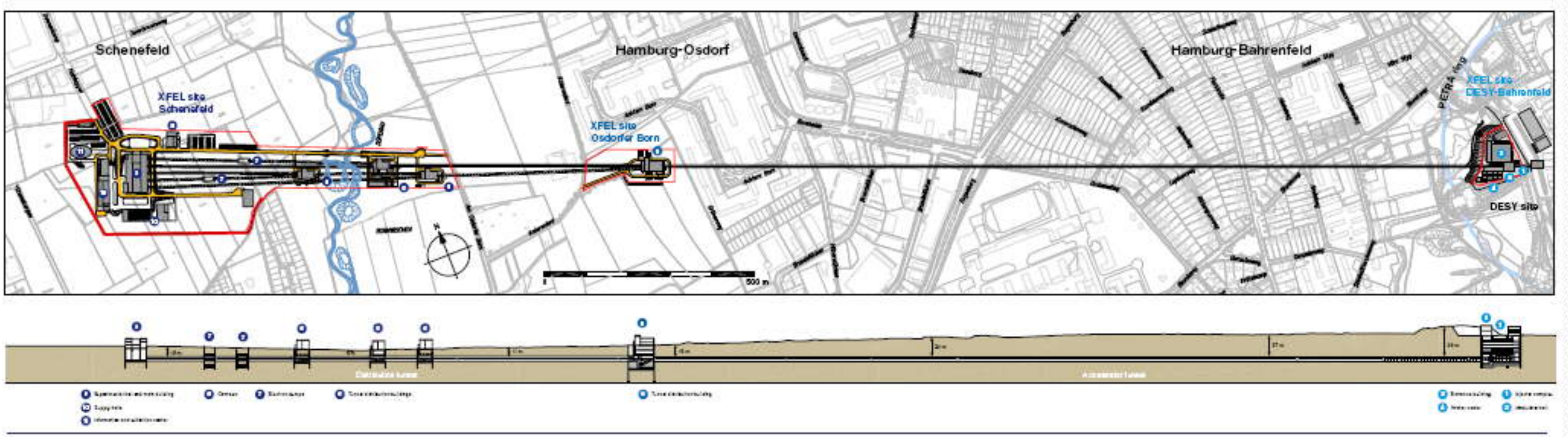
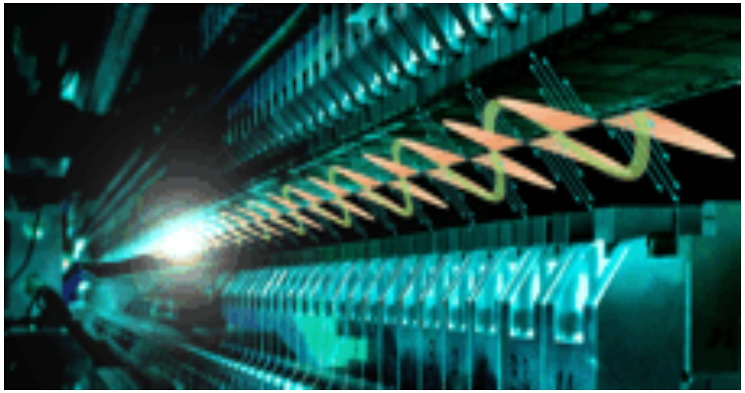
Science at X-Ray Free Electron Lasers (XFELs)

Serguei L. Molodtsov
European XFEL

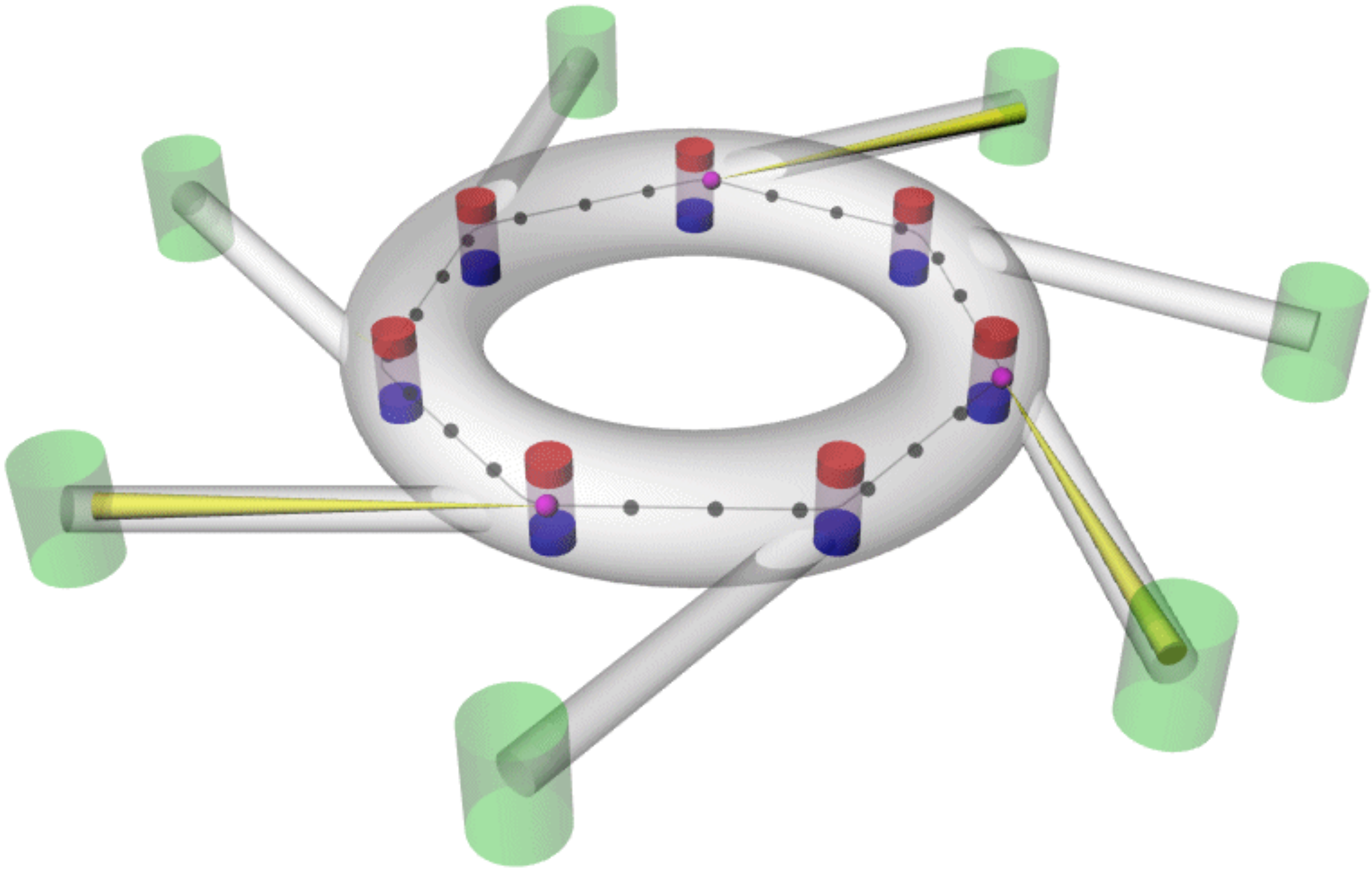


X-Rays

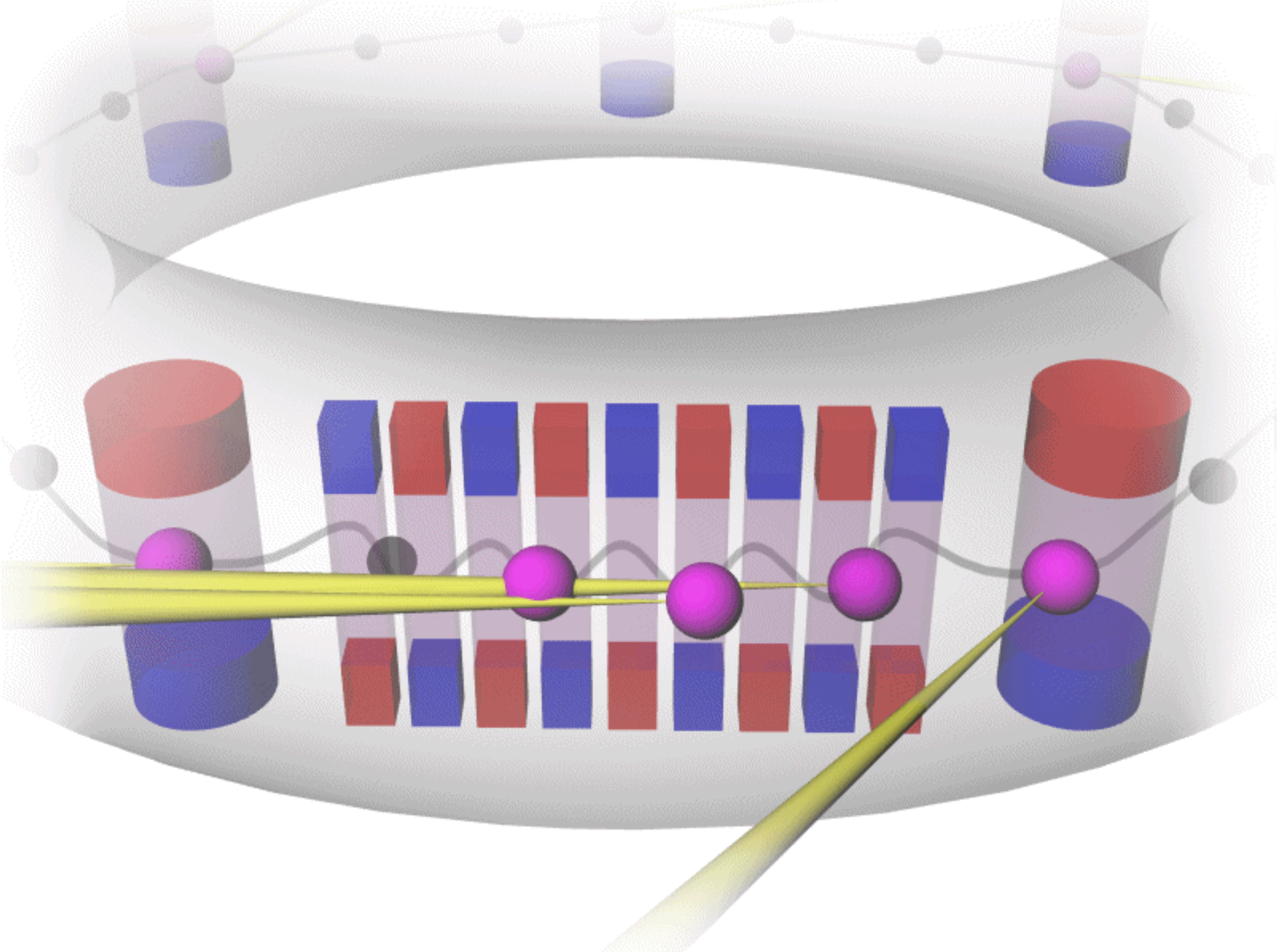
New (4th) Generation Sources
Free Electron Lasers



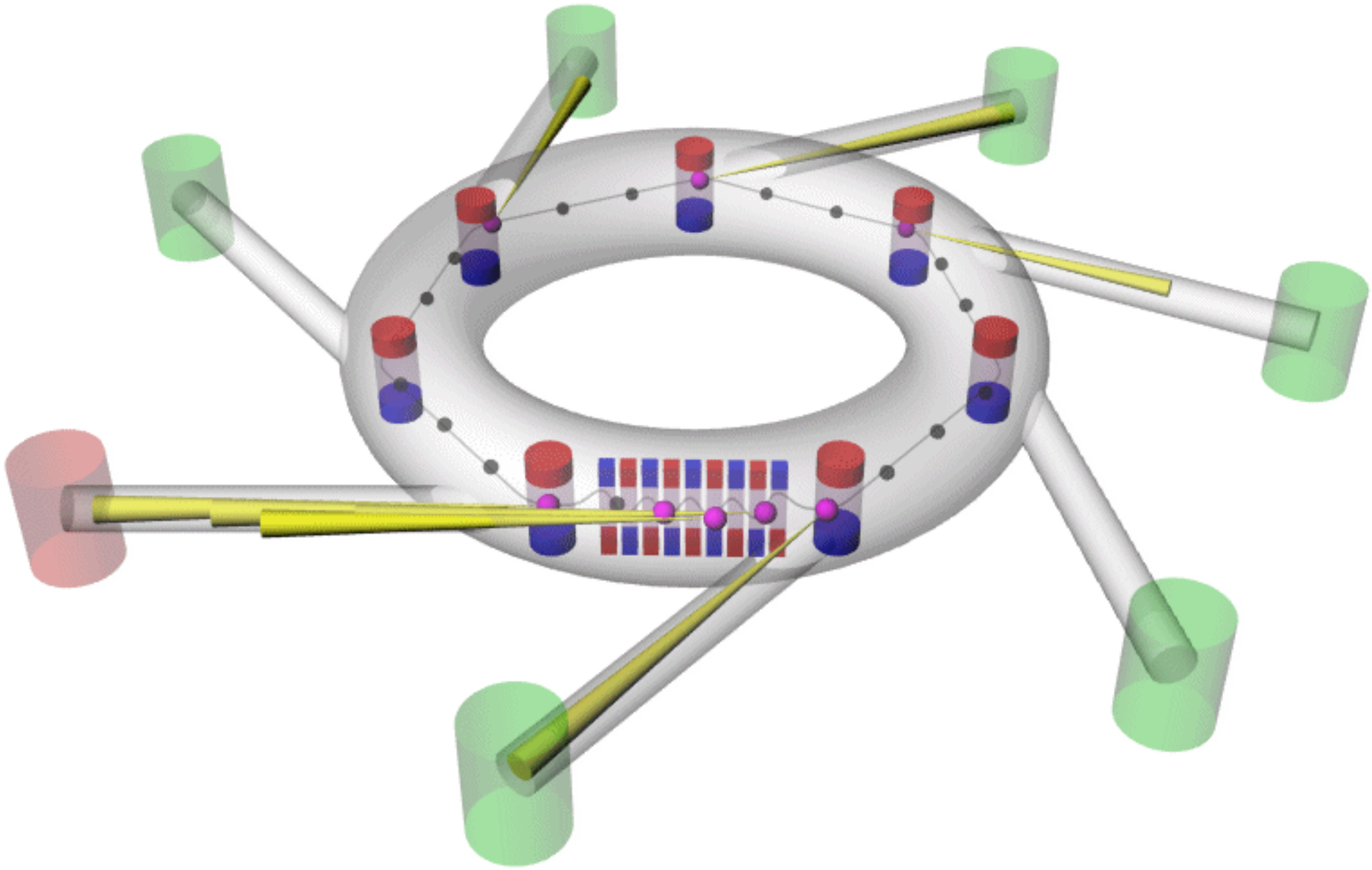
Synchrotron radiation (dipoles)



Synchrotron radiation (undulators)



Synchrotron radiation (sources + exp. stations)



Nobel prizes to synchrotron radiation work

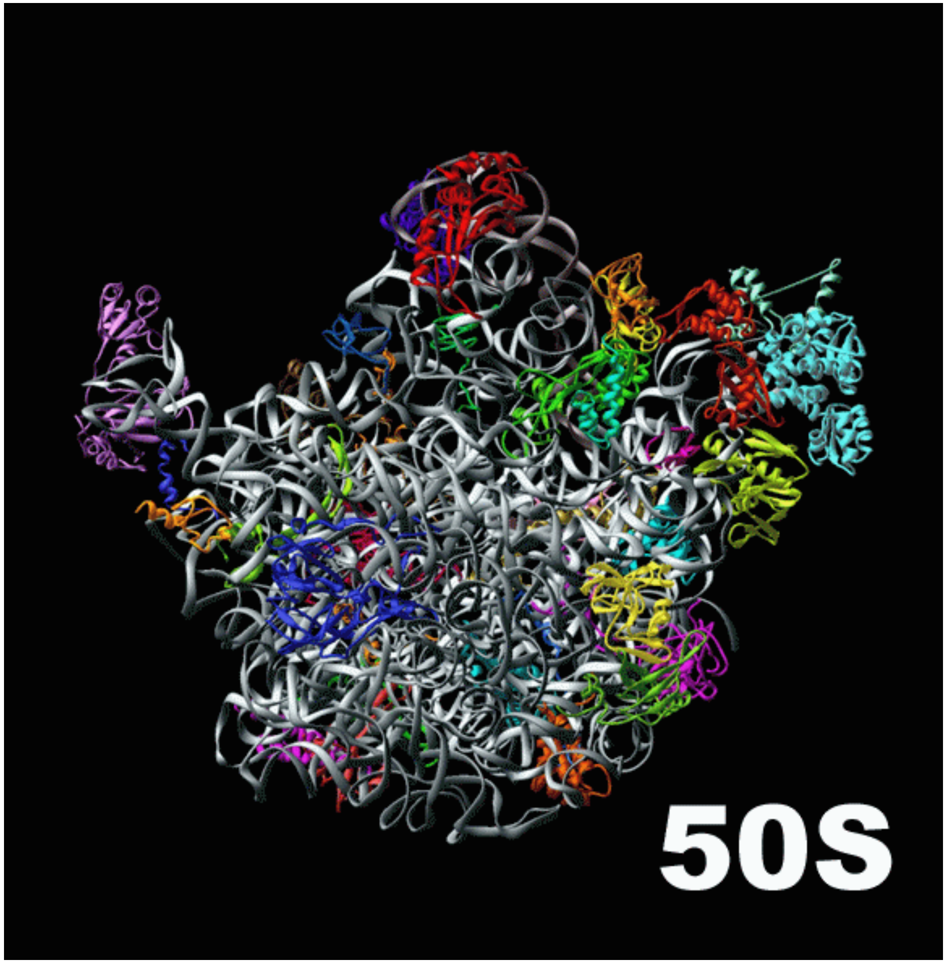
3 Win Nobel for Ribosome Research

From left, Venkatraman Ramakrishnan of the
Cambridge, England; Thomas A. Steitz of Yal
Institute of Science in Rehovot, Israel, will sha

