Introduction to (x-ray) photon science

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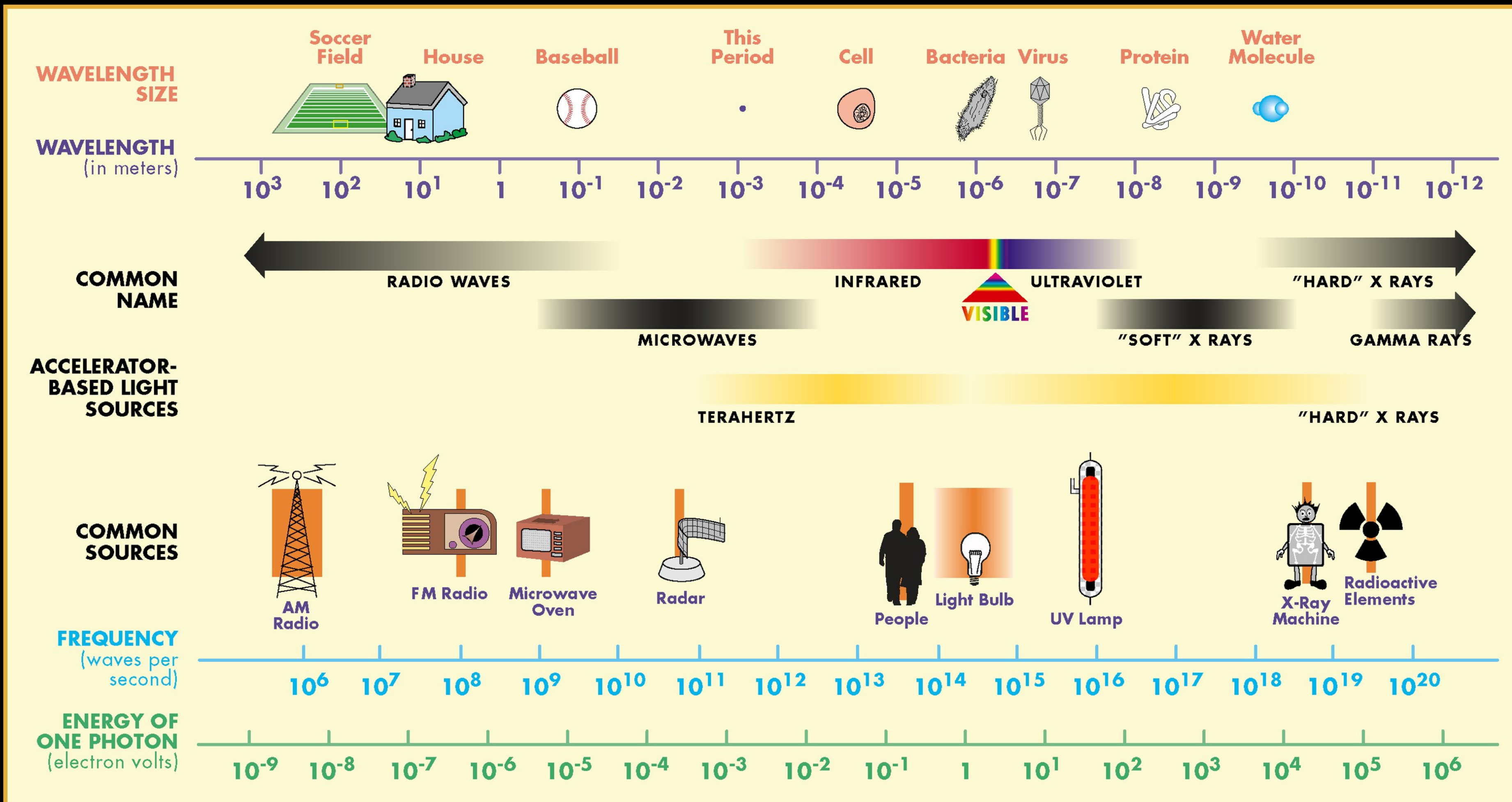
READi Workshop
Hamburg, Germany
April 7 – 9, 2014

What is photon science?

- Development and application of
  - new light sources (Hanus; Calendron; Ahr)
  - new techniques for controlling matter (Li; Höppner)
  - new techniques for probing matter (Baev)

THE ELECTROMAGNETIC SPECTRUM



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Basic x-ray techniques

Dominant x-ray–atom interaction process: photoabsorption

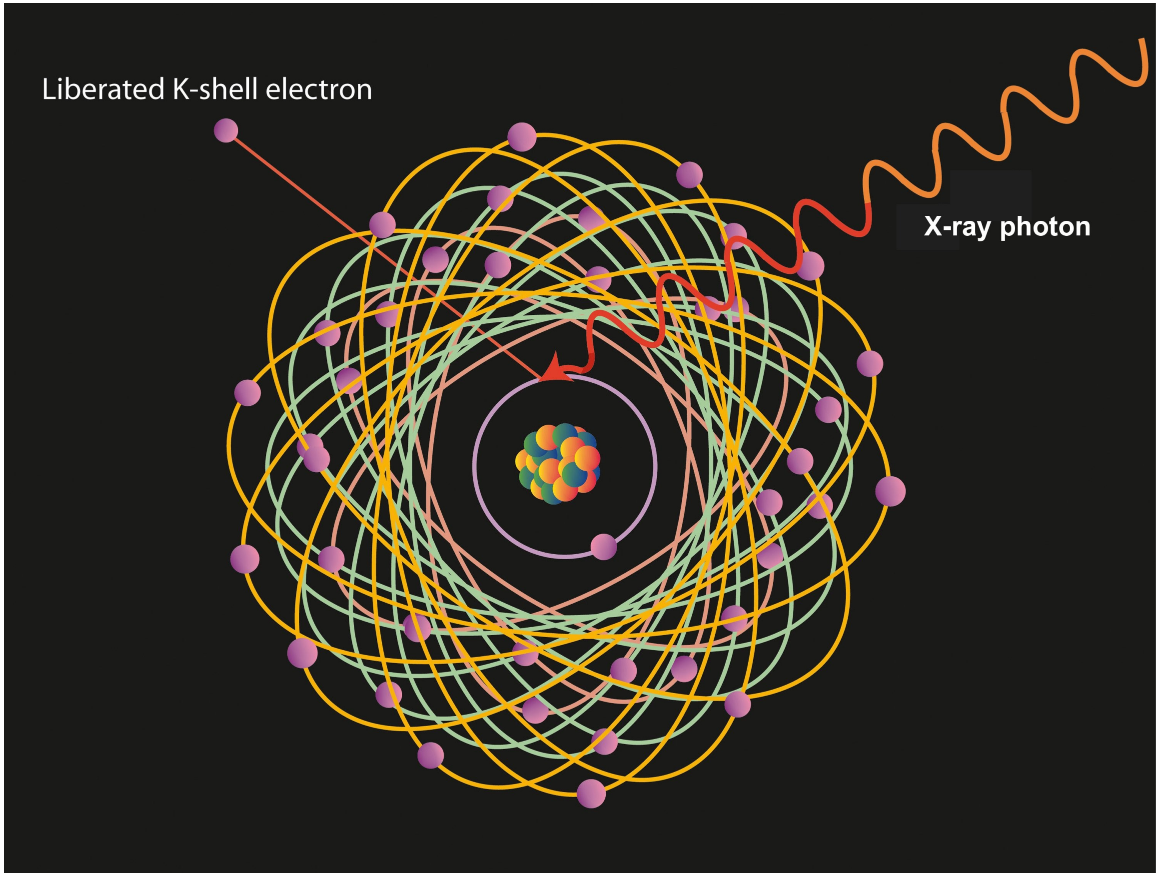

Table 1-1. *Electron binding energies, in electron volts, for the elements in their natural forms.*

Element	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$	N_1 4s	N_2 $4p_{1/2}$	N_3 $4p_{3/2}$
1 H	13.6											
2 He	24.6*											
3 Li	54.7*											
4 Be	111.5*											
5 B	188*											
6 C	284.2*											
7 N	409.9*	37.3*										
8 O	543.1*	41.6*										
9 F	696.7*											
10 Ne	870.2*	48.5*	21.7*	21.6*								
11 Na	1070.8†	63.5†	30.65	30.81								
12 Mg	1303.0†	88.7	49.78	49.50								
13 Al	1559.6	117.8	72.95	72.55								
14 Si	1839	149.7*b	99.82	99.42								
15 P	2145.5	189*	136*	135*								
16 S	2472	230.9	163.6*	162.5*								
17 Cl	2822.4	270*	202*	200*								
18 Ar	3205.9*	326.3*	250.6†	248.4*	29.3*	15.9*	15.7*					
19 K	3608.4*	378.6*	297.3*	294.6*	34.8*	18.3*	18.3*					
20 Ca	4038.5*	438.4†	349.7†	346.2†	44.3 †	25.4†	25.4†					
21 Sc	4492	498.0*	403.6*	398.7*	51.1*	28.3*	28.3*					
22 Ti	4966	560.9†	460.2†	453.8†	58.7†	32.6†	32.6†					

X-ray photoelectron spectroscopy (XPS)

