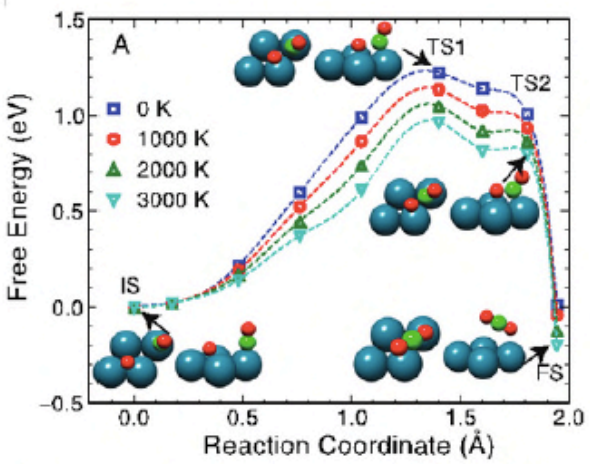
Spokesperson and Consortium Members			
Ulf Karlsson	*KTH Stockholm*	*Kai Rossnagel*	*Universität Kiel*
Wilfried Wurth	*Univ. Hamburg/L*	*Wolfgang Eberhardt*	*TU Berlin/DESY*
Yves Acremann	ETH Zürich	Victor Aristov	RAS Chernogolov
Alessandro Baraldi	Univ. Trieste/ Elet	Carlo Carbone	CNR-ISM
Stefano Colonna	CNR-ISM	Dan Dessau	Univ. of Colorad
Alexander Föhlisch	HZB	Gerd Ganteför	Universität Kons
Mats Göthelid	KTH	Nils Martensson	Uppsala Universi
Anders Nilsson	Stockholm Univ./	Henrik Öström	Stockholm Unive
Hirohito Ogasawara	SLAC	Giancarlo Pannacione	IOM-CNR
Eric Pellegrin	ALBA	Giorgio Rossi	UMilano/IOM-CN
Alexander Soldatov	So. Fed. Univ. Ros	Gerd Schönhense	Universität Mainz
Giovanni Stefani	Universita Roma T	Svante Svensson	Uppsala Universi
Oscar Tjernberg	KTH	Geoff Thornton	UCL
Martin Weinelt	FU Berlin	Jonas Weissenberger	KTH
Martin Wolf	FHI Berlin		
XFEL contacts			
Serguei Molodtsov	Harald Sinn	Andreas Scherz	

European XFEL

Science with TR-XPES

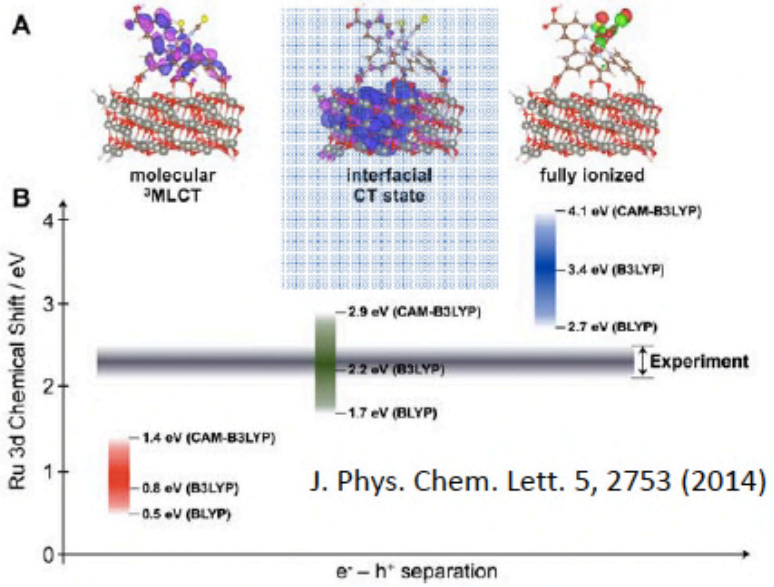
Science case for TR-XPES at EuXFEL

Surface and Interface Chemistry and Catalysis – observe transition states



H. Öström et al. Science 347,978 (2015)

Photovoltaics – follow charge transfer at interfaces



J. Phys. Chem. Lett. 5, 2753 (2014)

Methods

TR-XPS (ESCA) → **Element specific, chemical state selective,**
→ **Local charge state**