2009 Venkatraman Ramakrishnan, Thomas Steitz & Ada Yonath

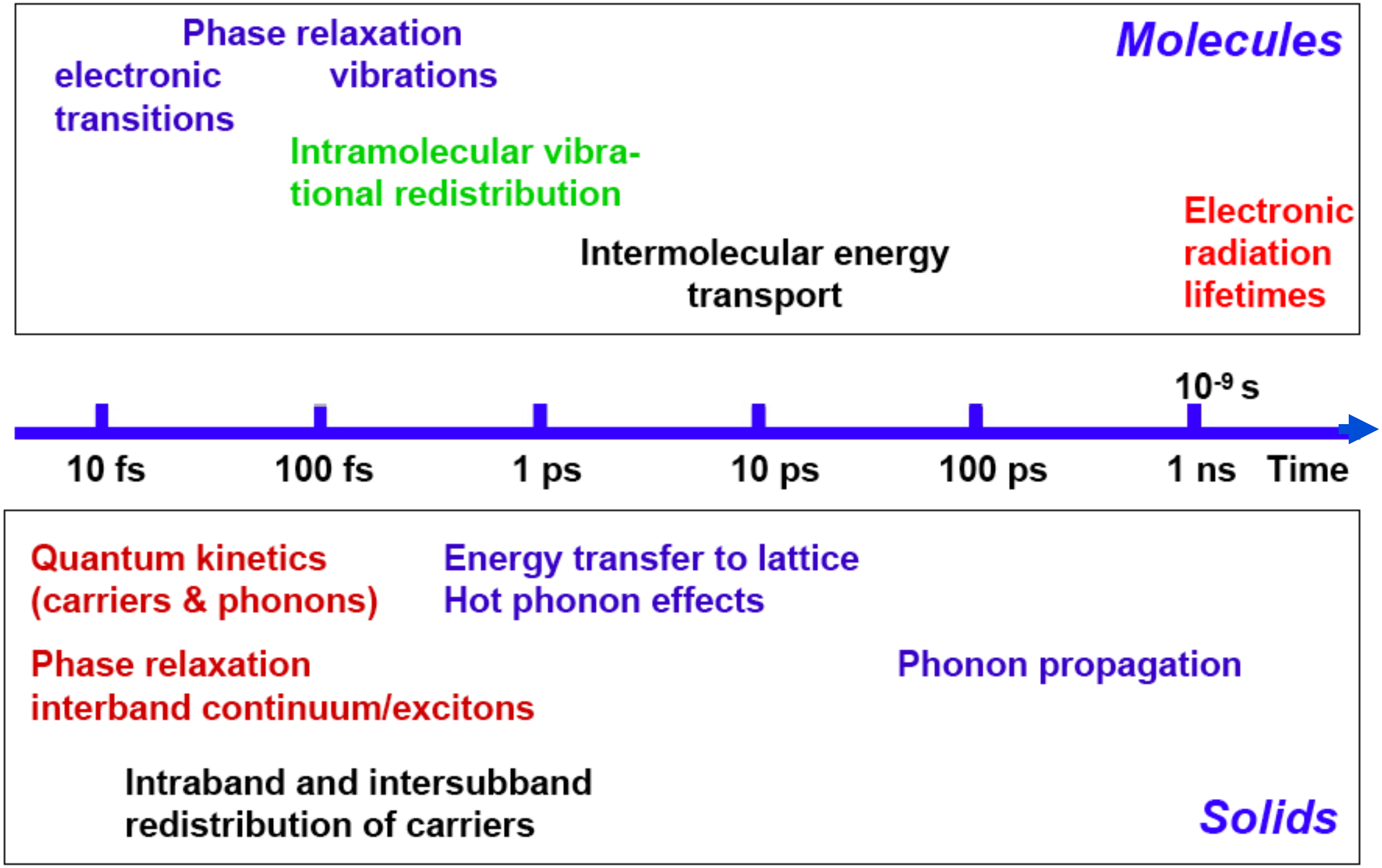
Working independently and using, among other things, the X-rays generated by powerful particle accelerators and prodigious computer calculations, the three winners and their colleagues succeeded in mapping the locations of the hundreds of thousands of atoms in the giant molecular complexes inside.

Ribosome: the Protein factory of the cell

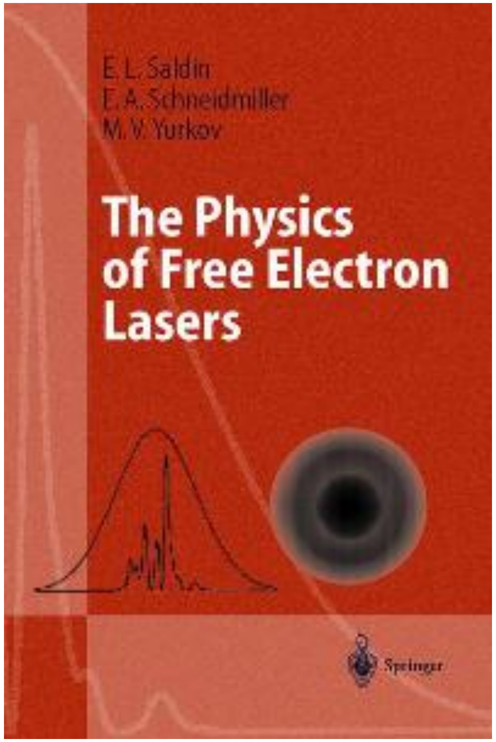


20 years of heroic efforts to crystallize Ribosomes!

Time scales for dynamics



Basics of SASE FEL process

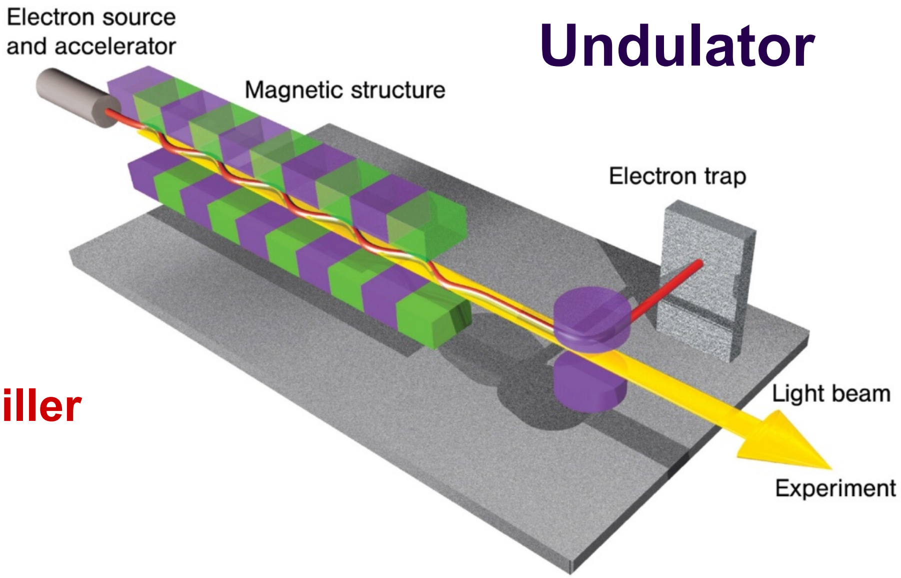

E. L. Saldin
E. A. Schneidmiller
M. V. Yurkov

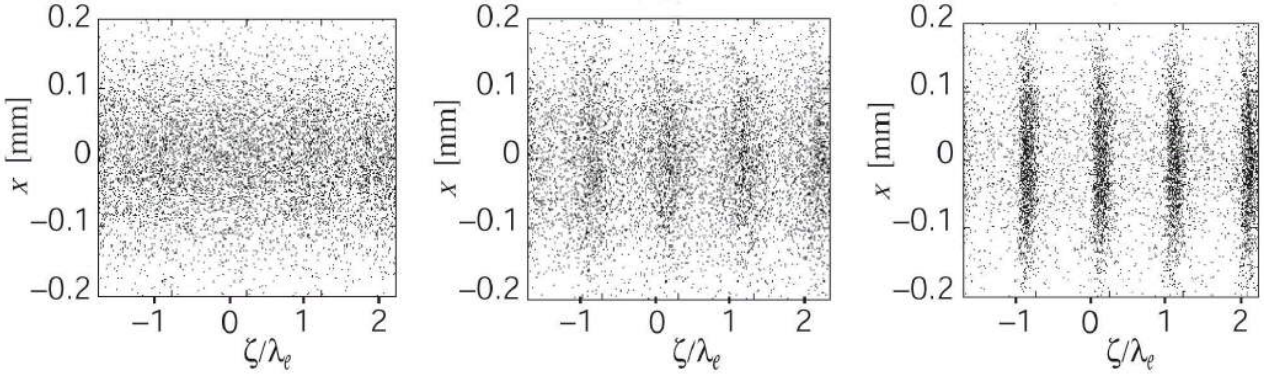
The Physics of Free Electron Lasers

Springer

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

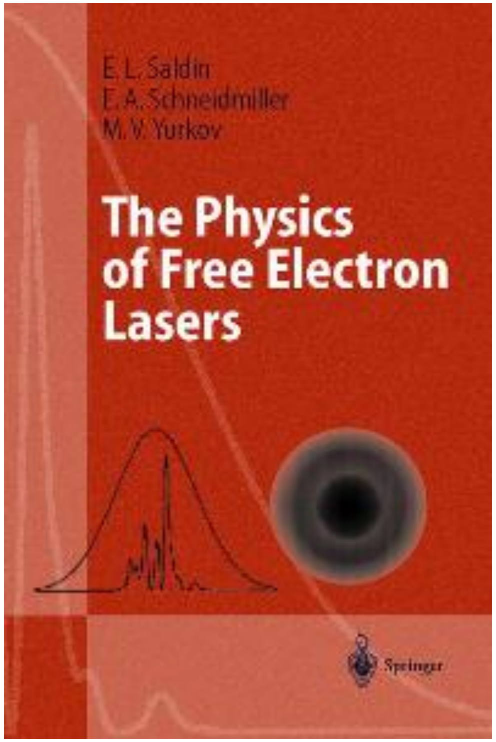
Undulator





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

Basics of SASE FEL process



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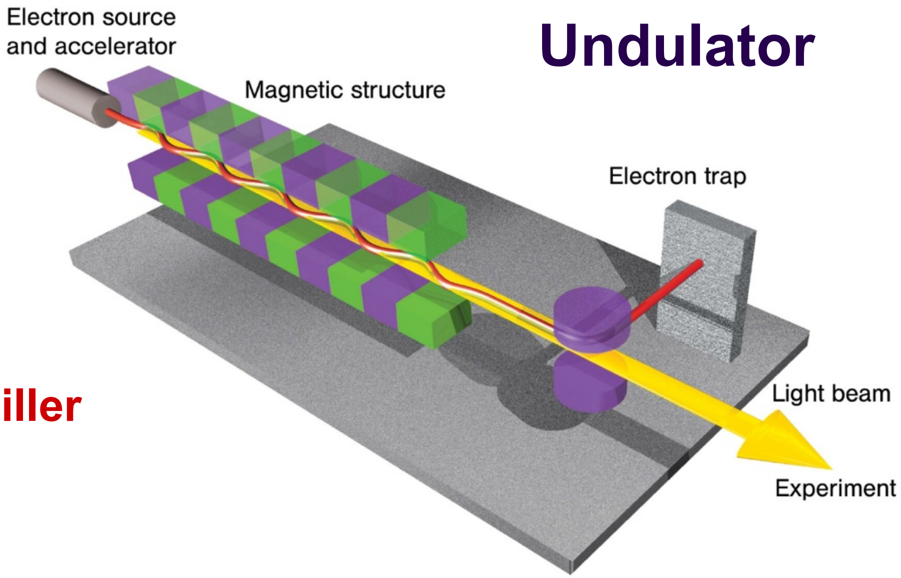
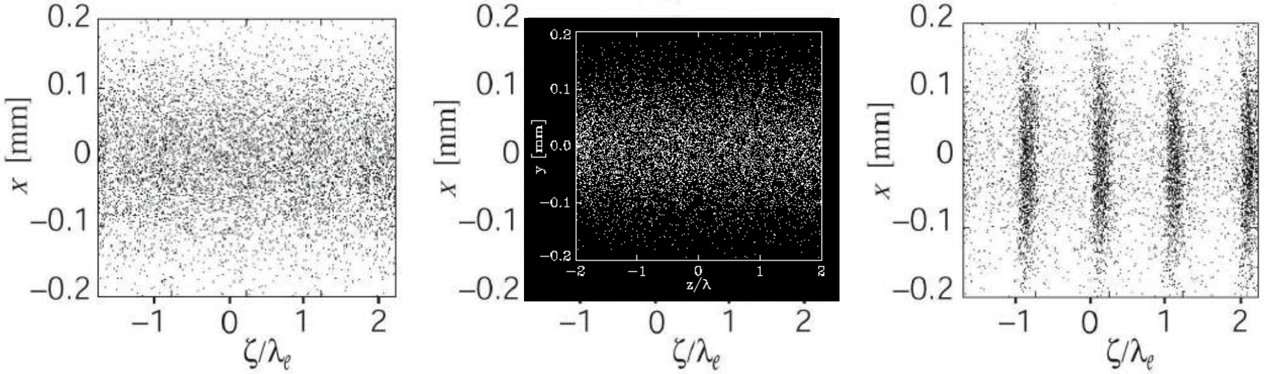
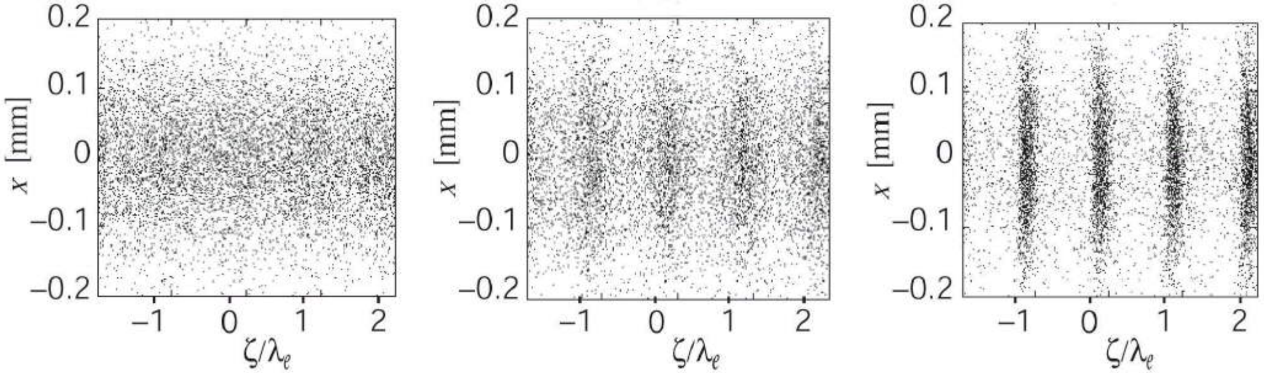
Undulator

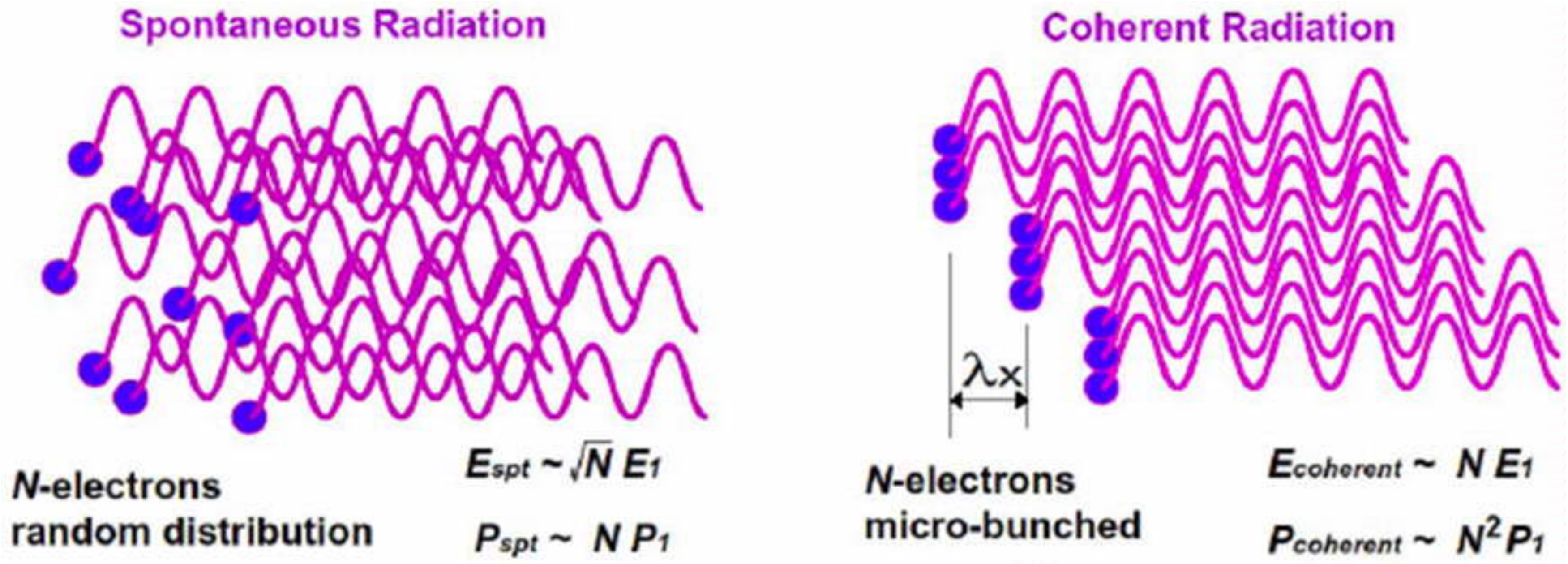




simulations at the radiation wavelength (λ_e), ζ – distance inside the undulator

Spontaneous vs. coherent radiation in undulators





Spontaneous Radiation

N-electrons
random distribution

$E_{spt} \sim \sqrt{N}\, E_1$

$P_{spt} \sim N\, P_1$

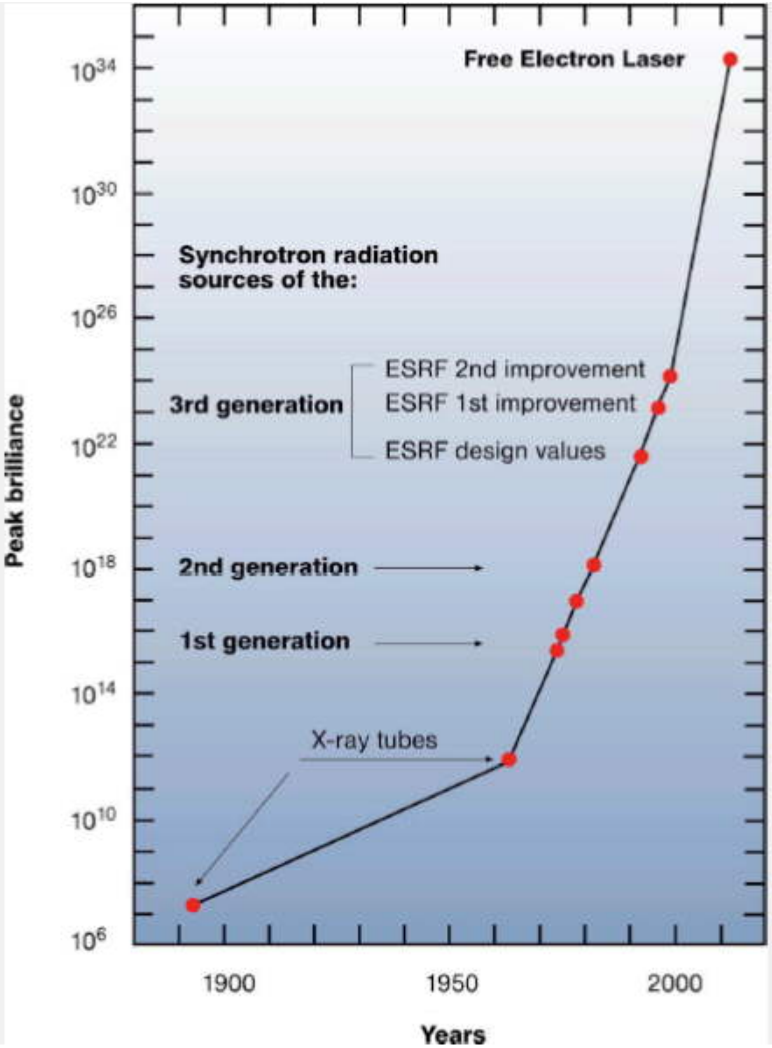
Coherent Radiation

N-electrons
micro-bunched

$E_{coherent} \sim N\, E_1$

$P_{coherent} \sim N^2 P_1$

Peak brilliance of X-Ray sources vs. time



Free Electron Lasers:

-Based on Linear Accelerator

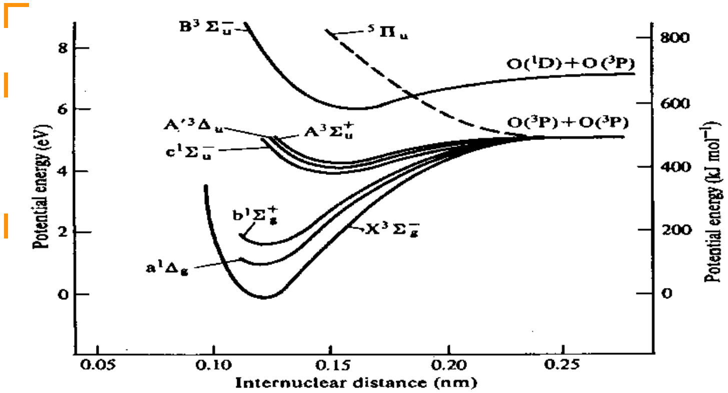
-Delivers ultrashort pulses

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

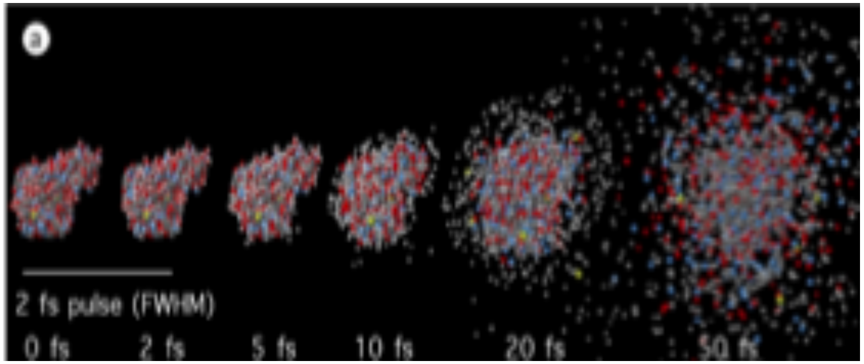
- (Transversely) Spatially coherent (laser-like) radiation

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

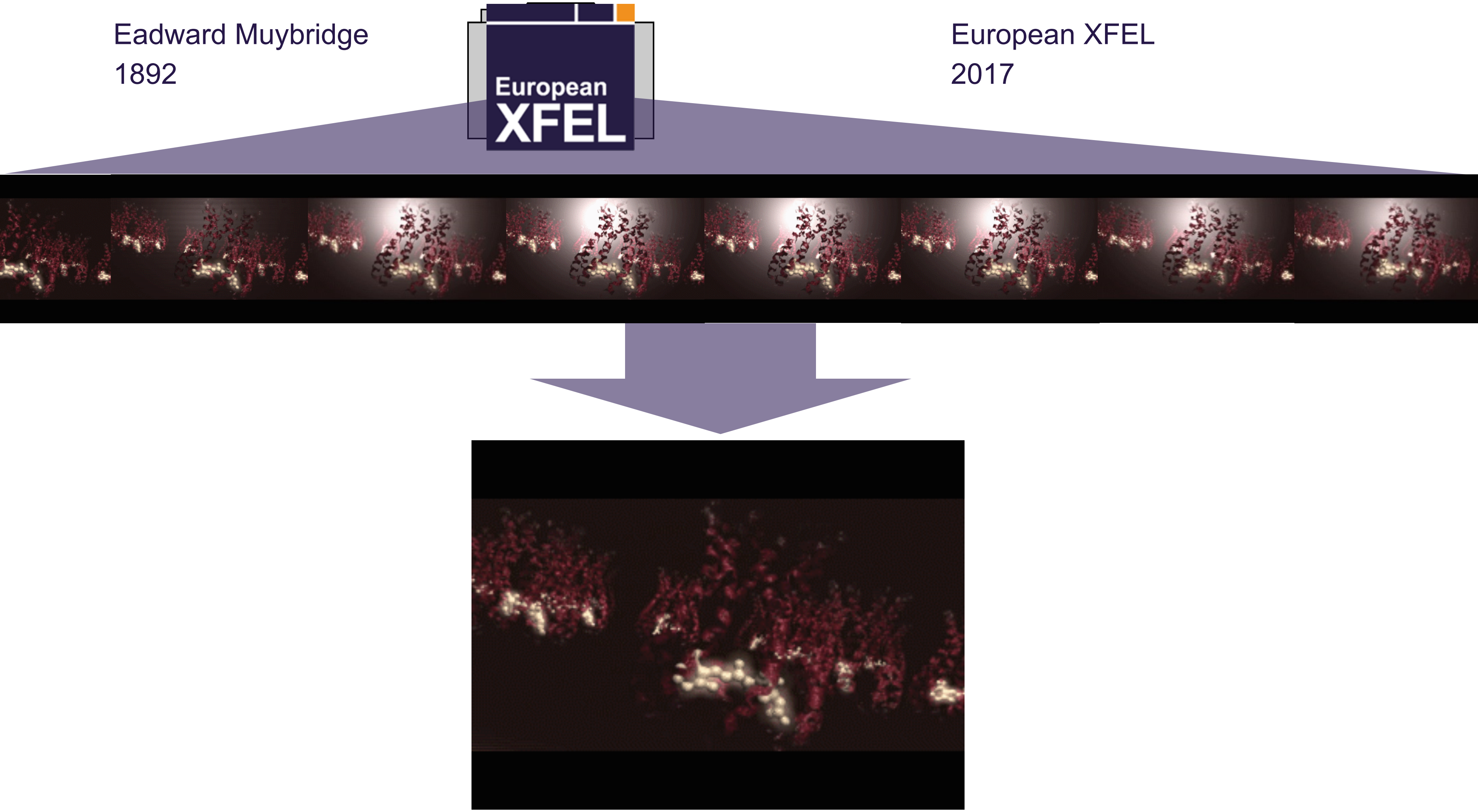
==> imaging of single nanoscale objects, possibly down to individual macromolecules (no crystals)

==> investigation of matter under extreme conditions…

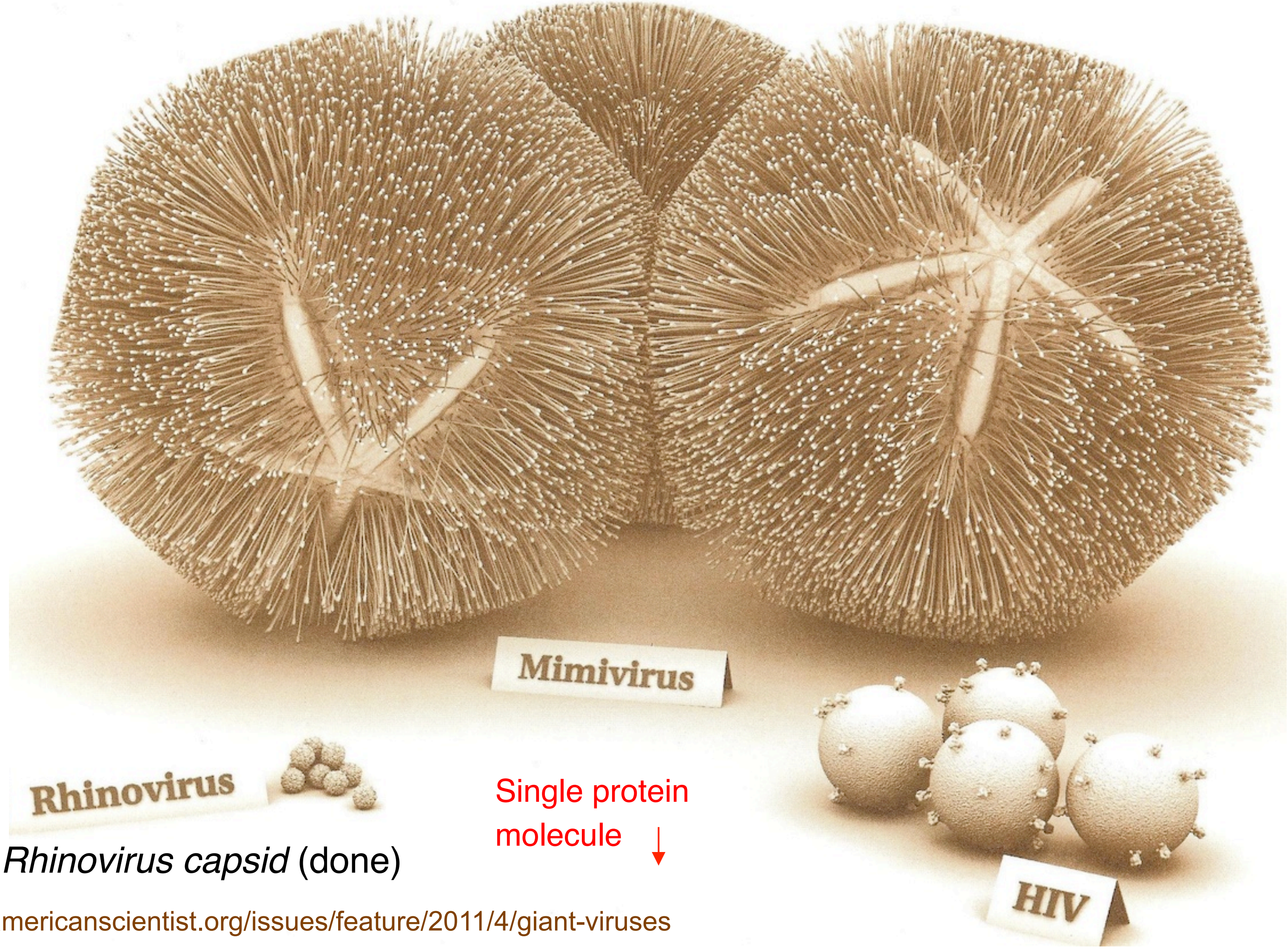
Making molecular movies

Eadward Muybridge
1892

European XFEL
2017



Tremendous variety of bio-objects to be studied



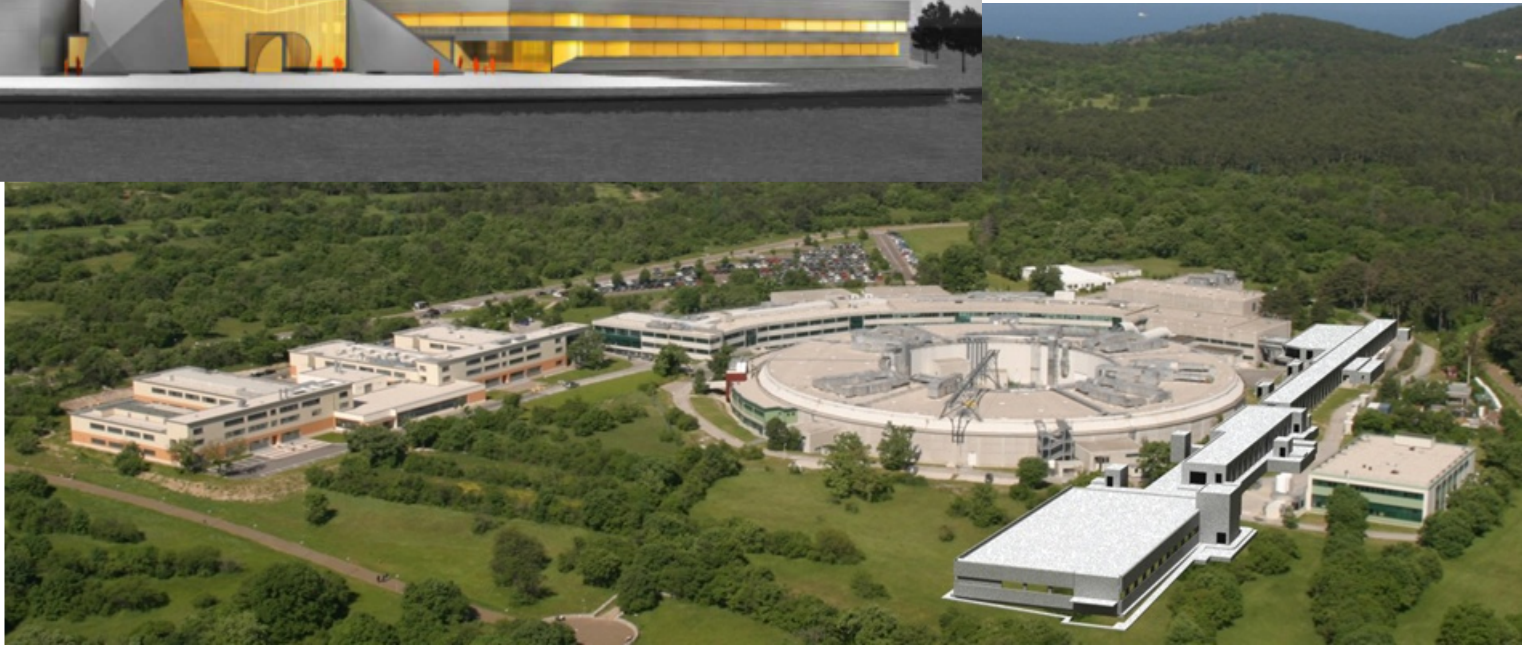
Single protein molecule ↓

Rhinovirus capsid (done)