A tool to measure inner-shell binding energies

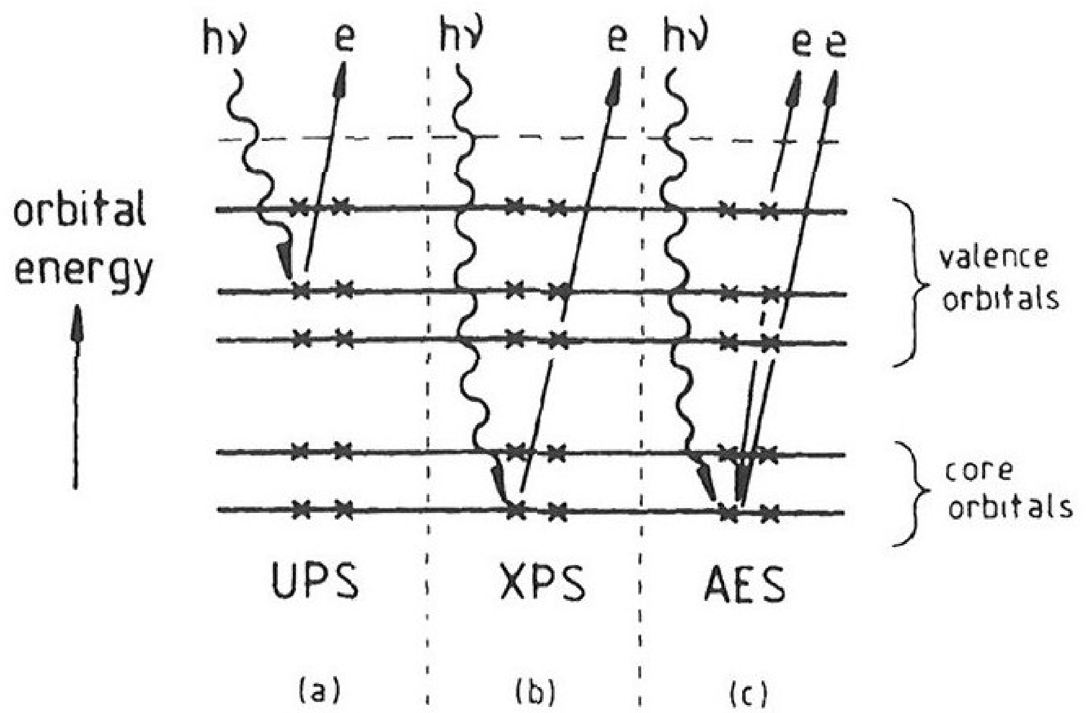

Figure 8.1 Processes occurring in (a) ultraviolet photoelectron spectroscopy (UPS), (b) X-ray photoelectron spectroscopy (XPS), (c) Auger electron spectroscopy (AES)

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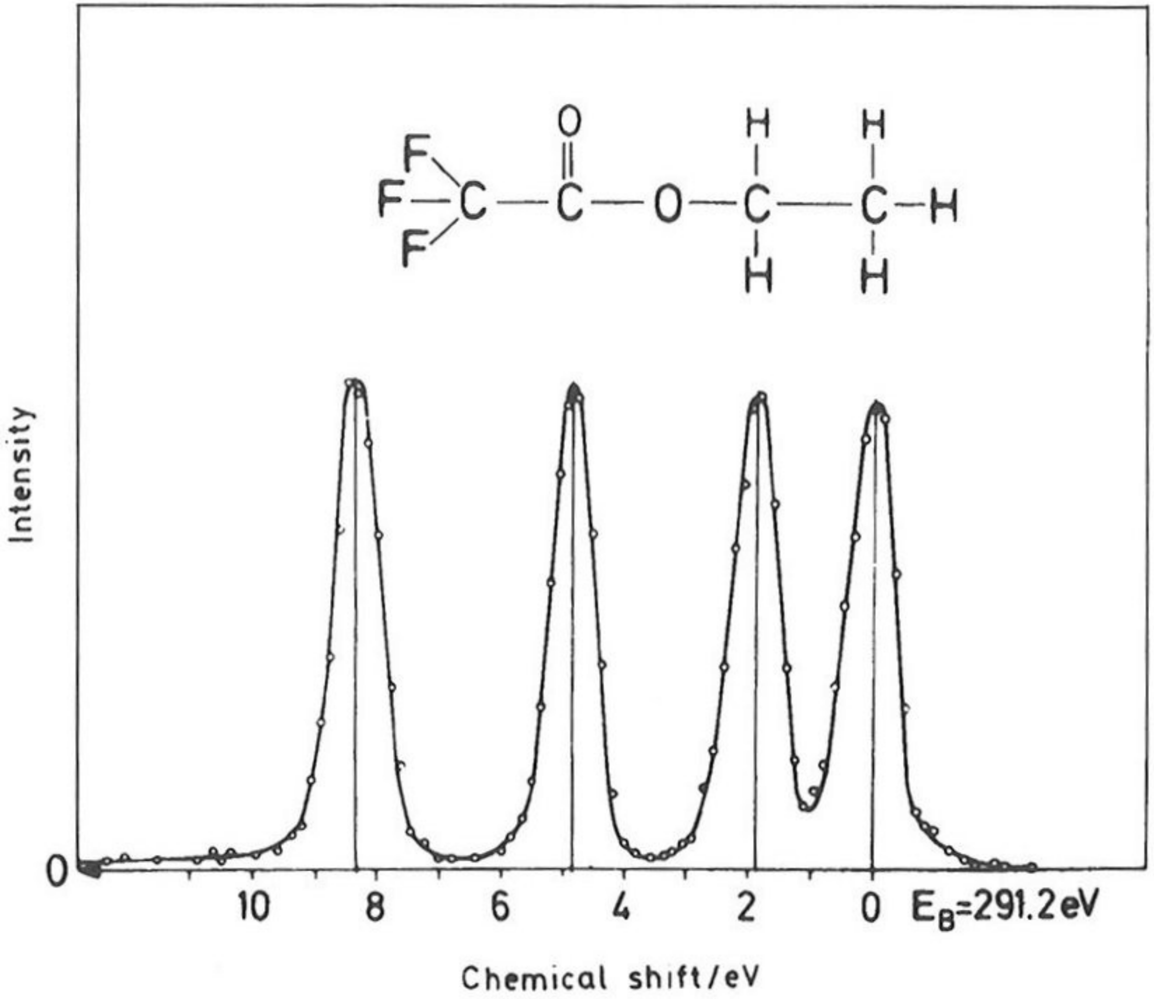


Figure 8.14 The monochromatized Al$K\alpha$ carbon 1*s* XPS spectrum of ethyltrifluoroacetate showing the chemical shifts relative to an ionization energy of 291.2 eV. (Reproduced, with permission, from Gelius, U., Basilier, E., Svensson, S., Bergmark, T., and Siegbahn, K., *J. Electron Spectrosc.*, **2**, 405, 1974)

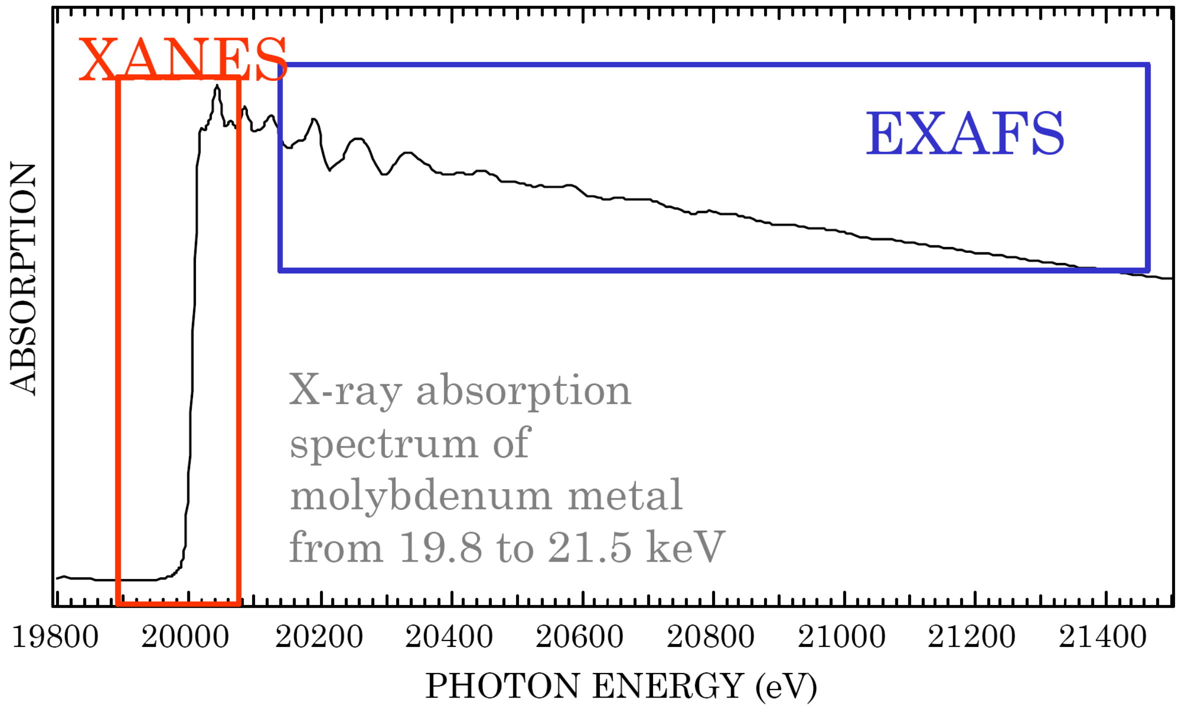
X-ray absorption spectroscopy

Exploiting the impact of the chemical environment on the x-ray-excited electron

- XANES (x-ray absorption near-edge structure) or NEXAFS (near-edge x-ray absorption fine structure)

- EXAFS (extended x-ray absorption fine structure)

What Is XANES?