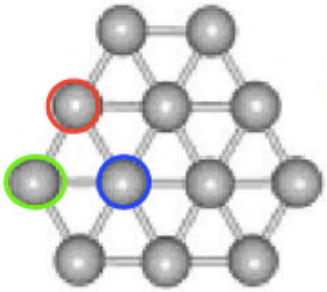
TR-XPED → **element specific, structural information**

Science with TR-XPES

Science case for TR-XPES at EuXFEL

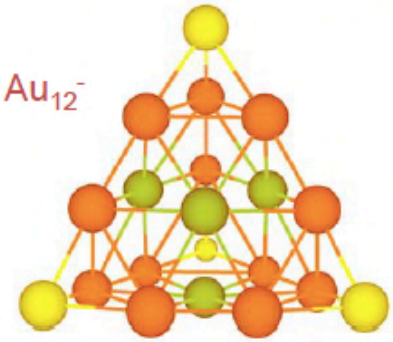
Cluster physics

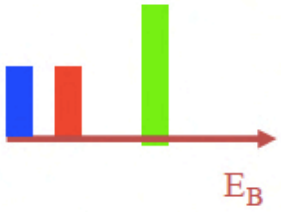
– structure and dynamics (e.g. dissociation, non-thermal melting) as function of size



planar clusters up to at least Au_{12}^-

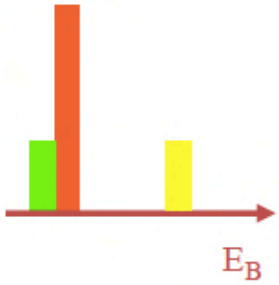
vs. tetrahedral Au_{20}^-





Methods

TR-XPS (ESCA)



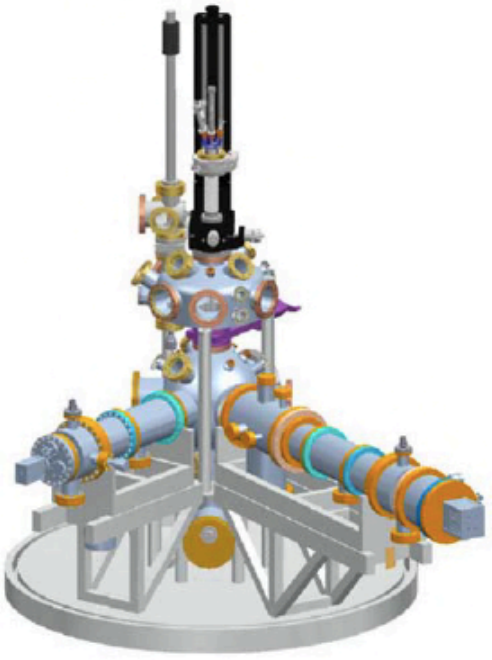
→ Element specific, chemical state selective,