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

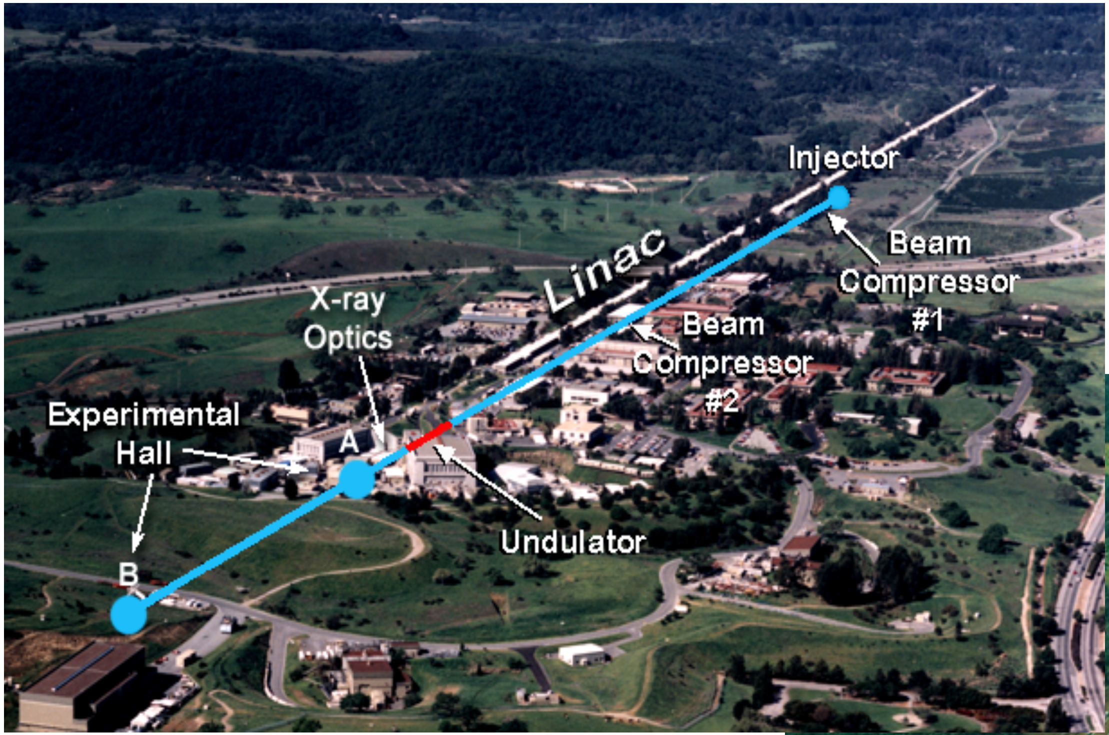
Soft X-Ray FEL facilities

FLASH /
DESY



FERMI /
ELETTRA

Hard X-Ray FEL facilities



2009 -120 p/s

LCLS

LINAC COHERENT

LIGHT SOURCE

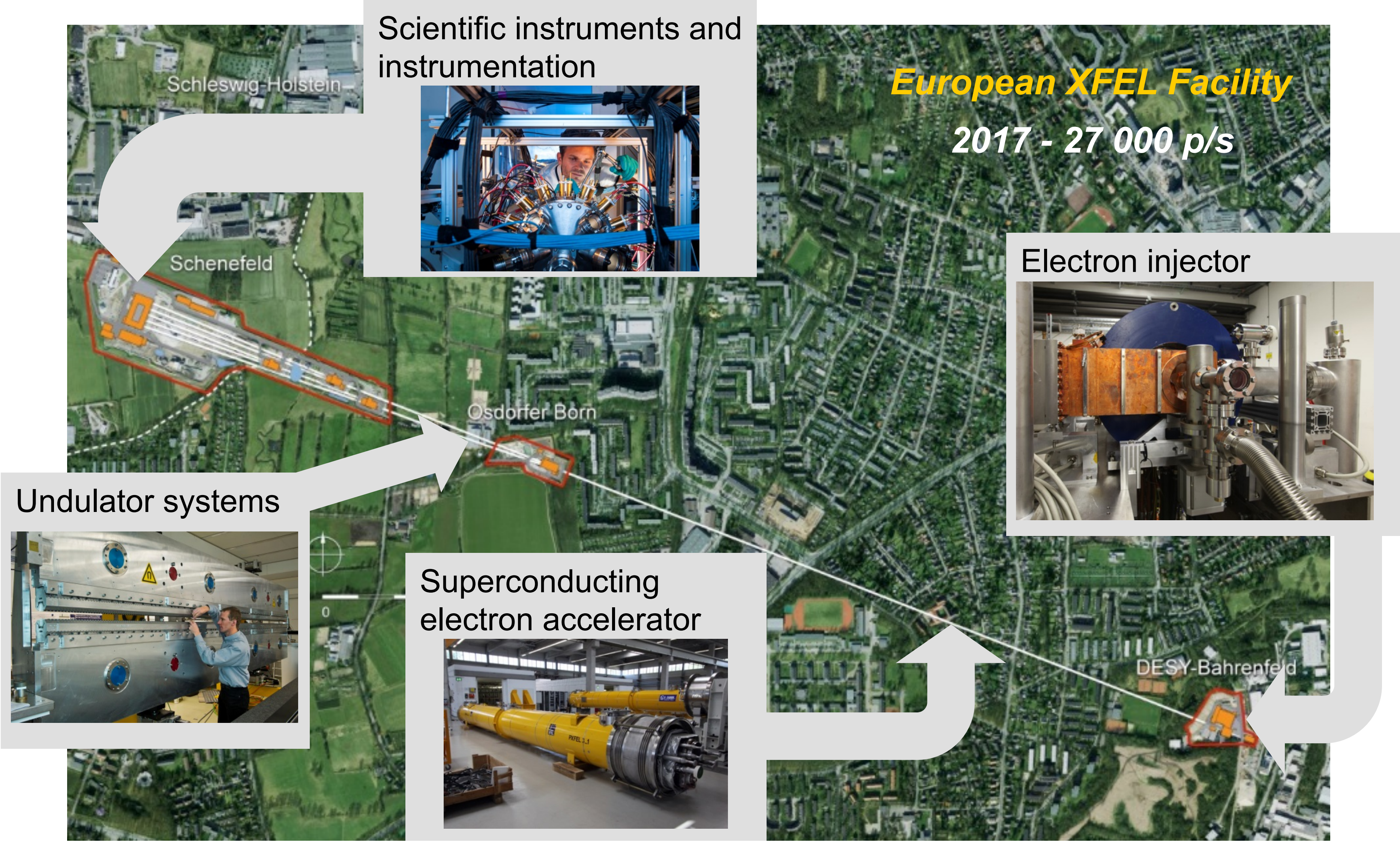
2011 - 60 p/s

SCSS

SPring-8 Compact

SASE Source

European XFEL



European XFEL Facility

2017 - 27 000 p/s

Scientific instruments and instrumentation

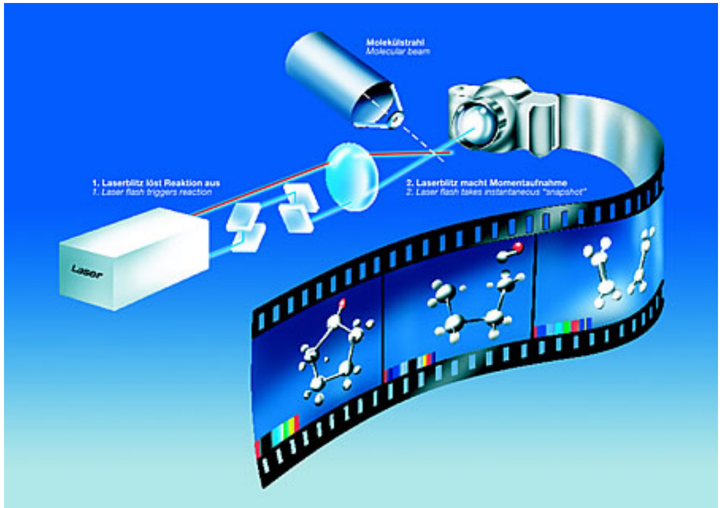
Electron injector

Undulator systems

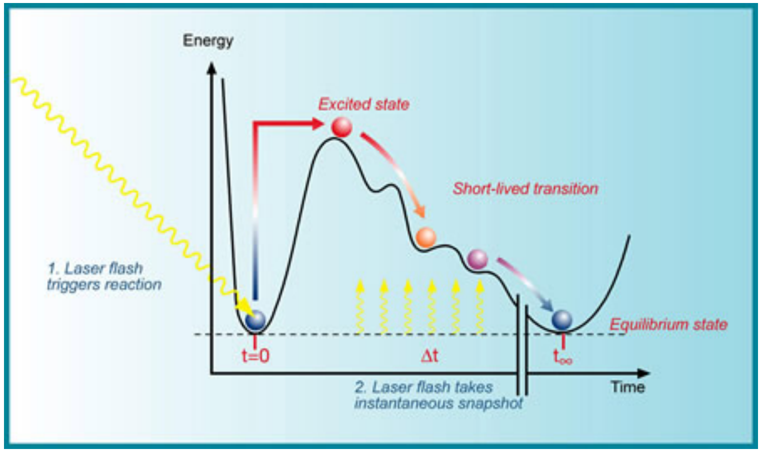
Superconducting electron accelerator

Femtochemistry

- Capturing chemical reactions on film



"Filming" chemical reactions using ultra-fast lasers.

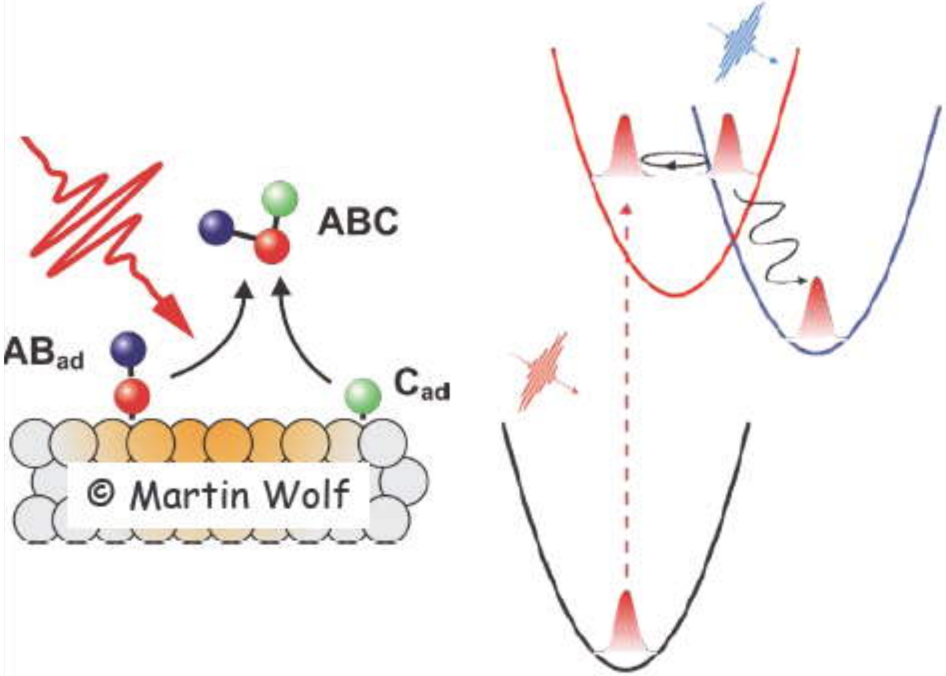


A chemical reaction is triggered by a laser flash. A second laser pulse is then sent at varying intervals after the first one to take instantaneous snapshots.

Surface chemical reactions: capturing and controlling the transition states

Photoinduced reaction dynamics

THz/IR/VIS pump /X-ray probe

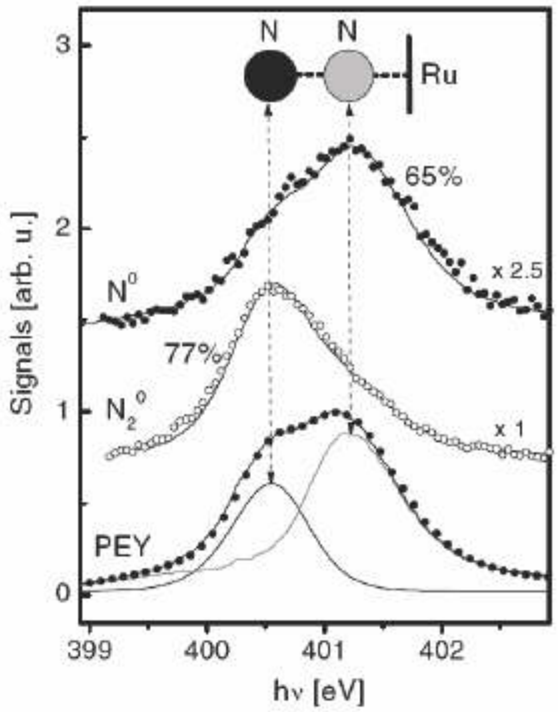


© Martin Wolf

Radiation chemistry

X-ray pump-X-ray probe

selective bond breaking

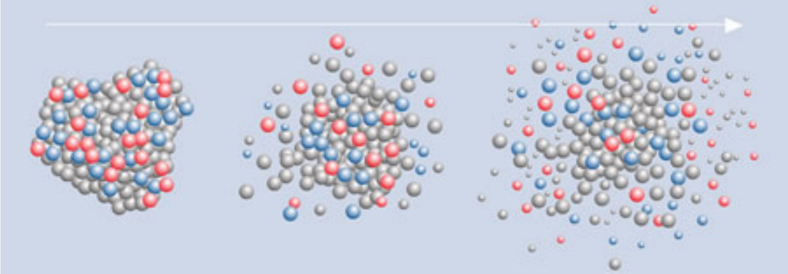


R. Romberg et al, PRL 84, 374 (2000)

Structural biology

- Shedding light on biomolecules

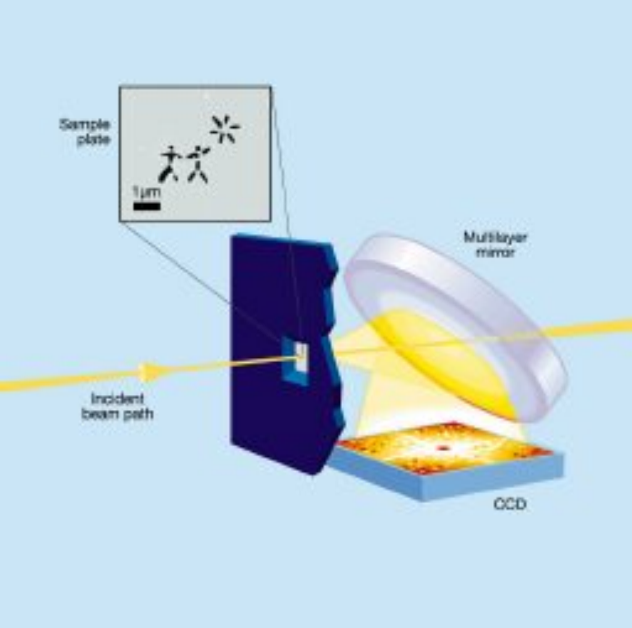
Protein DNA complexes are often very large and difficult to crystallize. The X-ray laser opens up possibilities to unravel their structure and function in the living organism without the need for crystallization.



Biomolecules are destroyed by intense X-ray radiation. In order to obtain a usable image of the biomolecule, the image must be recorded very quickly.

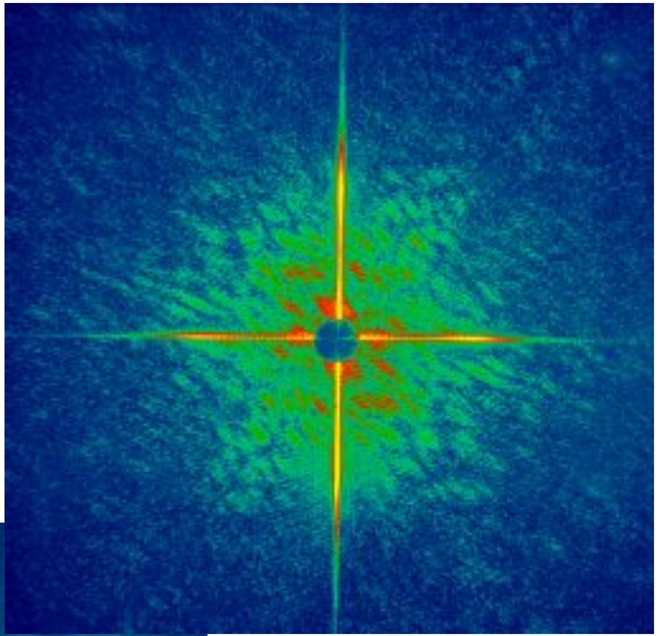
Experiments at FLASH (H. Chapman, CFEL, Hamburg)

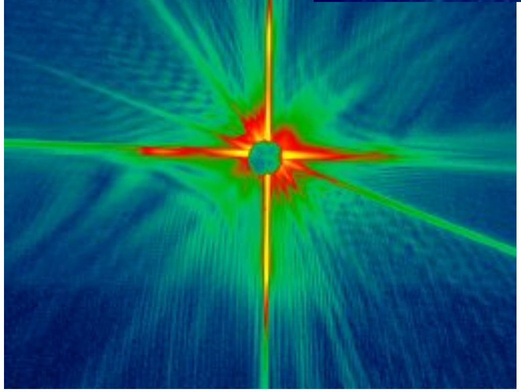
A single shot image



A nanoscale object can be imaged by a single femtosecond FEL pulse before the sample explodes

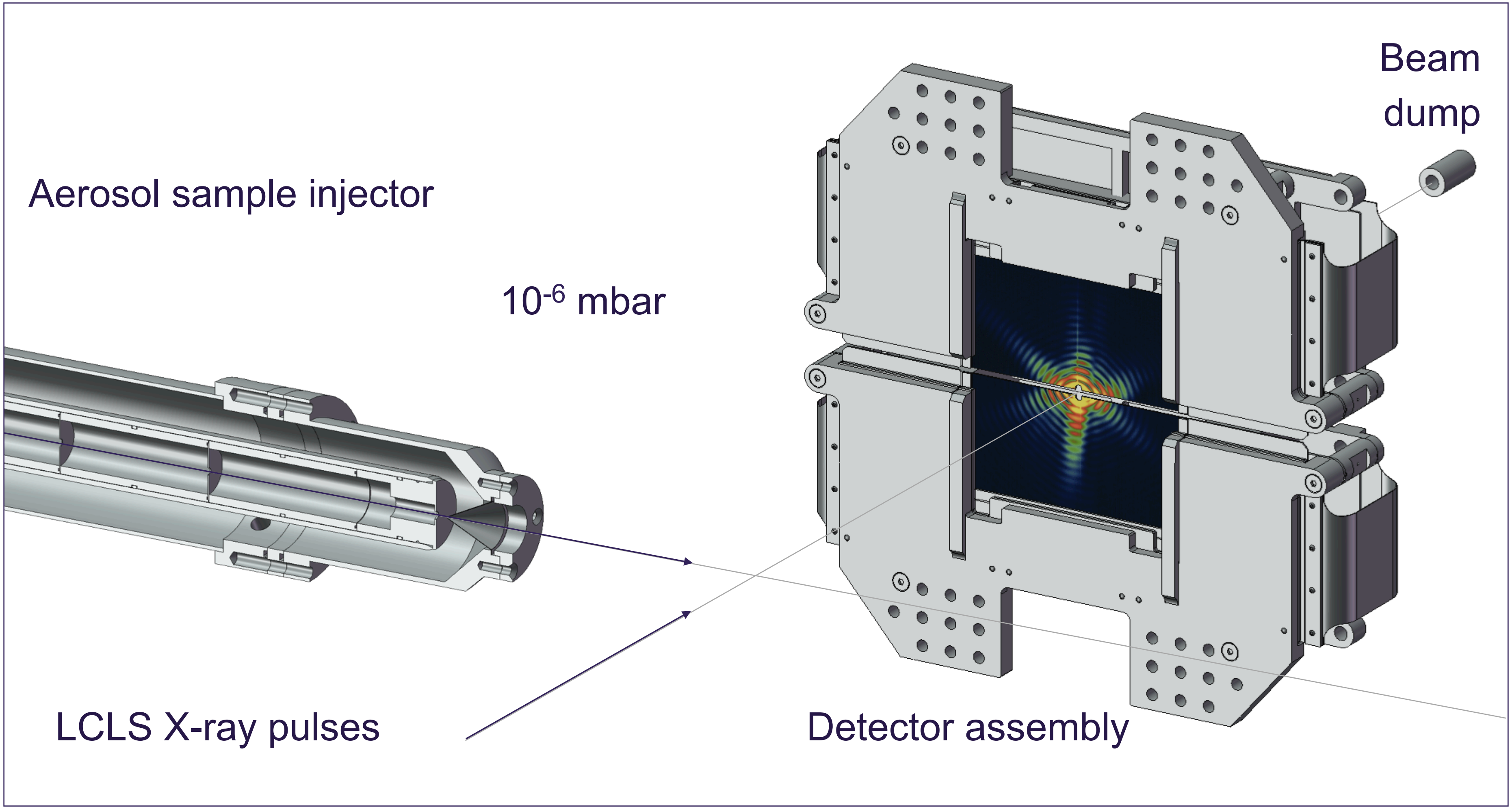
A coherent diffraction pattern recorded from a single 25 fs pulse





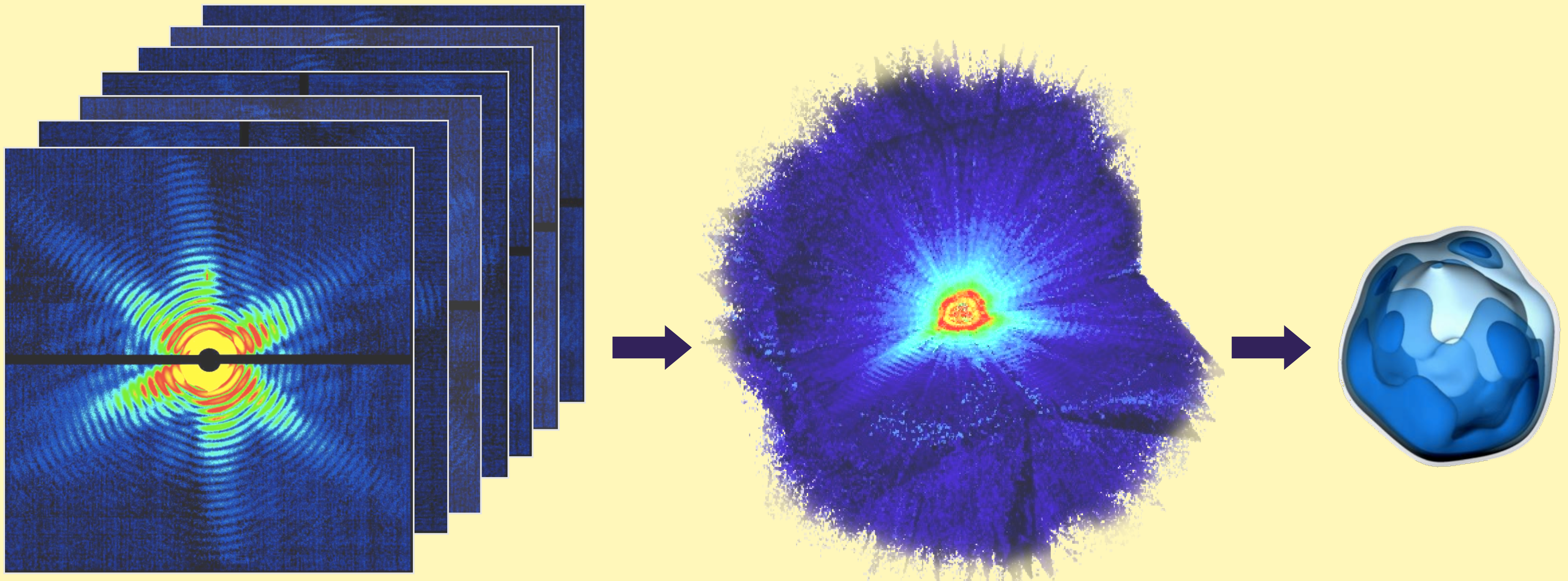
Diffraction pattern from a subsequent pulse showing that the sample was destroyed after recording the image

Single particle imaging (J. Hajdu, Uni Uppsala)



Measured hit rates match theoretical values

Single particle imaging (J. Hajdu, Uni Uppsala)



From 2D to 3D structure determination

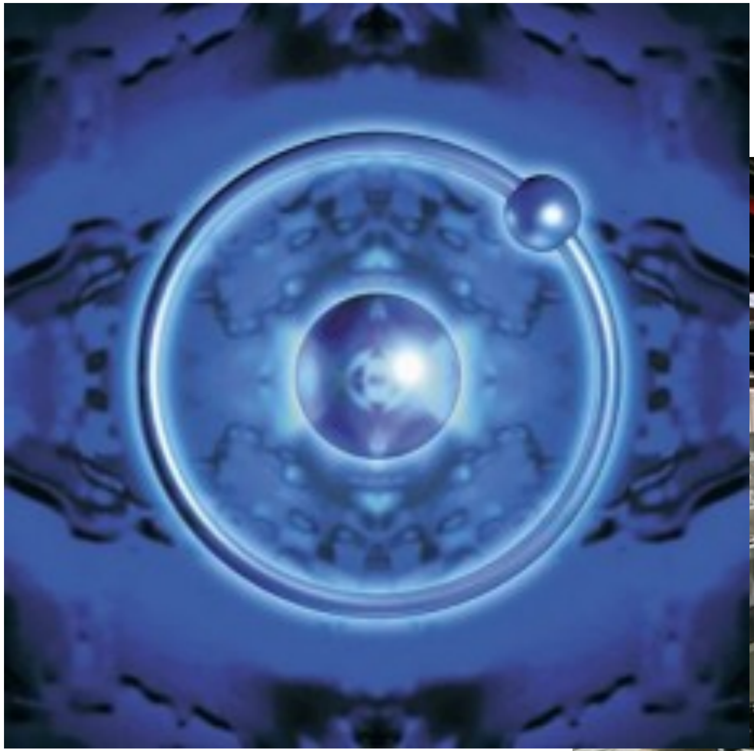
Energy research

- Alternative (hydrogen, solar cells, etc.) economies

A *solar cell* (also called a *photovoltaic cell*) is an electrical device that converts the energy of light directly into electricity by the photovoltaic effect.