- XANES is region of x-ray absorption spectrum within ~50eV of the absorption edge.
- Suggested that division is that at which wavelength of excited electron is equal to distance between absorbing atom and its nearest neighbor. (λ (Å) $\approx 12/[e(eV)]^{1/2}$.

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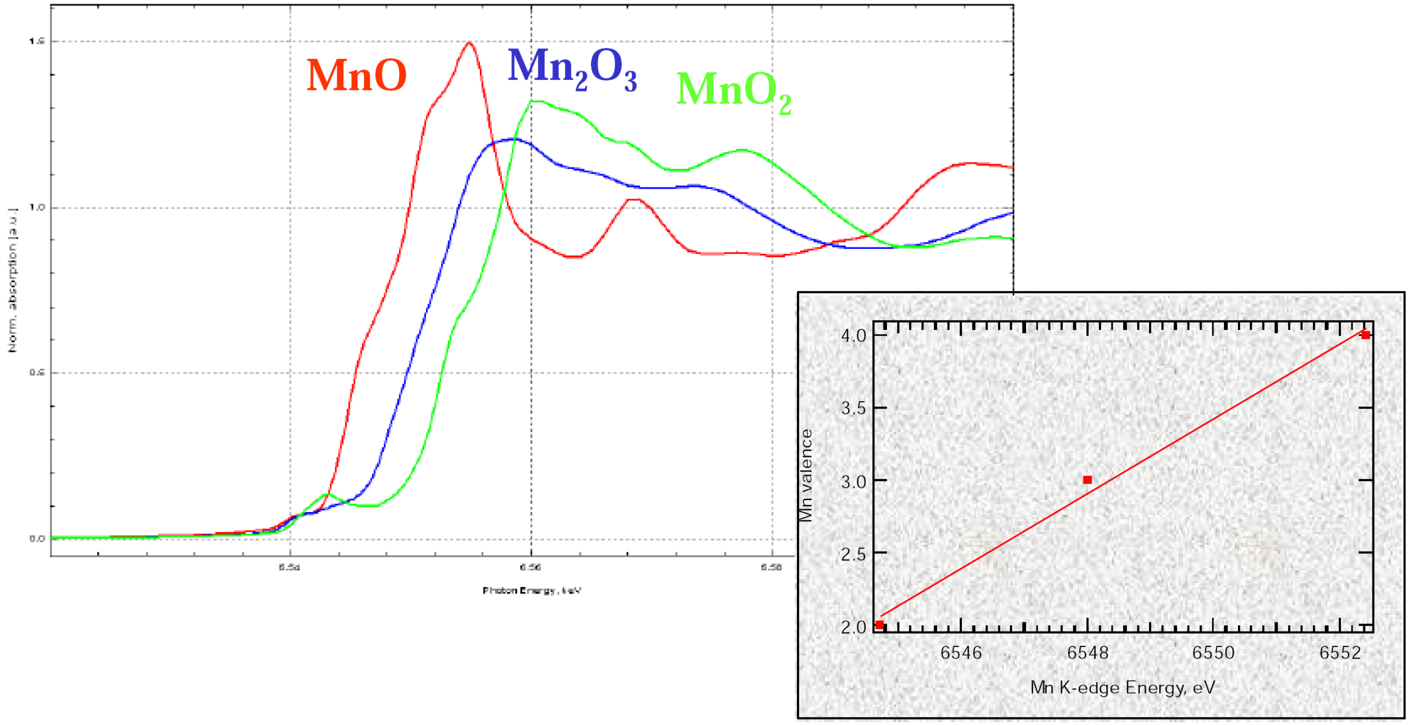
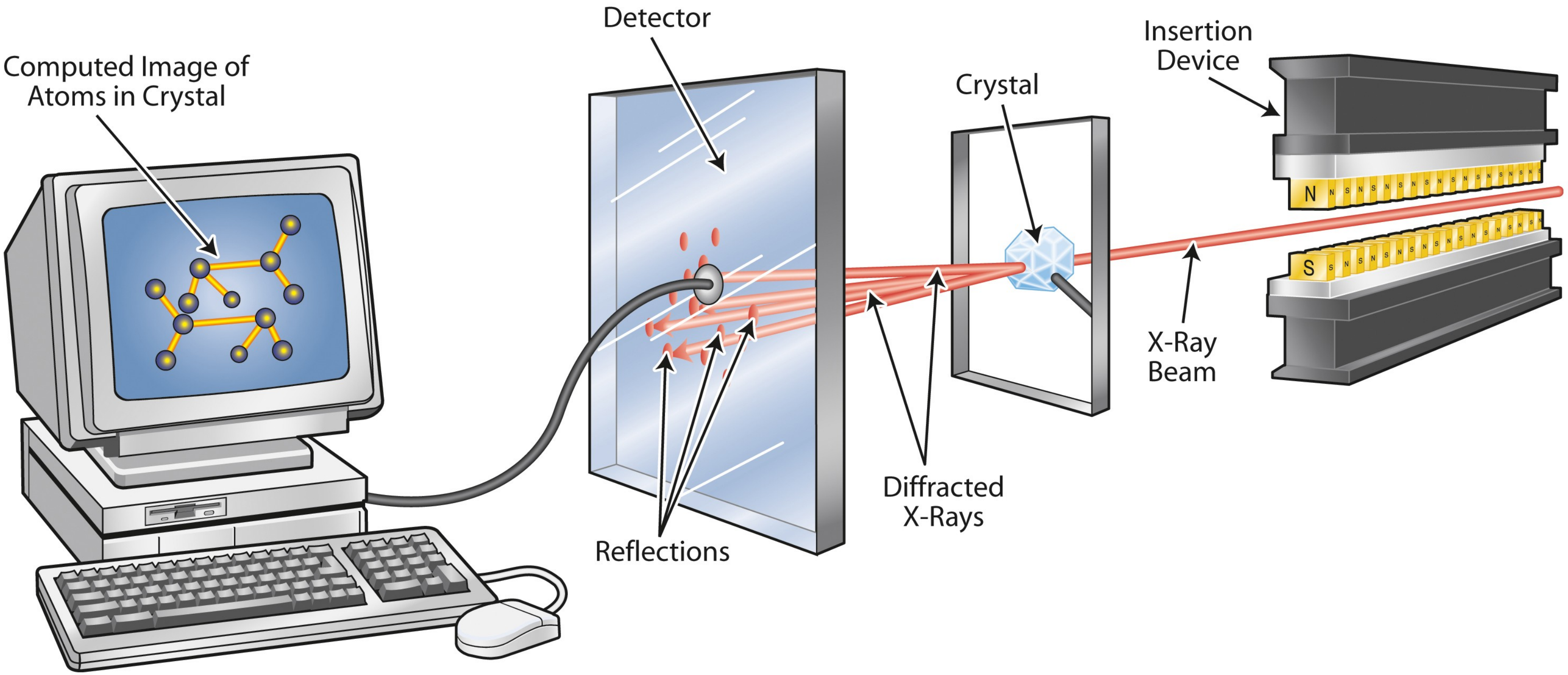
Why Are We Interested In XANES? Oxidation State