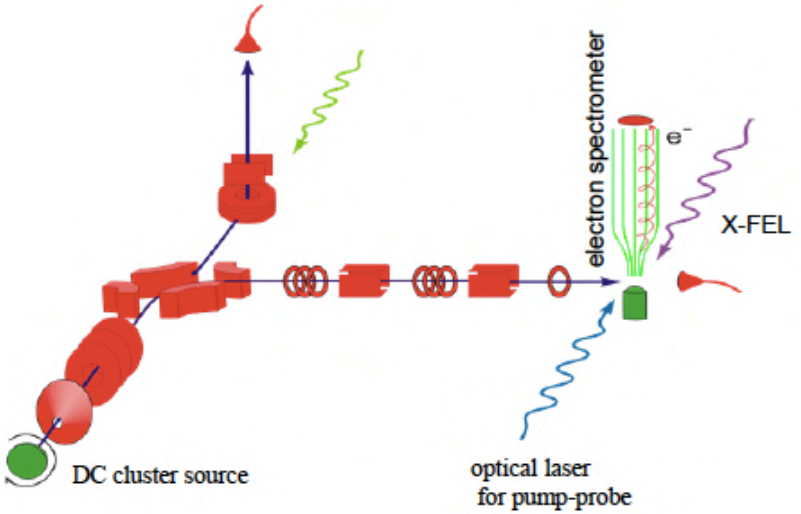
→ Local coordination

TR-XPES: Endstations

Technical concept - Endstations

Stage 1 (2016/2017) – use existing endstations





TR-PES instrument (Wurth)

Cluster instrument (Eberhardt, Ganteför)

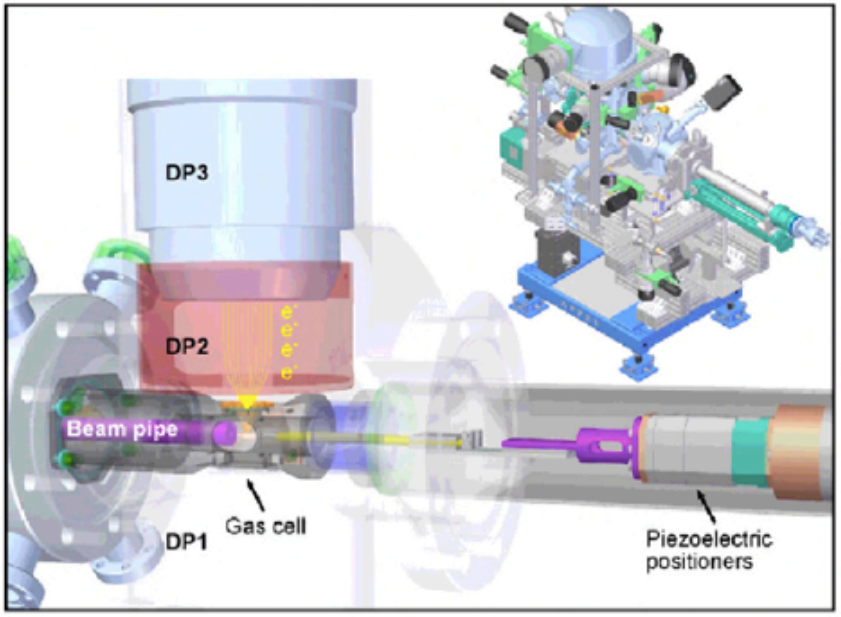
European XFEL

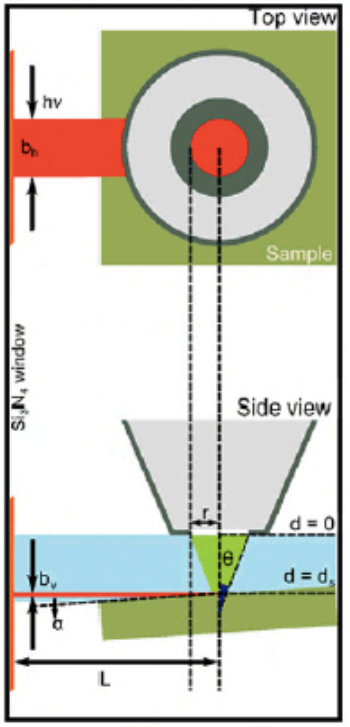
TR-XPES: Endstations

Technical concept - Endstations

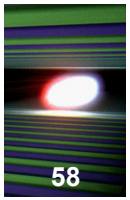
Stage 2 – dedicated instruments under development

e.g. Nilsson group - Ambient Pressure XPS





S. Kaya, et al, *Catal. Today* **205**, 101 (2012).



You are very welcome

to plan your experiments

at the European XFEL