The *hydrogen economy* is a system of delivering energy using hydrogen. The technological challenge of providing safe, energy-dense storage of hydrogen on-board the vehicle must be overcome.

Hydrogen storage

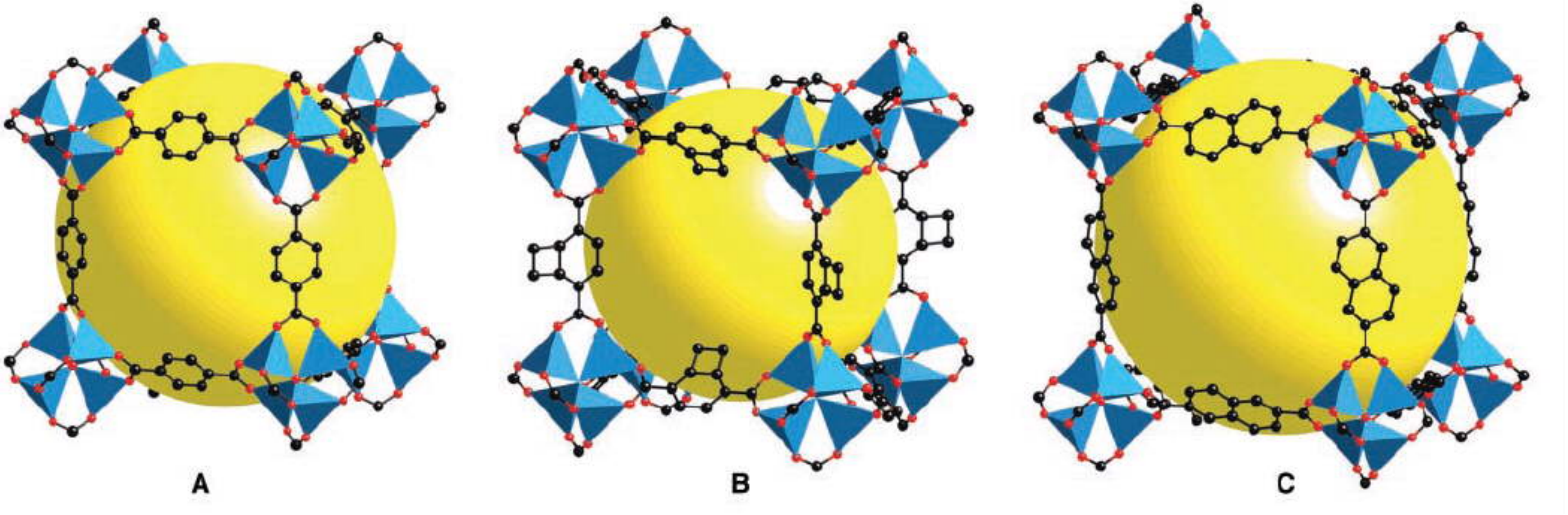


H atom

High pressure bottle storage

Real structure, MOF storage (J. Eckert, UC Santa Barbara)

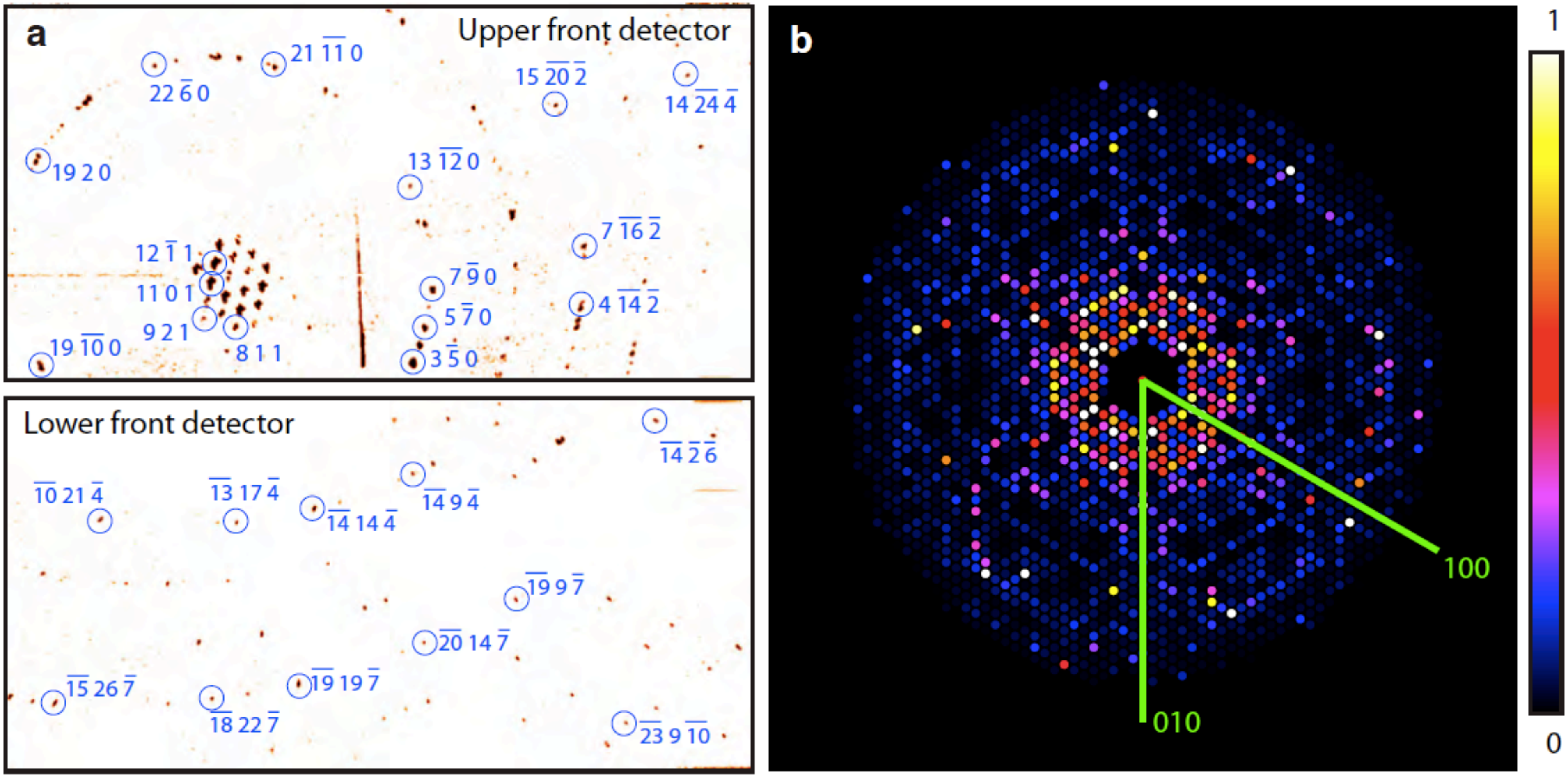
Metal-organics frameworks (MOF): single-crystal study

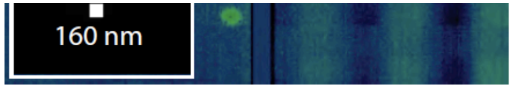


Single-crystal x-ray structures of MOF-5 (**A**), IRMOF-6 (**B**), and IRMOF-8 (**C**) [MOF-5: $Zn_4O(BDC)_3$ (BDC = 1,4-benzenedicarboxylate)]

Real nanocrystals structure (H. Chapman, CFEL)

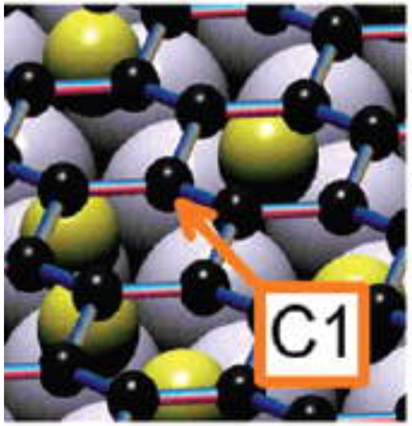
H.N. Chapman et al., *Nature 2010* Photosystem I, nanocrystals >100 nm

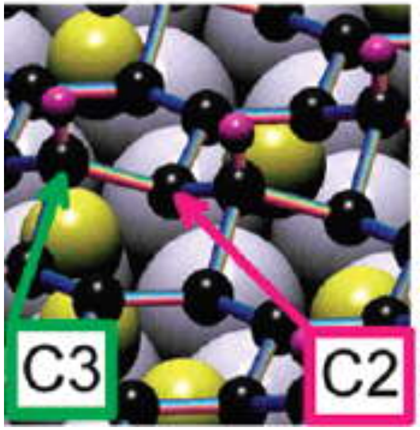




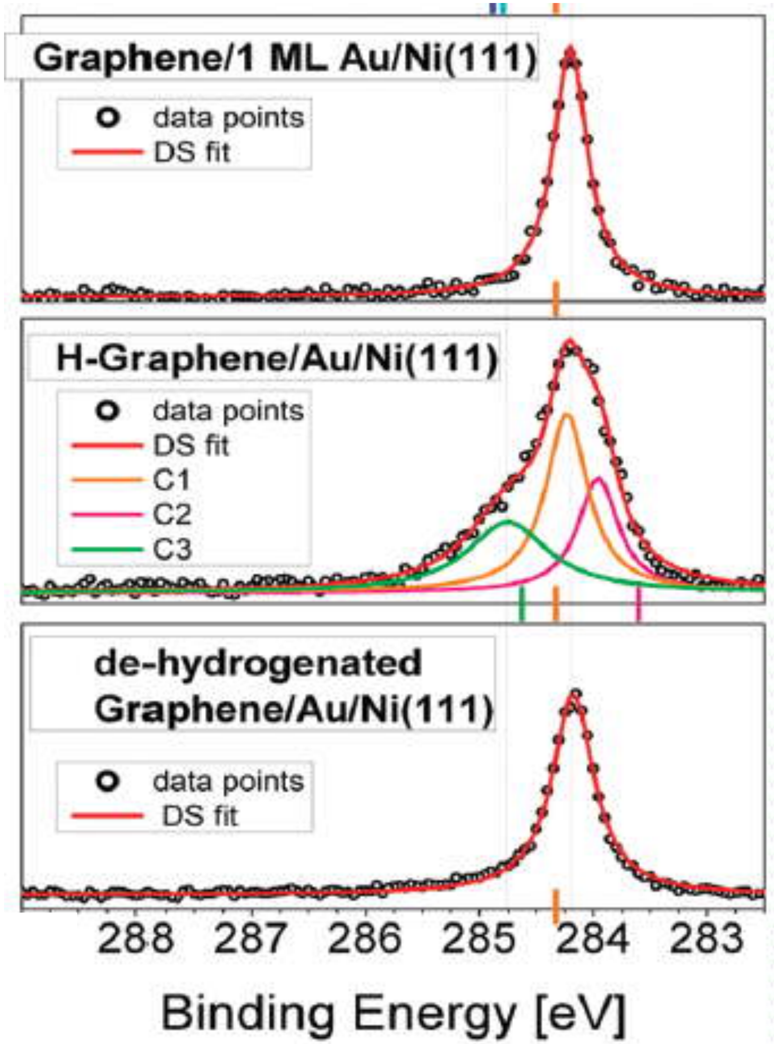
Electronic structure, graphene (A. Grüneis, D. Vyalikh, TUD)

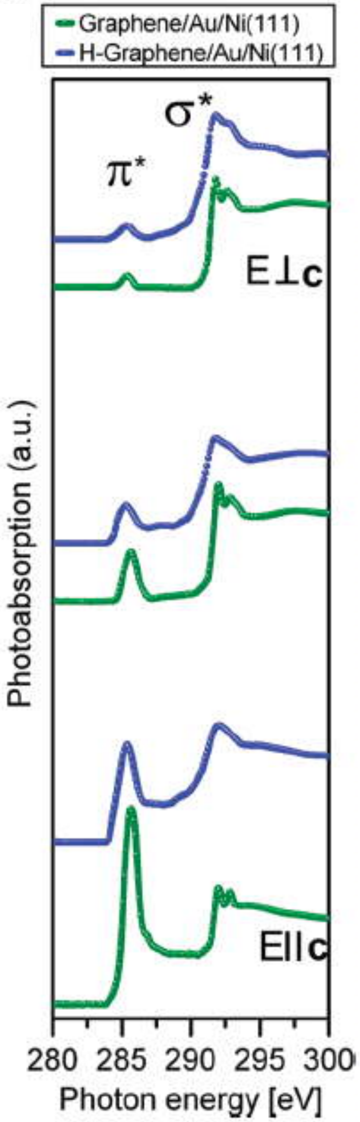
Graphene/Au/Ni(111)



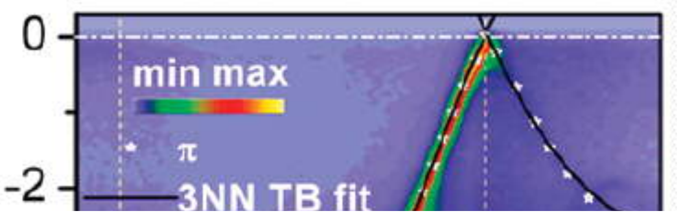


H-Graphene/Au/Ni(111)

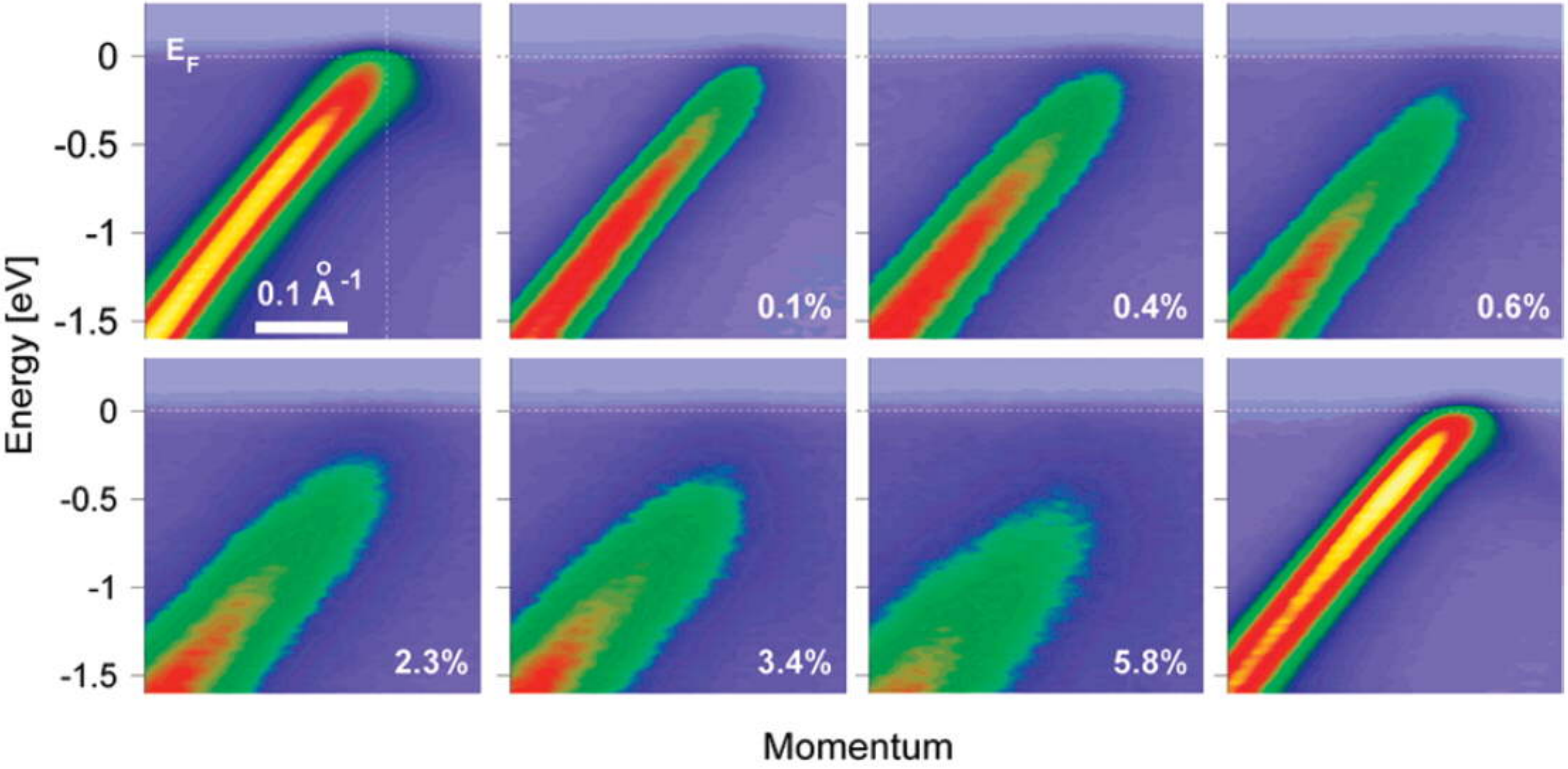




Electronic structure, graphene (A. Grüneis, D. Vyalikh, TUD)

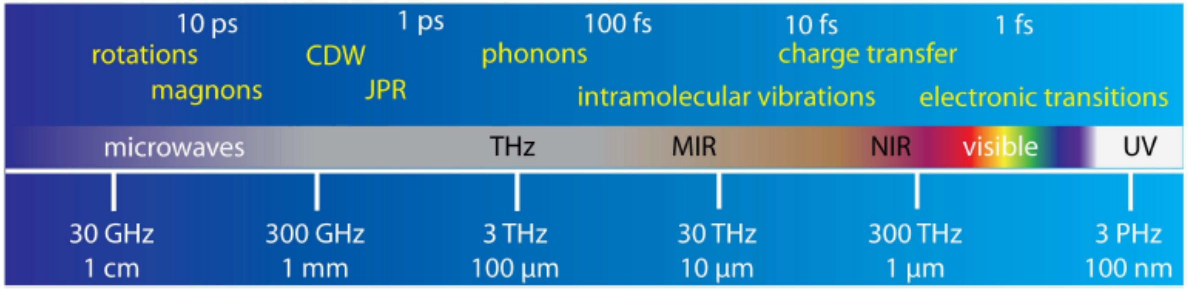


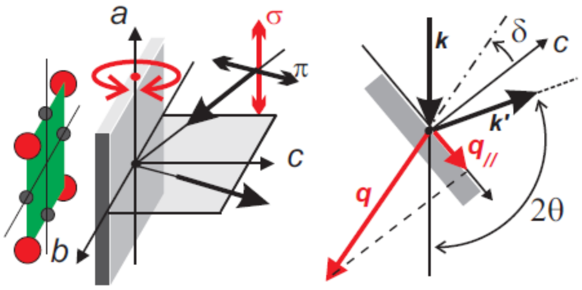
Gap opening (H storage) is reversible!