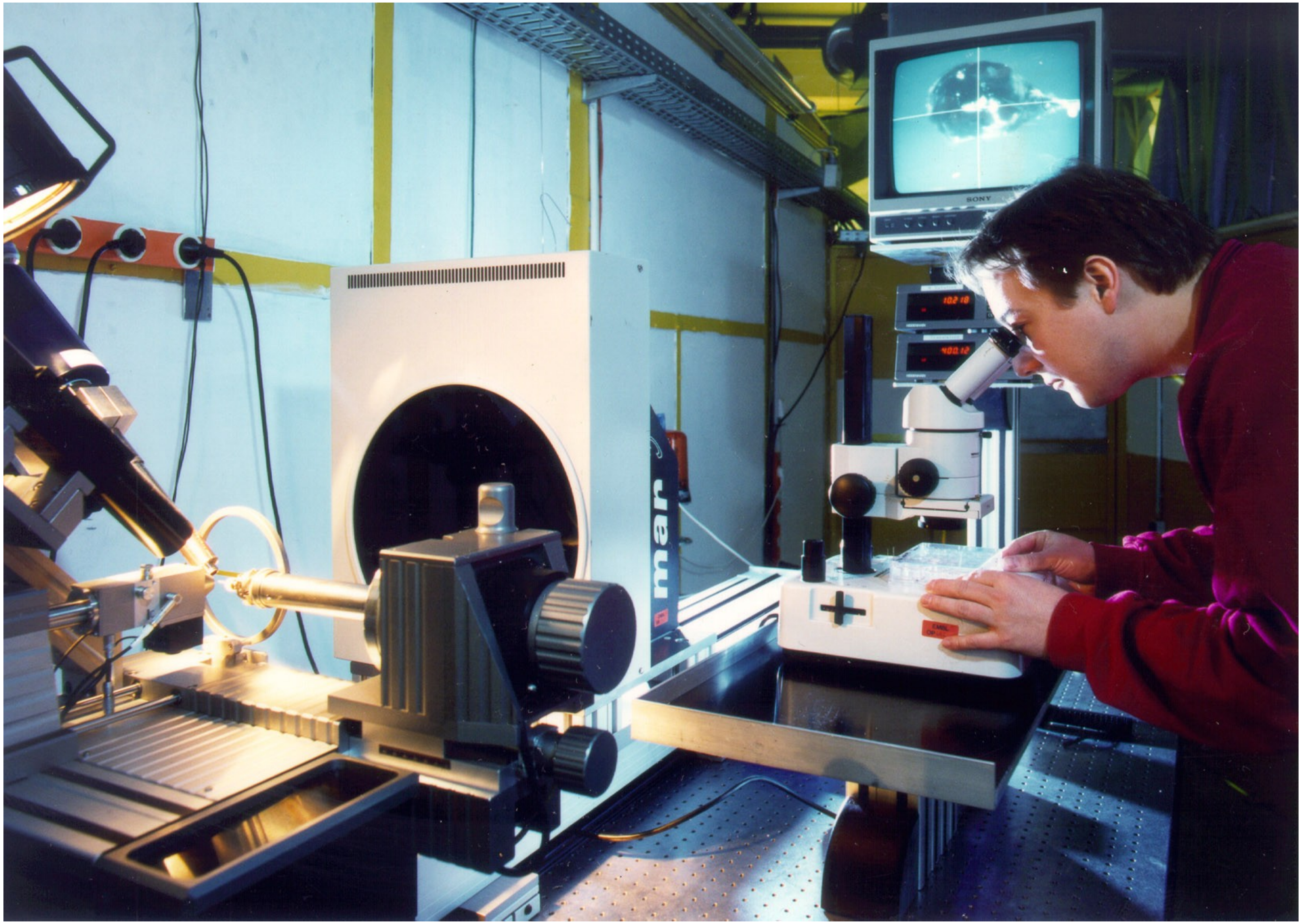
- Many edges of many elements show significant edge shifts (binding energy shifts) with oxidation state.

X-ray scattering

X-ray crystallography: principle



X-ray crystallography: application to biomolecules



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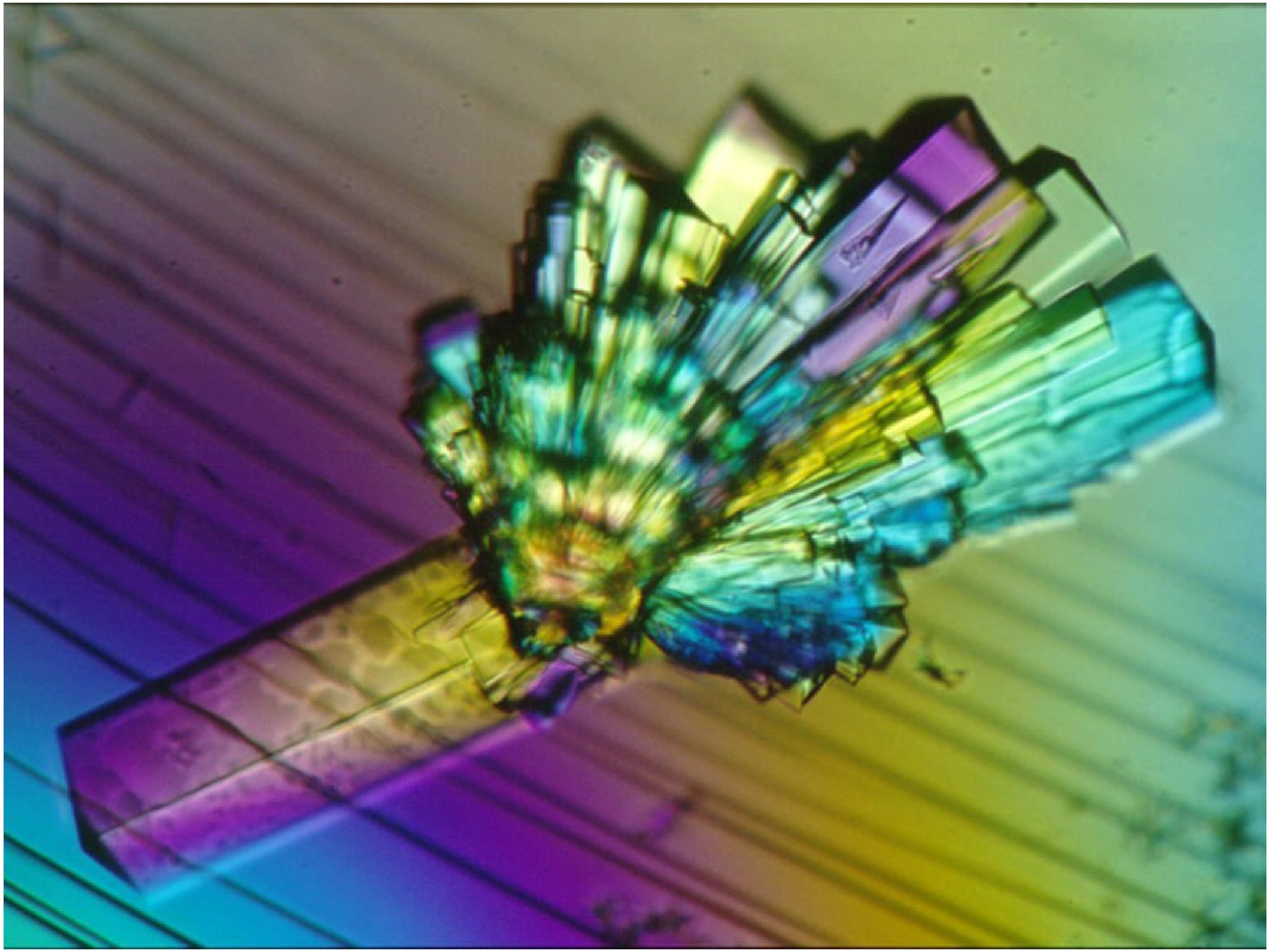
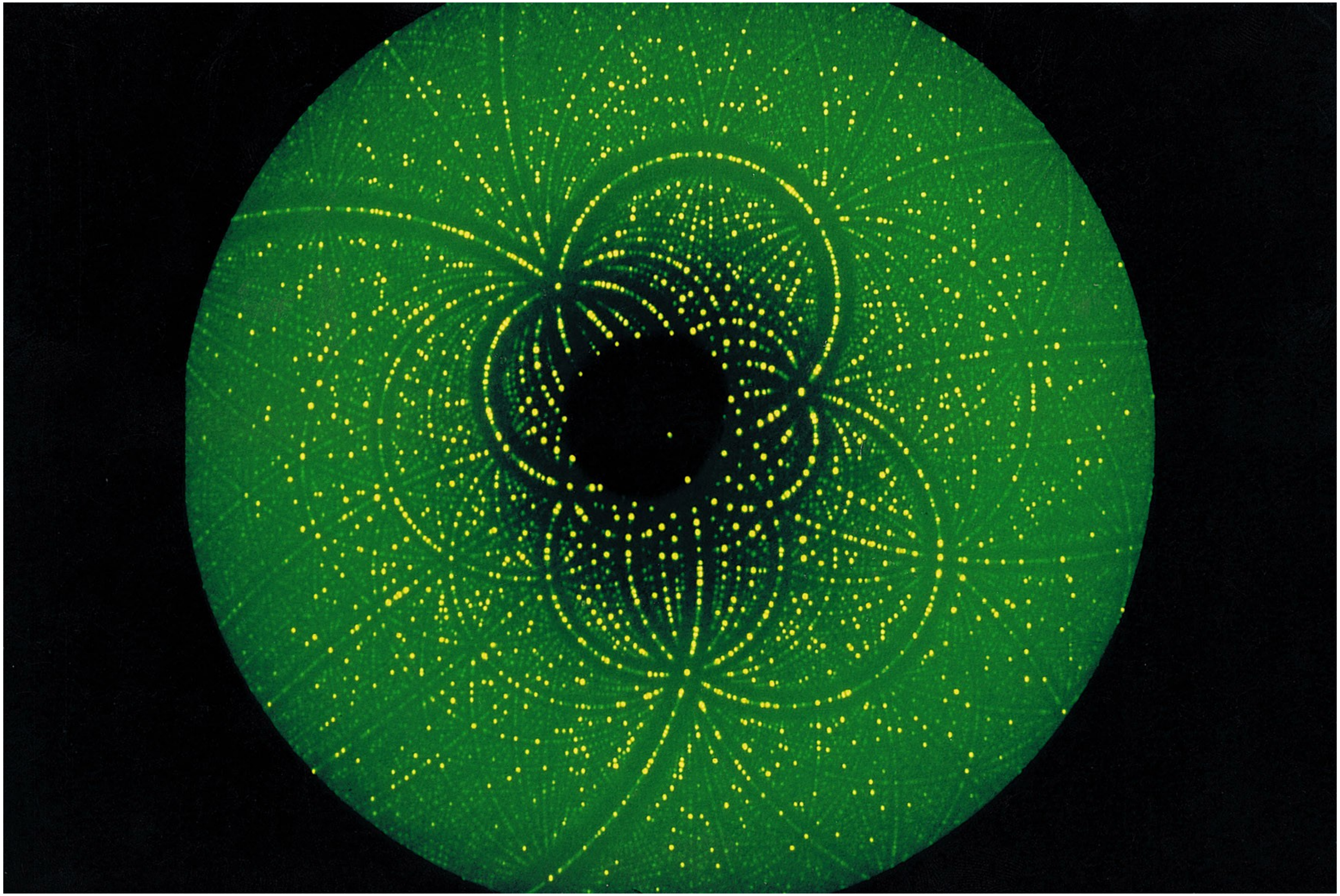
Protein crystal



X-ray diffraction pattern



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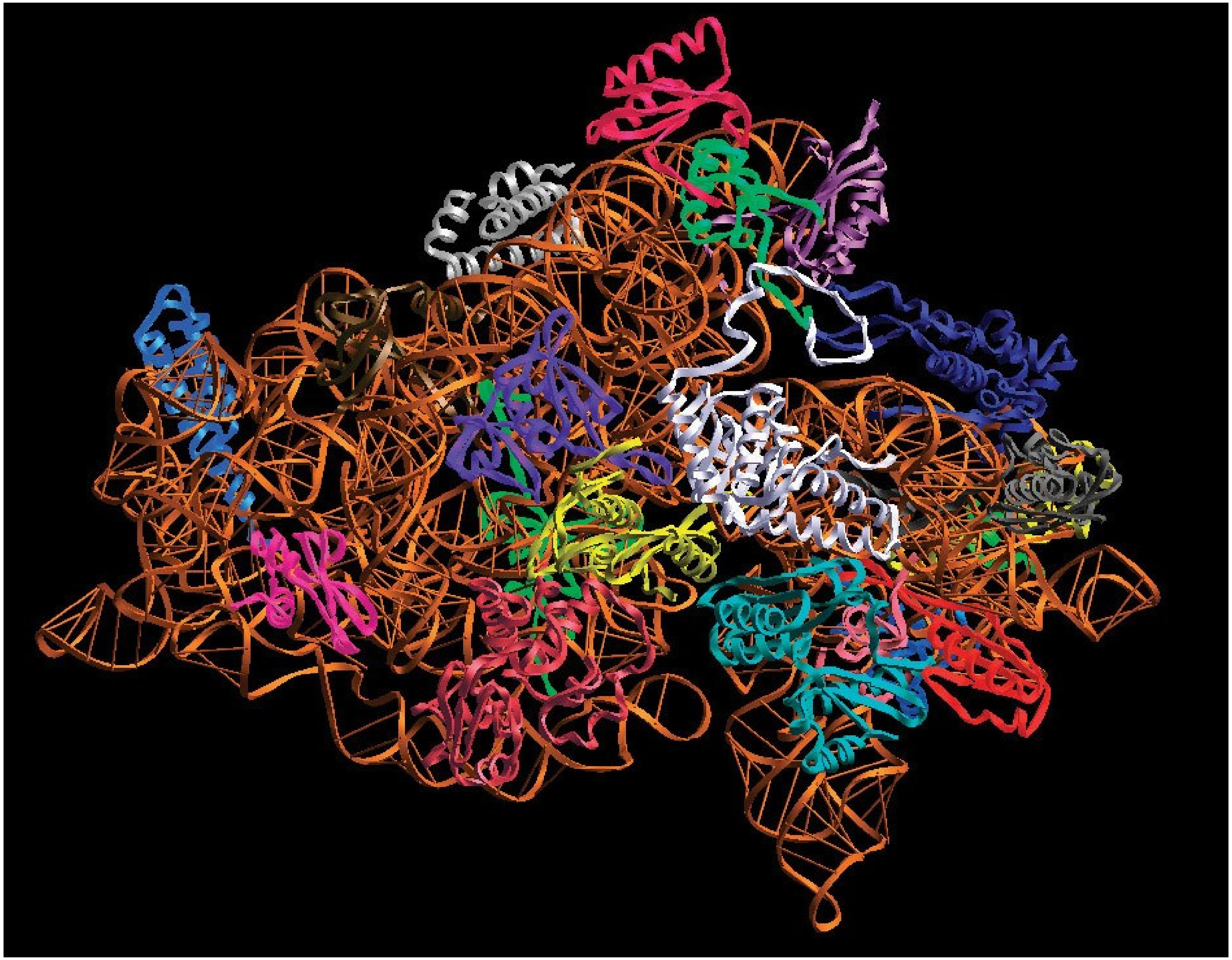
Molecular structure of a protein



Decay of inner-shell-excited systems

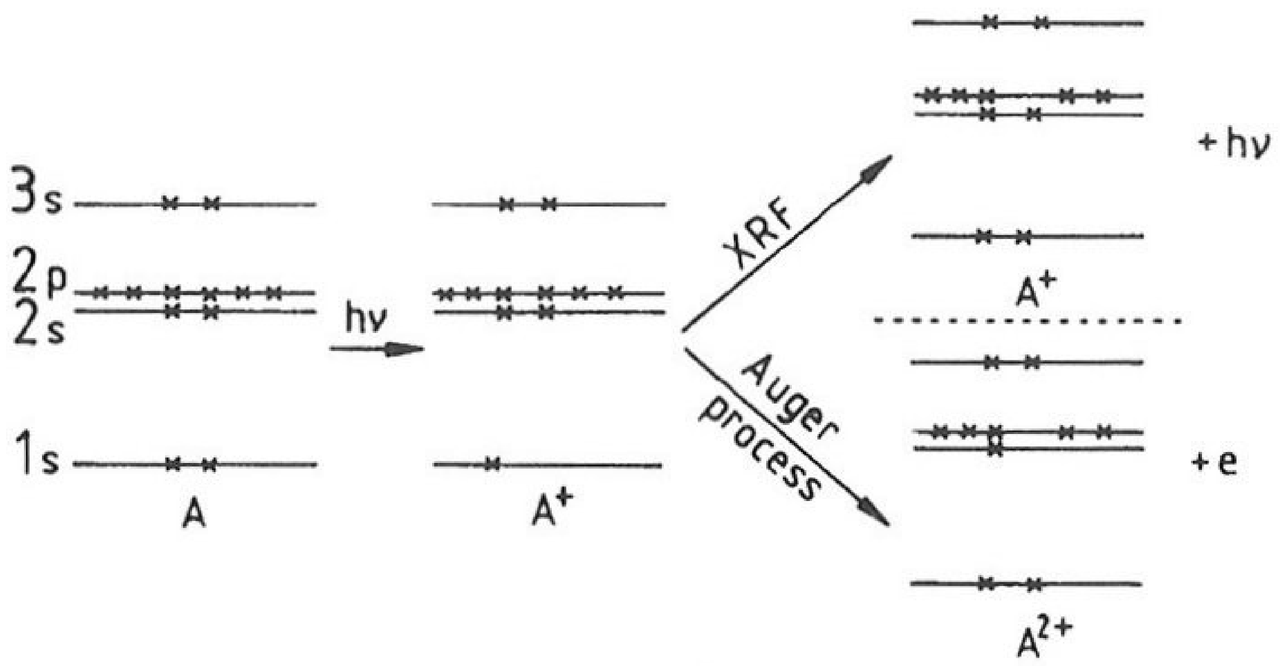
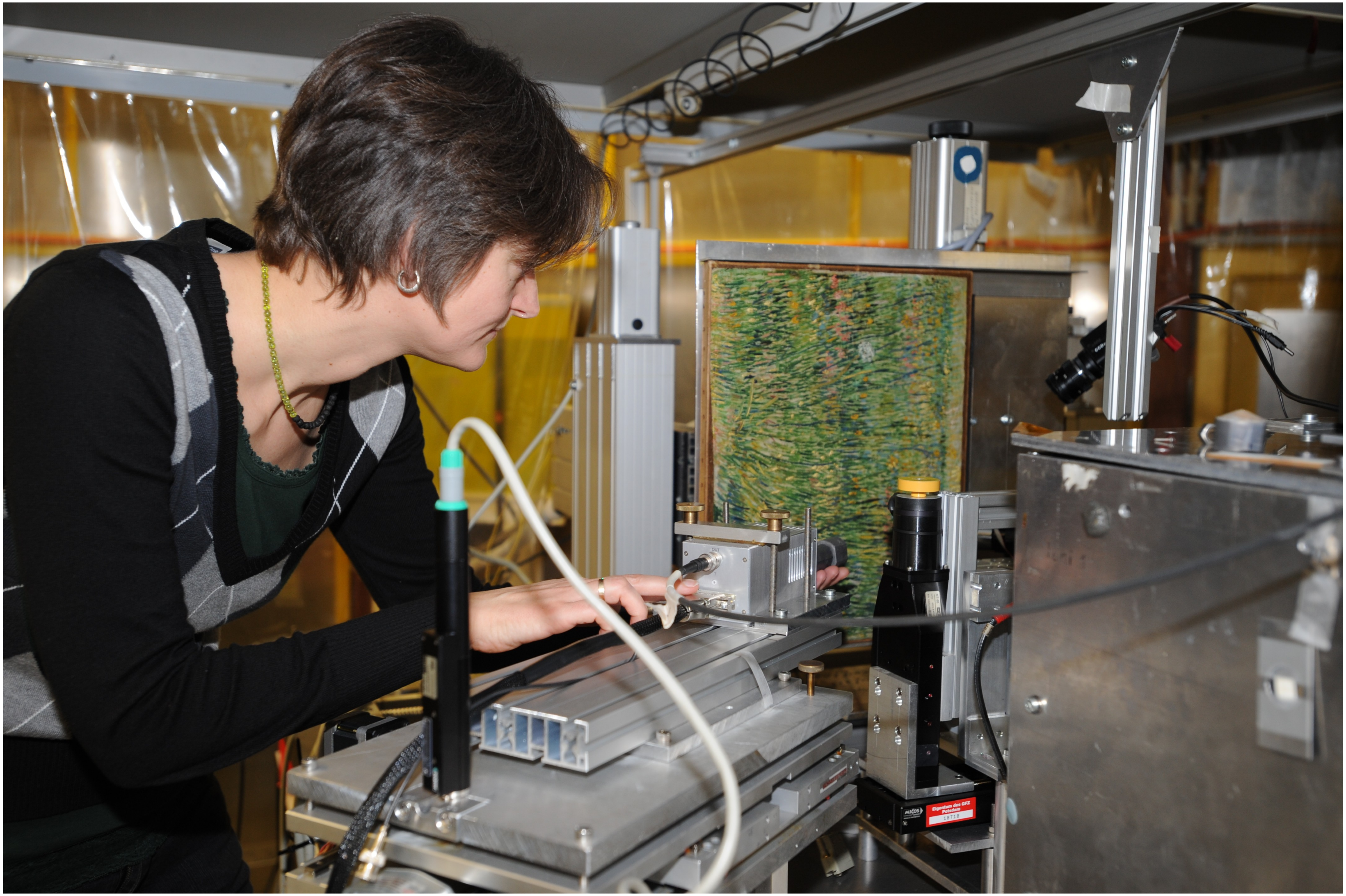