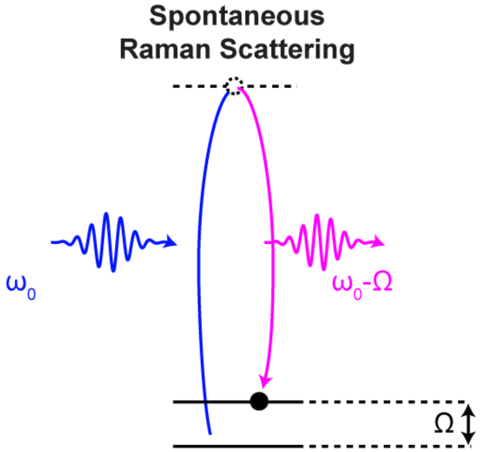
Resonant Inelastic X-ray Scattering: RIXS

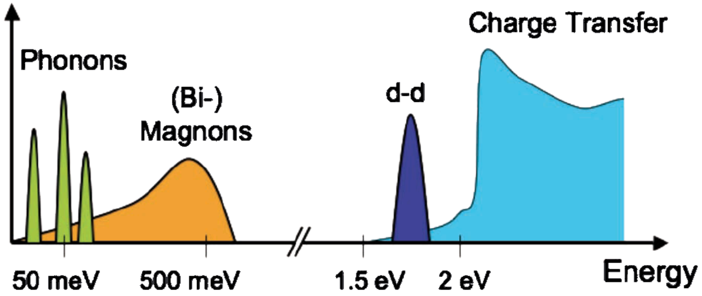
- Selective excitations pump

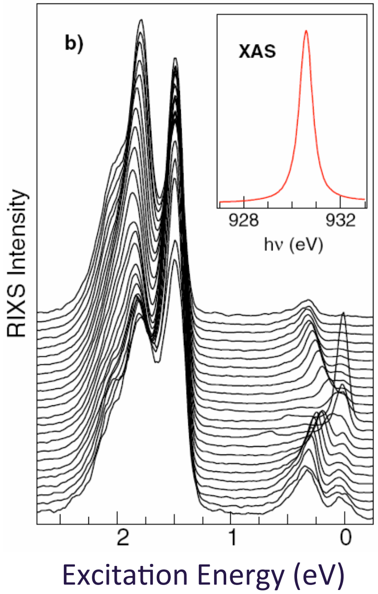




- Selective excitations probe (RIXS)





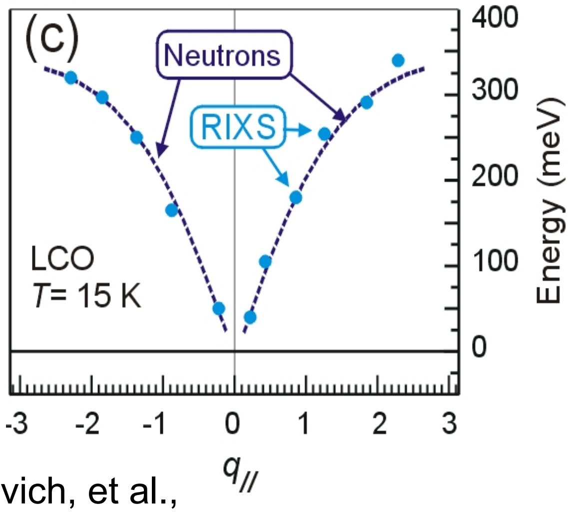


Ament et al., Rev.Mod.Phys. **83**, 75 (2011)

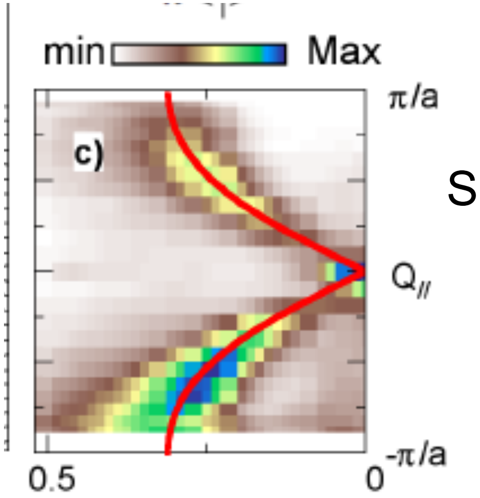
Guarise et al., PRL **105**, 157006 (2010)

Role of high resolution RIXS: low energy excitations in solids

La_2CuO_4

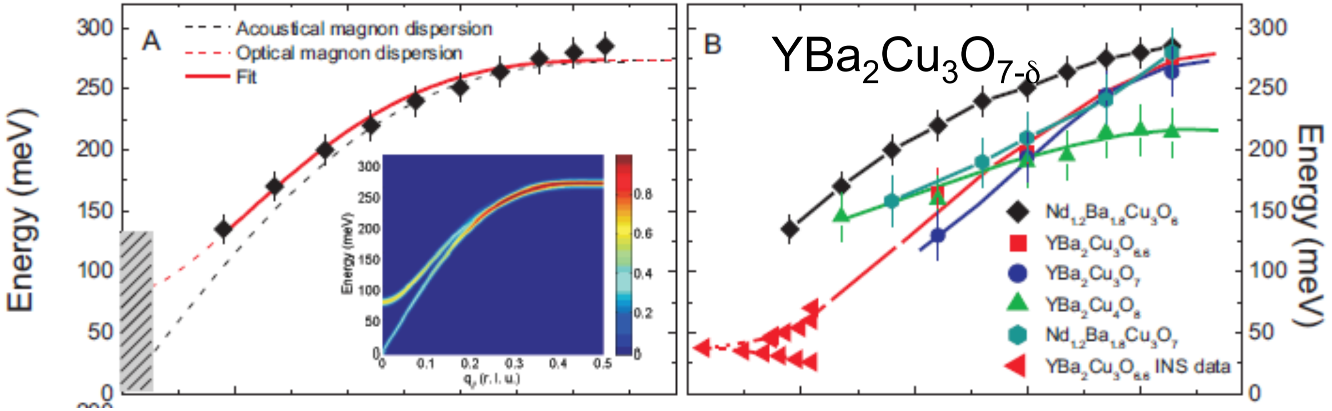


L. Braicovich, et al.,
Phys. Rev. Lett. 104, 077002 (2010)



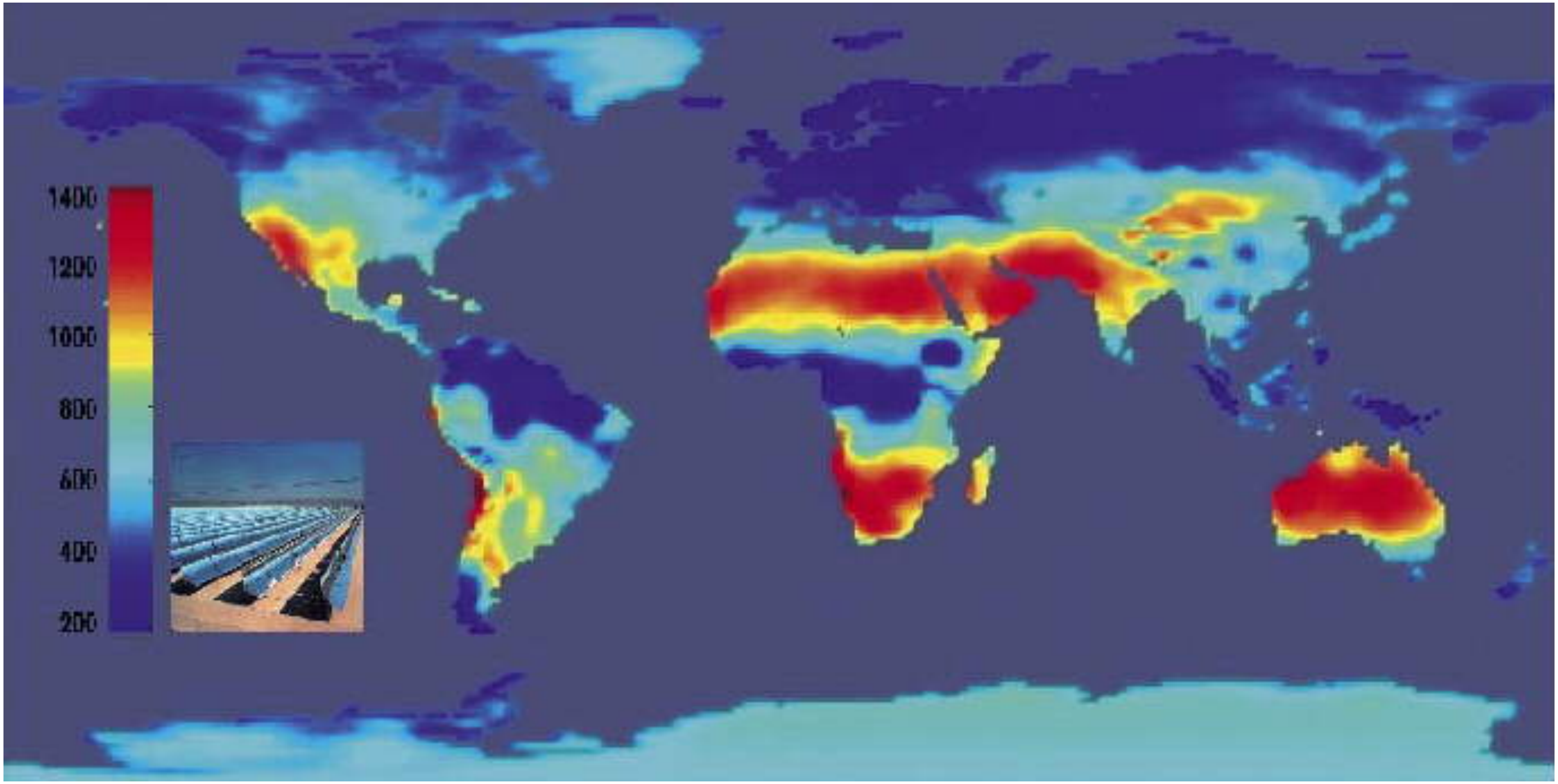
$Sr_2CuO_2Cl_2$

M. Guarise, et al.,
Phys. Rev. Lett. 105, 157006 (2010)



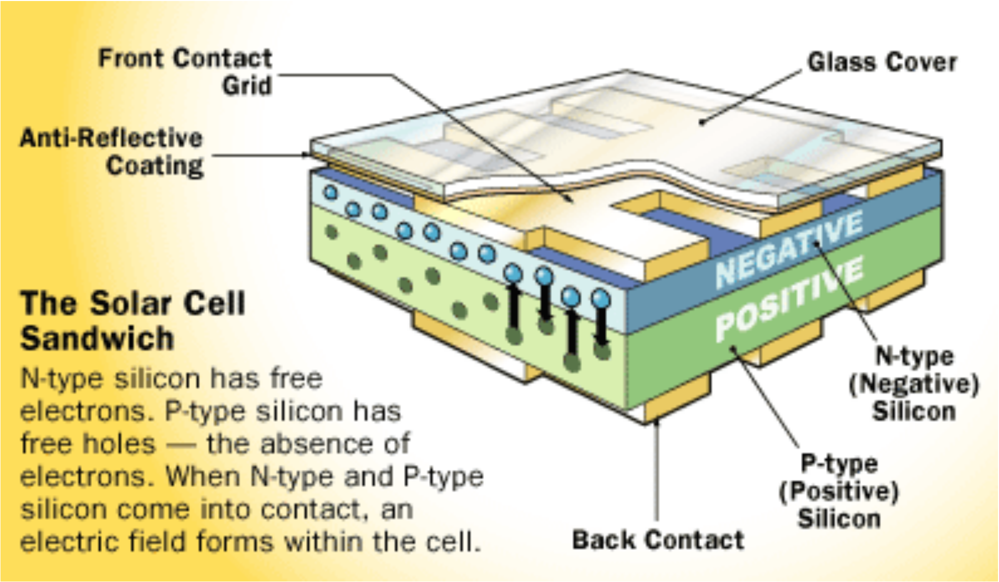
M. Le Tacon, et al., Nature Phys. 7, 725 (2011)

Solar energy



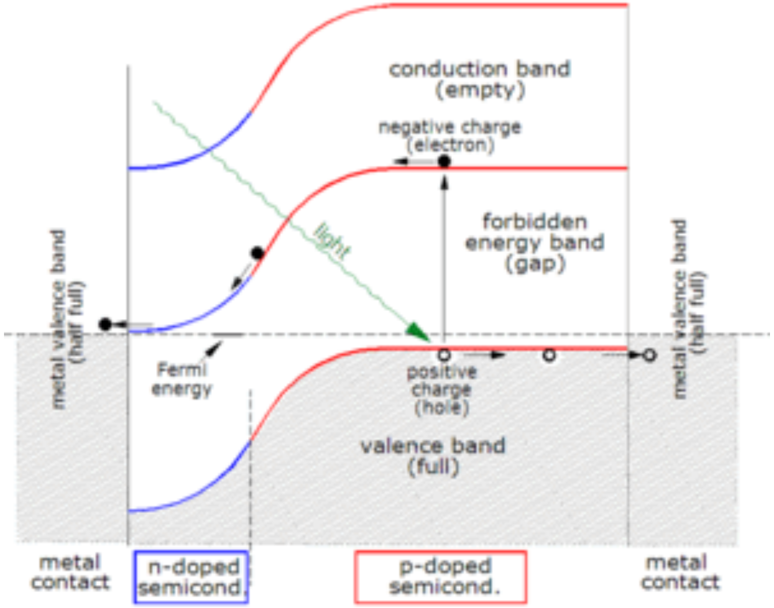
Potential annual thermal yields (kWh/m²) from solar parabolic troughs.

Solar cells



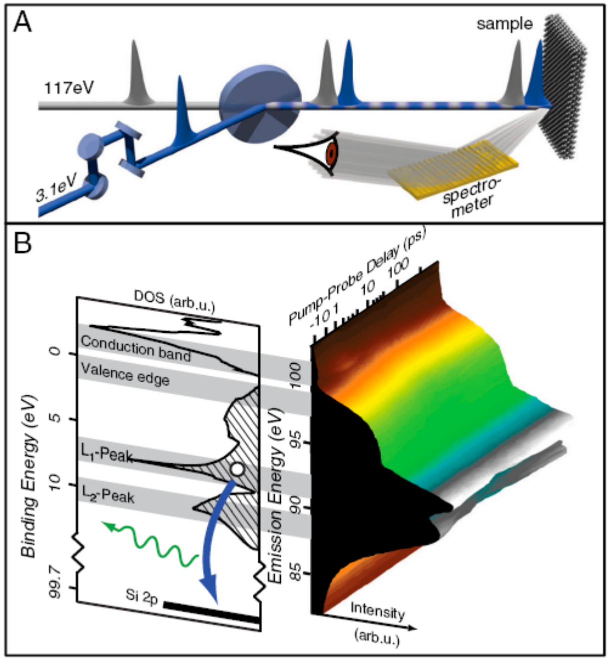
The Solar Cell Sandwich

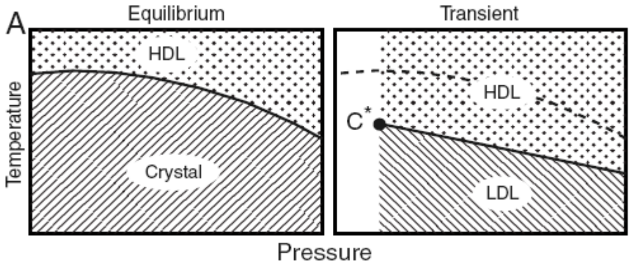
N-type silicon has free electrons. P-type silicon has free holes — the absence of electrons. When N-type and P-type silicon come into contact, an electric field forms within the cell.