Figure 8.21 The competitive processes of X-ray fluorescence and Auger electron emission

An application in art history



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Hidden painting by Van Gogh made visible

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Female portrait underneath *Grasgrond* by Vincent van Gogh

Accelerator-based x-ray sources

Synchrotrons

- A synchrotron is a circular accelerator of fixed radius *R*
- Bending magnets of field strength *B* keep the charged particles (charge *q*) on circular path
- As energy *E* of particles increases (using high-frequency acceleration techniques), *B* must be increased in a *synchronous* manner →

$$B = \frac{E}{qR}$$

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Synchrotron radiation

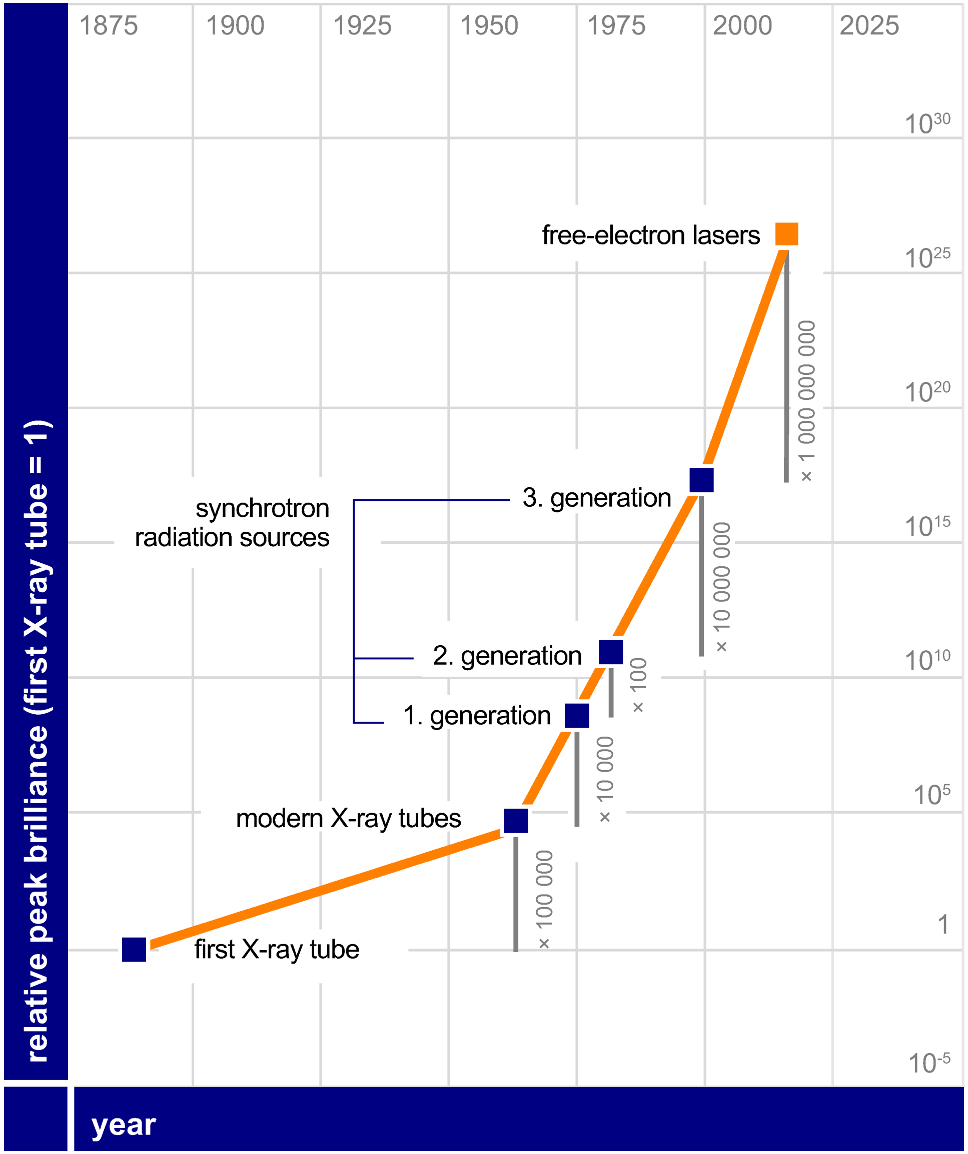
- Charged, accelerated particles emit electromagnetic radiation
- Synchrotron radiation losses severe in electron synchrotrons
- This limits the maximum electron energy attainable

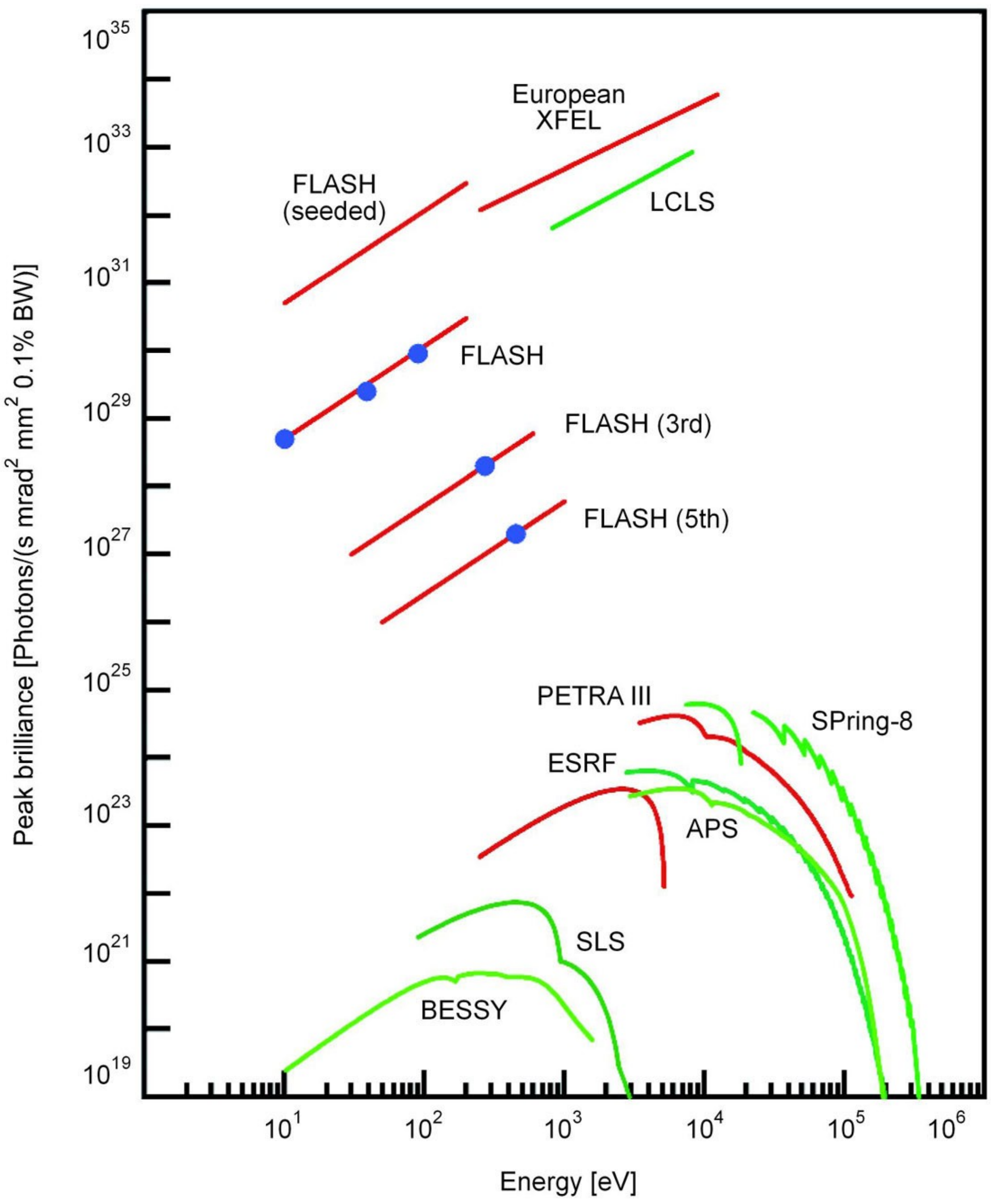
$$P_{\mathrm{syn}} = \frac{2}{3} c q^2 \frac{1}{R^2} \left(\frac{E}{mc^2} \right)^4$$

Synchrotron radiation sources: storage rings and free-electron lasers

- Synchrotron radiation sources are not synchrotrons (in a strict sense)
- 1st generation: storage rings built for particle physics; used in parasitic mode
- 2nd generation: storage rings dedicated to the generation of synchrotron radiation; radiation emitted in bend magnets is used
- 3rd generation: insertion devices (wigglers and undulators) provide more intense synchrotron radiation
- 4th generation: free-electron lasers

A brief history of x-ray intensity





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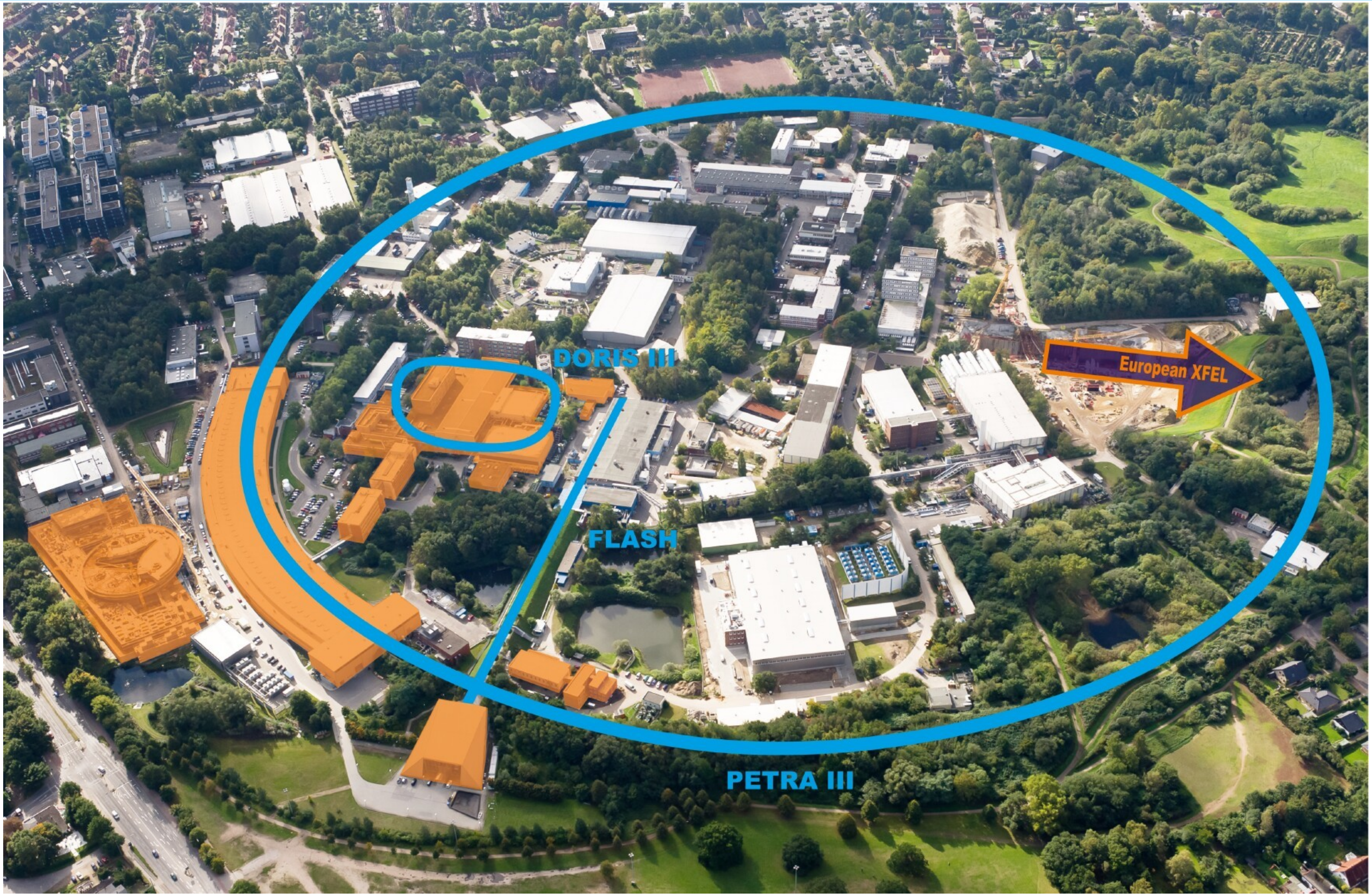
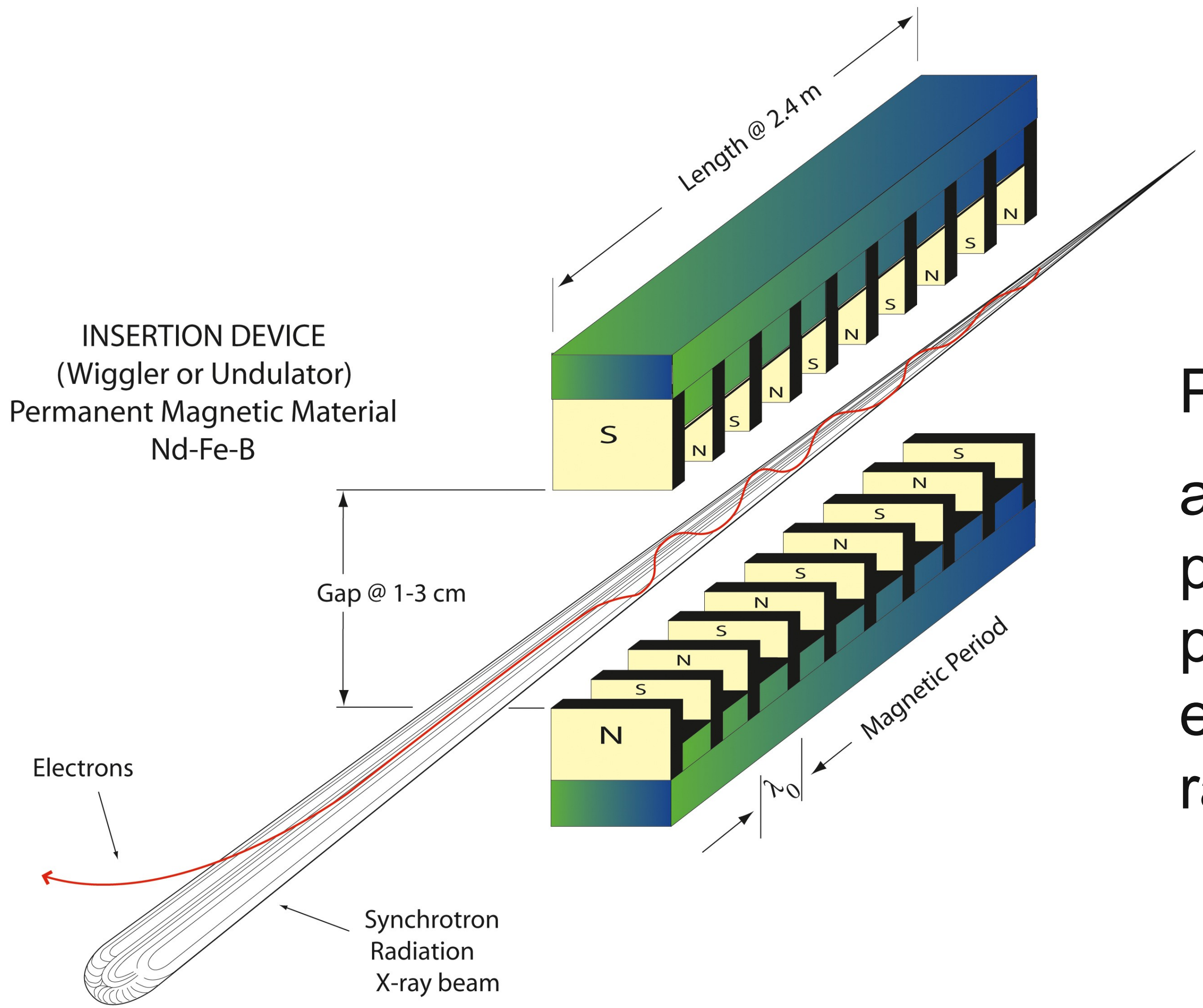
X-ray photon science in Hamburg