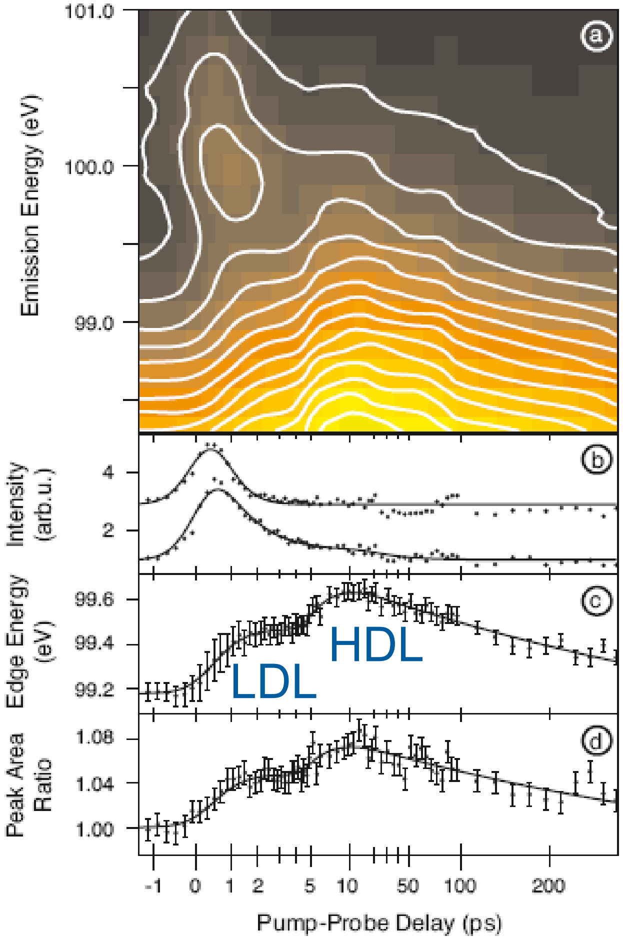


Role of time resolved RIXS: Transient phases and chemistry

The liquid-liquid phase transition in silicon revealed by snapshots of valence electrons
M. Beye, F. Sorgenfrei, W. F. Schlotter, W. Wurth, A. Föhlisch,
PNAS 2010 107 (39) 16772-16776

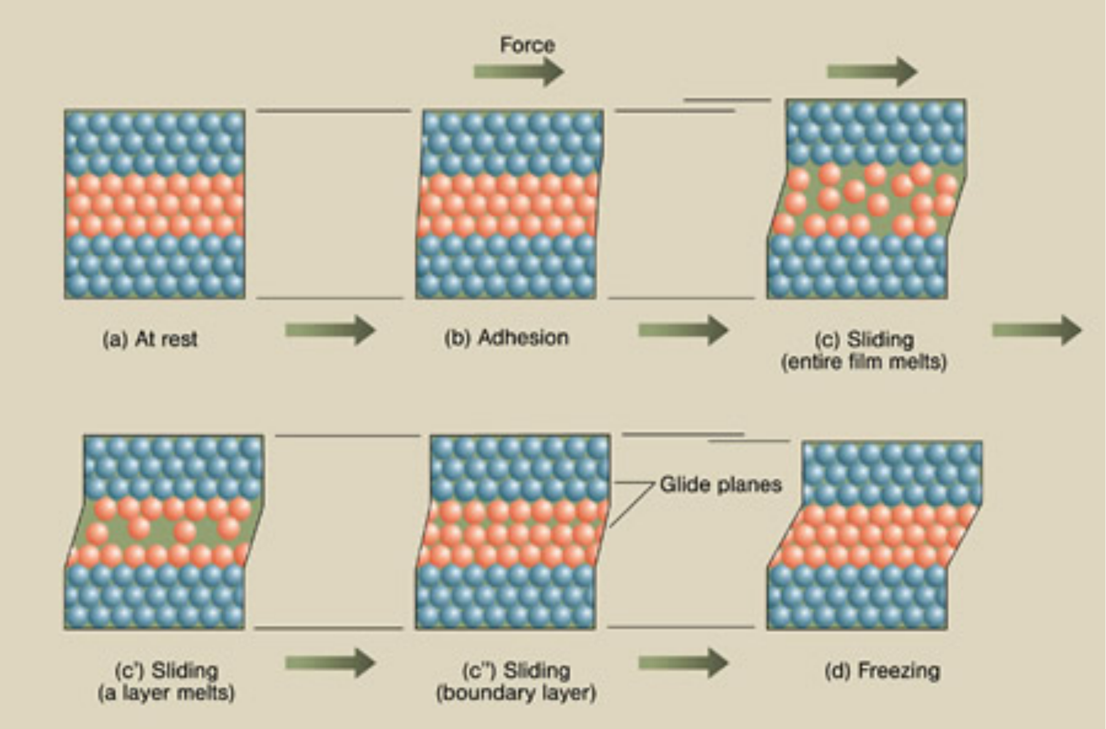






Materials research

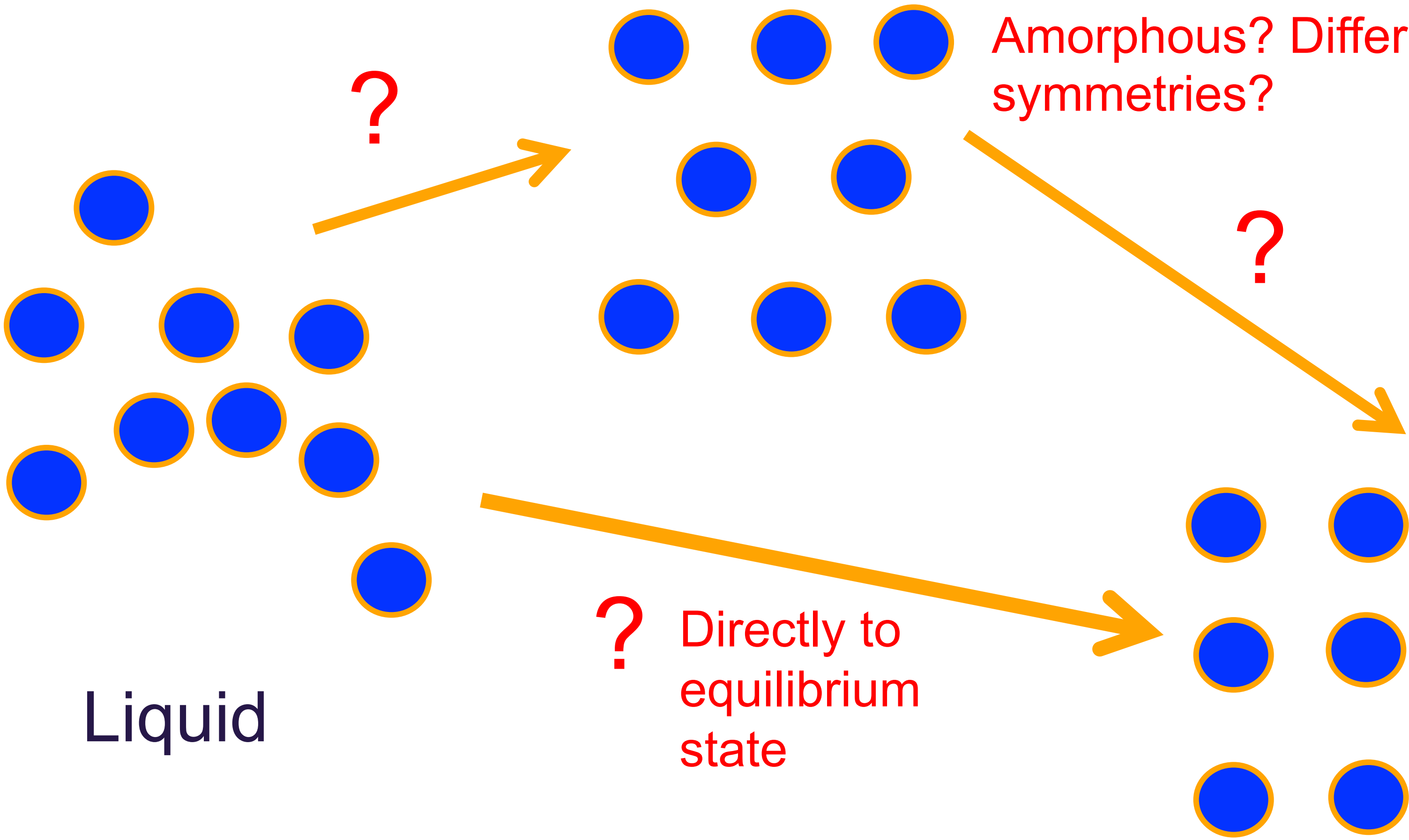
- Developing new materials



Various models explaining stick-slip friction. This phenomenon arises when a sliding film alternately melts (due to shear force) and freezes. A better understanding of the sliding phase (c) and how to prevent freezing (d) could help reduce frictional losses. Using intense X-ray radiation physicists investigate friction on an atomic level.

Formation of solid materials from liquids

XFEL allows "snapshots"



Via intermediate states?

Amorphous? Different bonding symmetries?

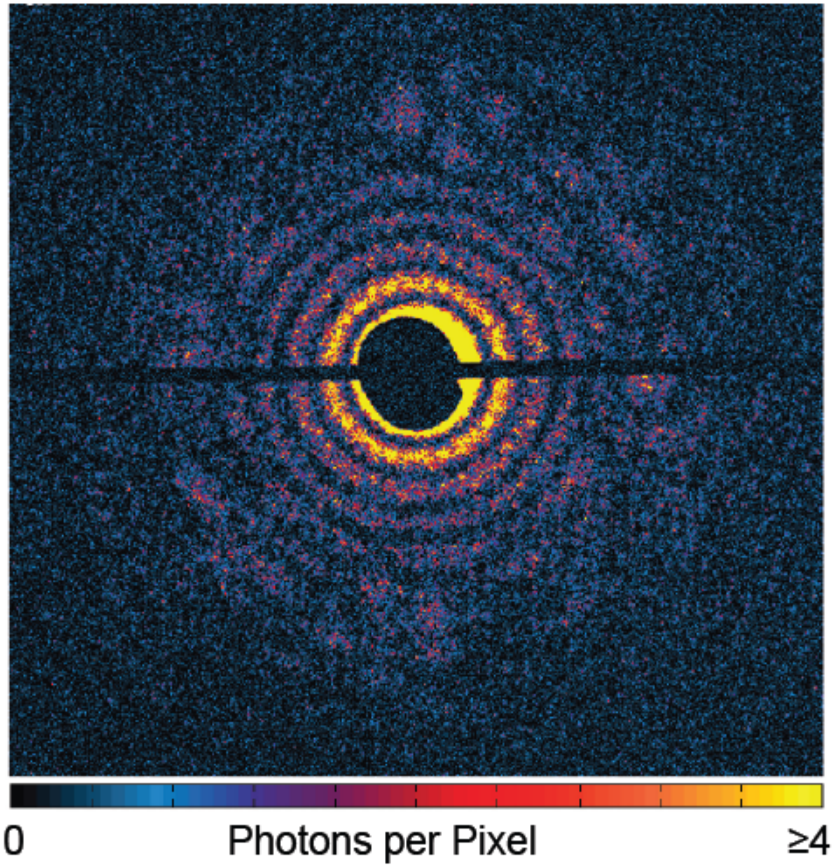
Directly to equilibrium state

Liquid

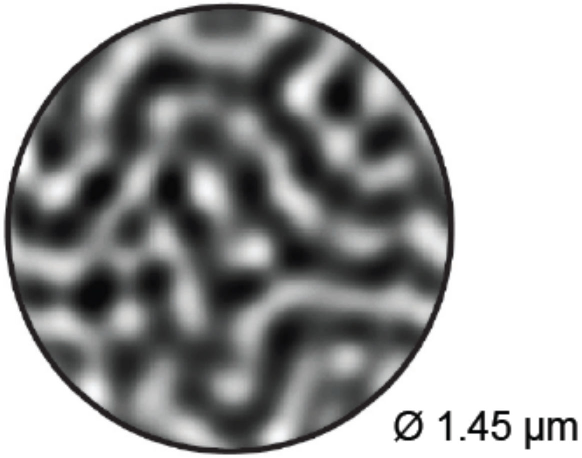
Crystalline Solid

fs Single short FTH image of magnetic domains (circular)

single shot- hologram



reconstruction
(magnetization contrast)



Co L_3 edge

FEL:

- 80 fs pulse
- 778 eV
- 1.5×10^5 photons
- 15 references

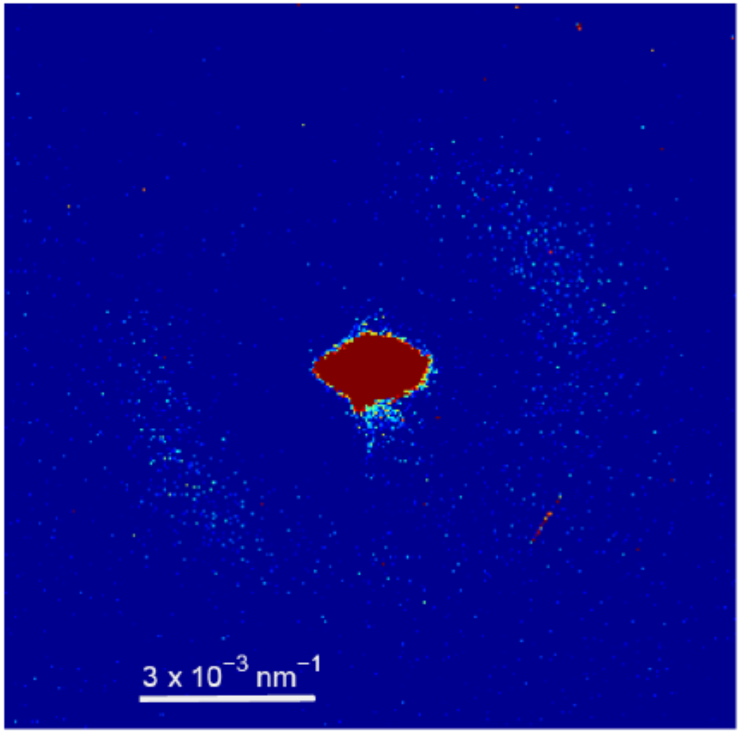
T. Wang et al., Phys. Rev. Letters ,**108**, 267403 (2012)

→ **Andreas Scherz**

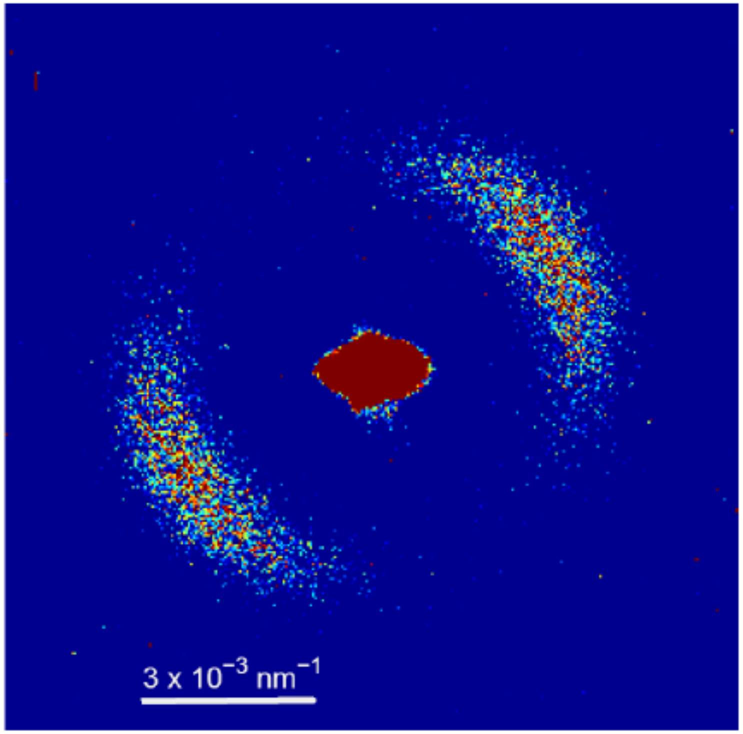
AGs Scherz/Stöhr, Eisebitt, Grübel, Lüning, Beaurepaire, Boeglin, Acremann +++

Magnetic SAXS of CoPd multilayer at Co L_3 edge (linear)

λ =1.58 nm
off resonance



λ =1.59 nm
on resonance



first magnetic signal at FLASH

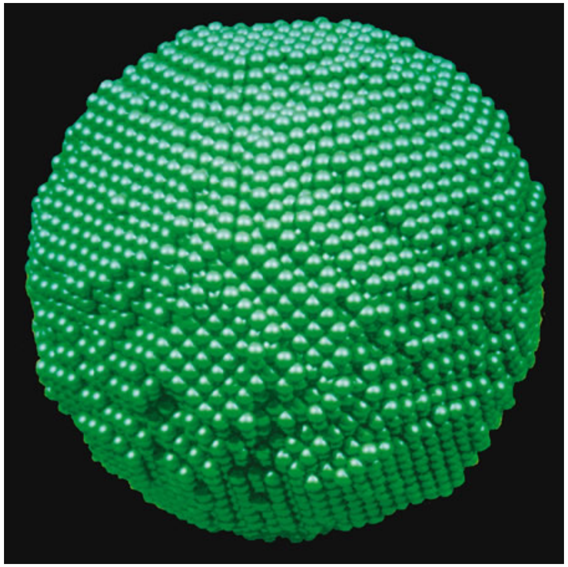
(5th harmonic, non-adapted optics)

exposure time 1000 s (Io=3×10^3)

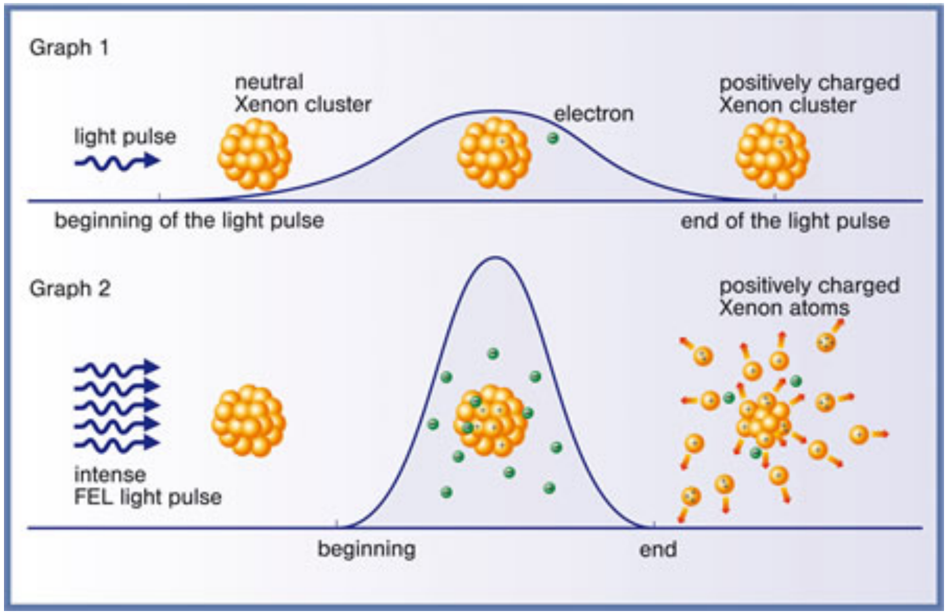
Gutt et al., PRB 79, 212406 (2009)

Cluster physics

- When less is more



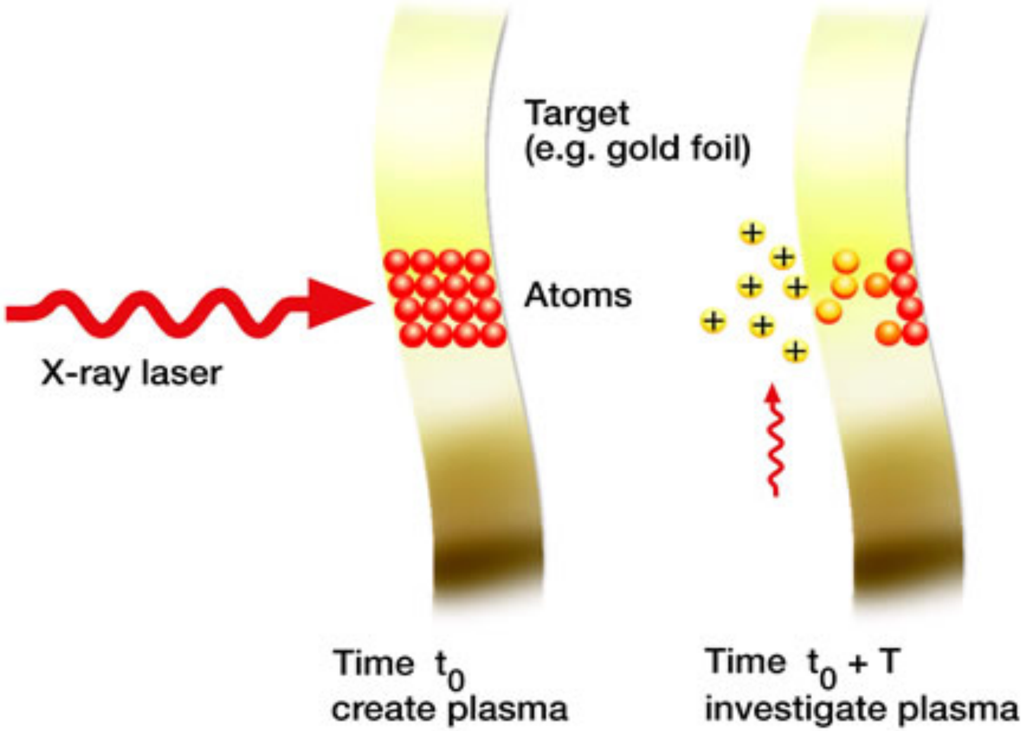
Model calculation of a copper particle with 17000 atoms - a cluster which plays a role in catalytic processes.



When matter is irradiated with very intense light, unusual processes occur which do not happen after irradiation with less intense light.

High energy density (HED Instrument)

- A different state of matter, extreme conditions

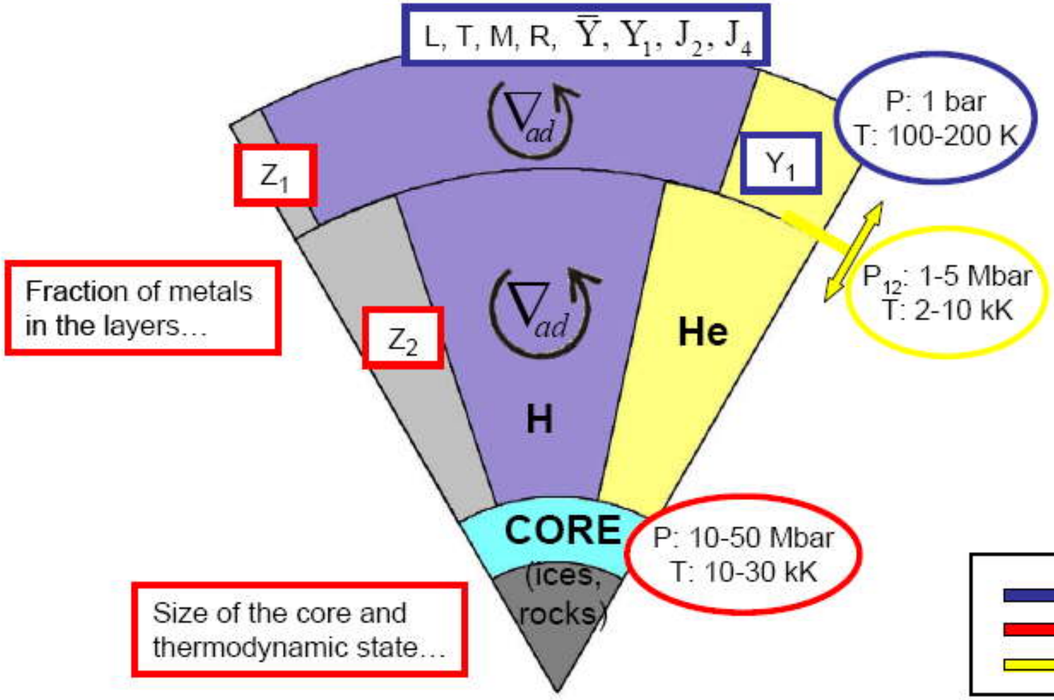


With an X-ray laser, plasmas can be created that are as hot as the interiors of giant stars. At the same time, it will be possible to investigate the plasmas so created at varying intervals with another part of the laser beam and thus to conduct research into the plasma state.

European XFEL

Planetarial models

Standard three-layer structure model



Y: fraction of He

Z: fraction of metals

J_2, J_4: gravitational moments

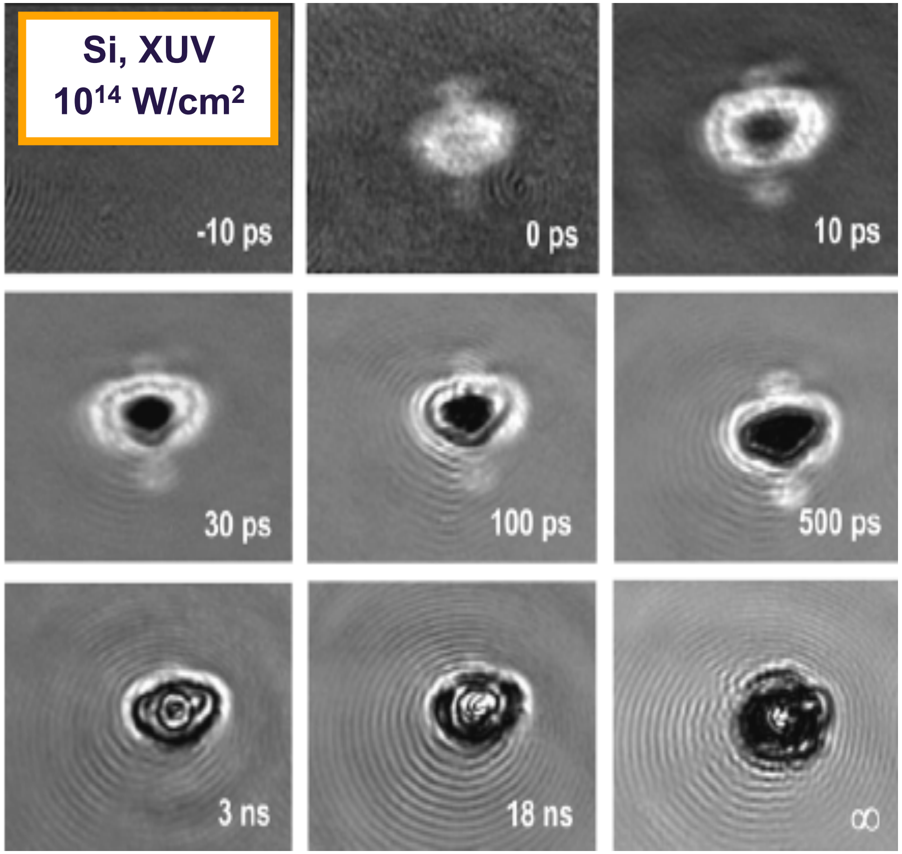
Physical origin and location of the layer boundary…
→ MIT (PPT)
→ H-He demixing

🟦 constraints
🟥 results from modeling
🟨 free parameter

Apart from the transition pressure, interior models of this structure type are uniquely defined by the observables.

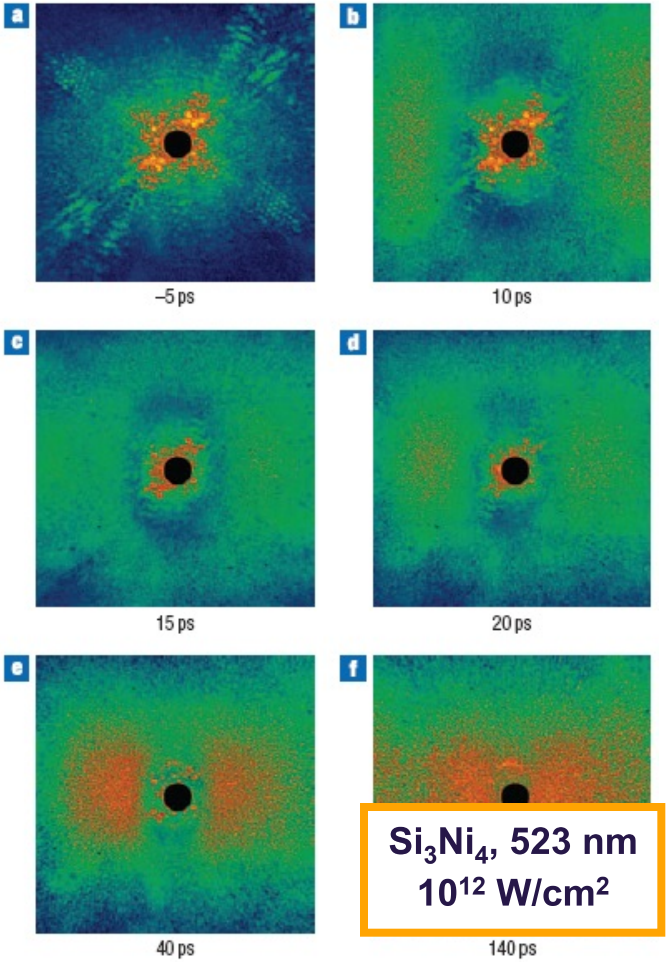
Most important input: Accurate EOS data for H and He as well as the representative of metals, e.g. H2O.

Exciting solids: Onset of ablation (FLASH)



Si, XUV
10^{14} W/cm^2

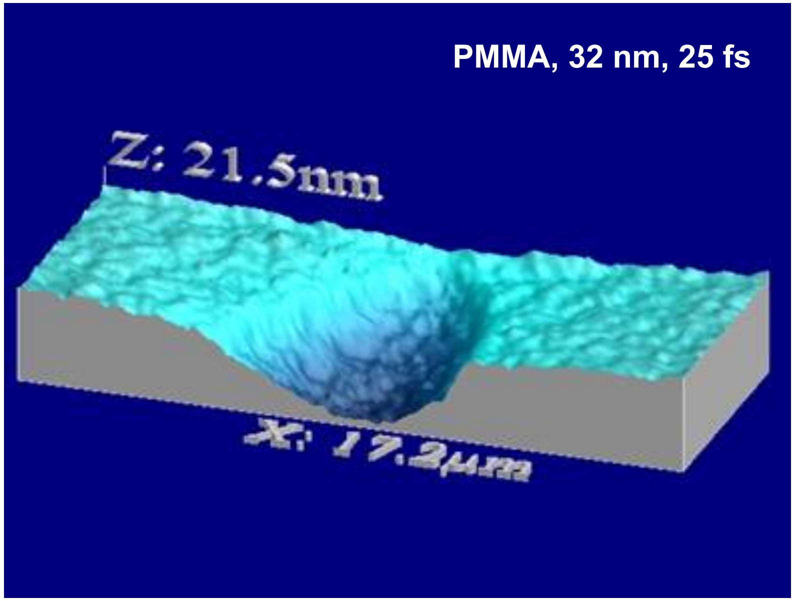
N. Stojanovic et al., APL 89, 241909 (2006)

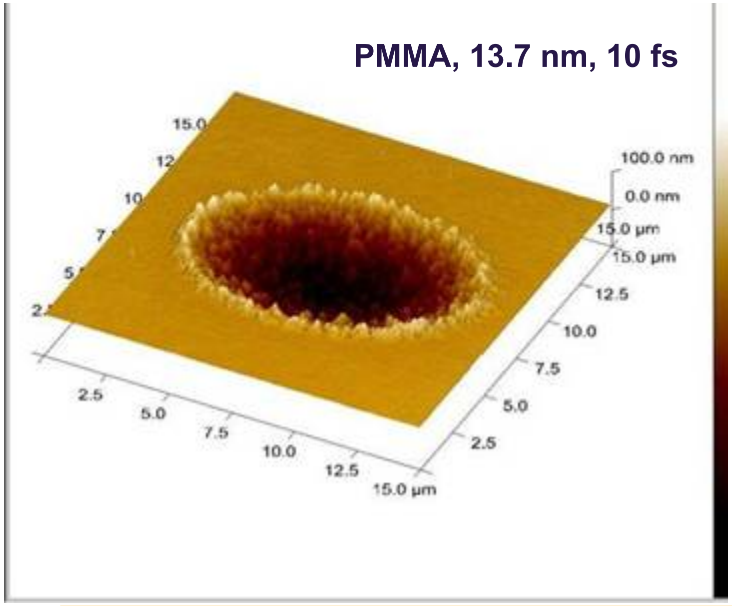


Si_3Ni_4, 523 nm
10^{12} W/cm^2

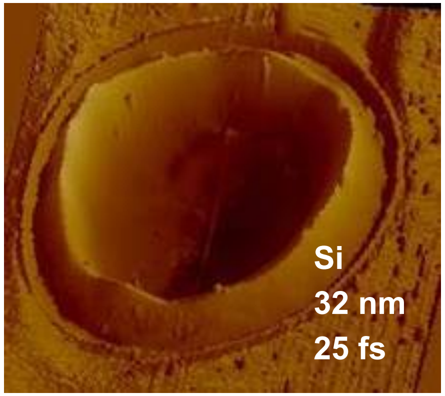
A. Barty et al., Nature Photonics 2, 415 (2008)

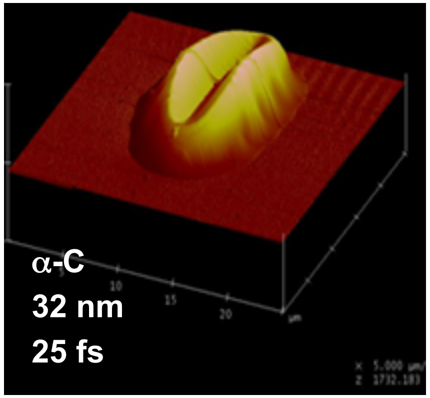
X-ray ablation





~10^{13} W/cm^2





- Thresholds for optical damage
  - SiC, 0.14 ± 0.07 J/cm^2
  - Si, 0.087 ± 0.04 J/cm^2
  - B_4C, 0.20 ± 0.1 J/cm^2
  - amorph. C, 0.06 ± 0.03 J/cm^2
  - cvd-diamond 0.14 ± 0.07 J/cm^2

S. Hau-Riege et al., APL 90, 173128(2007)

European XFEL, Campus

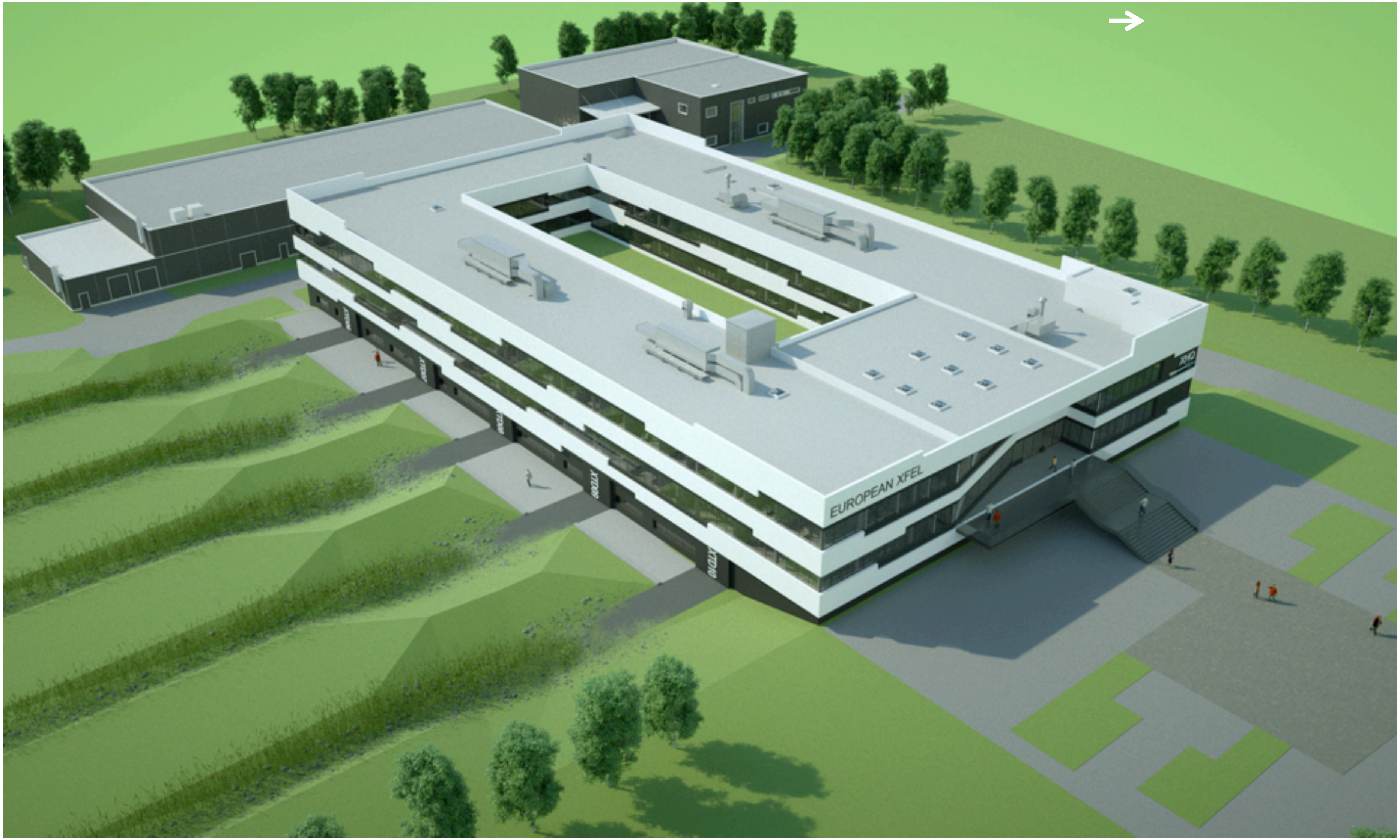
European XFEL: Modules installed in tunnel

European XFEL experiment hall infrastructure, 18.09.2014

European XFEL building, Jan. 2015

Richtfest, 18.02.2015!

European XFEL main quarter



European XFEL / DESY Users' Meeting 2015

> 600 people!

You are very welcome

to plan your experiments

at XFEL facilities