PETRA III is a synchrotron radiation source based on **insertion devices** (third-generation source)



Principle:

accelerated charged particles (light ones, in particular) emit electromagnetic radiation

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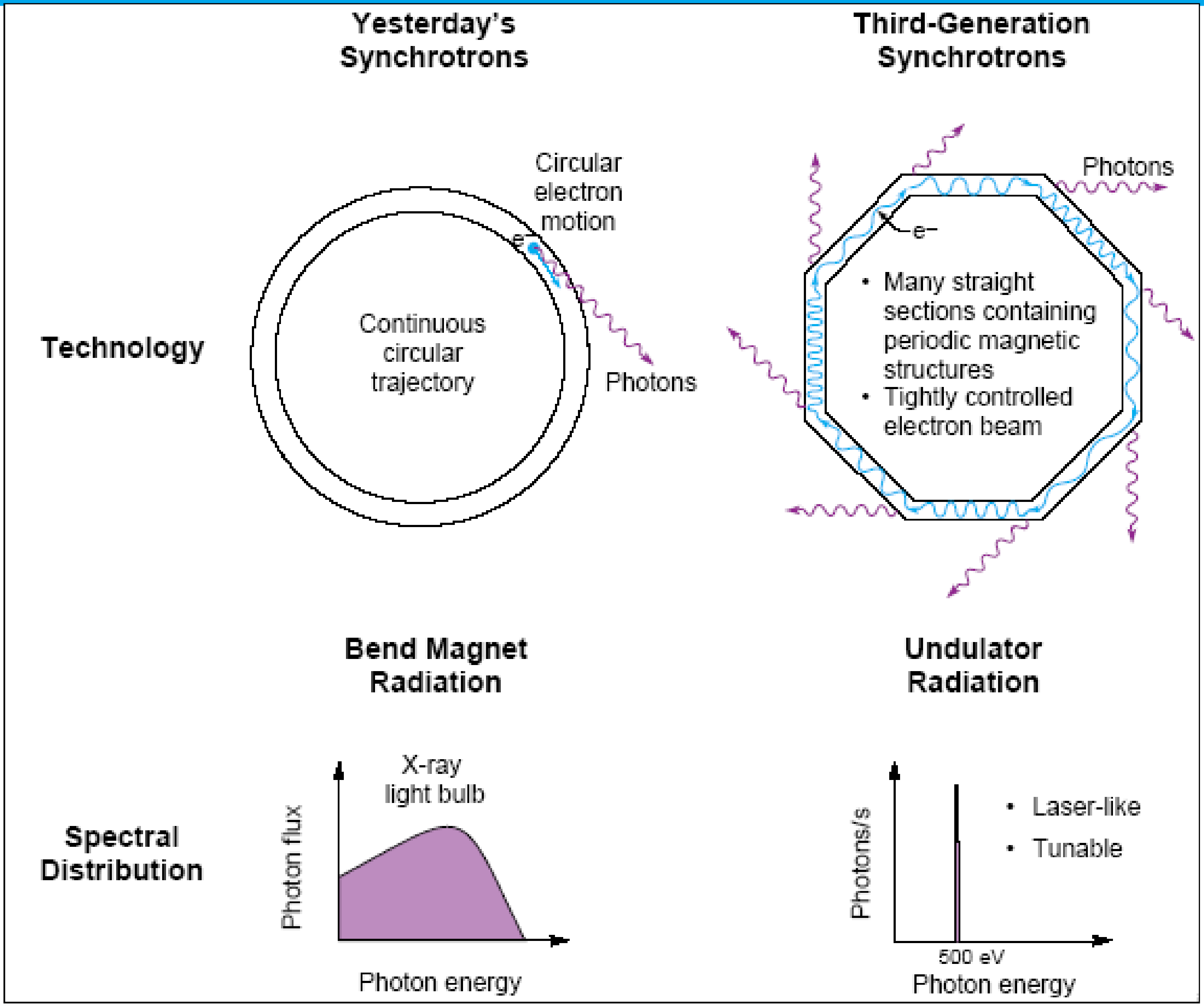
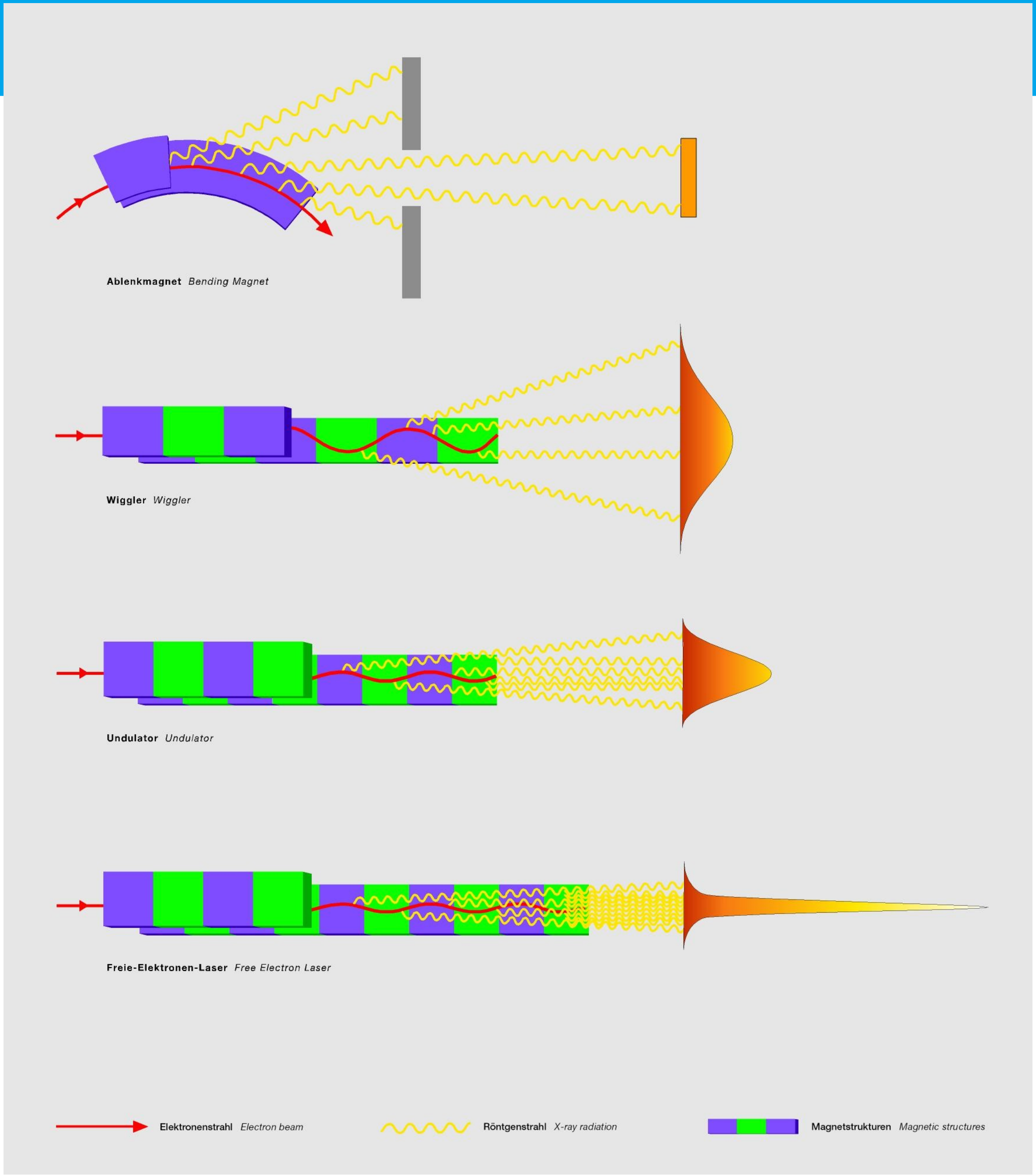
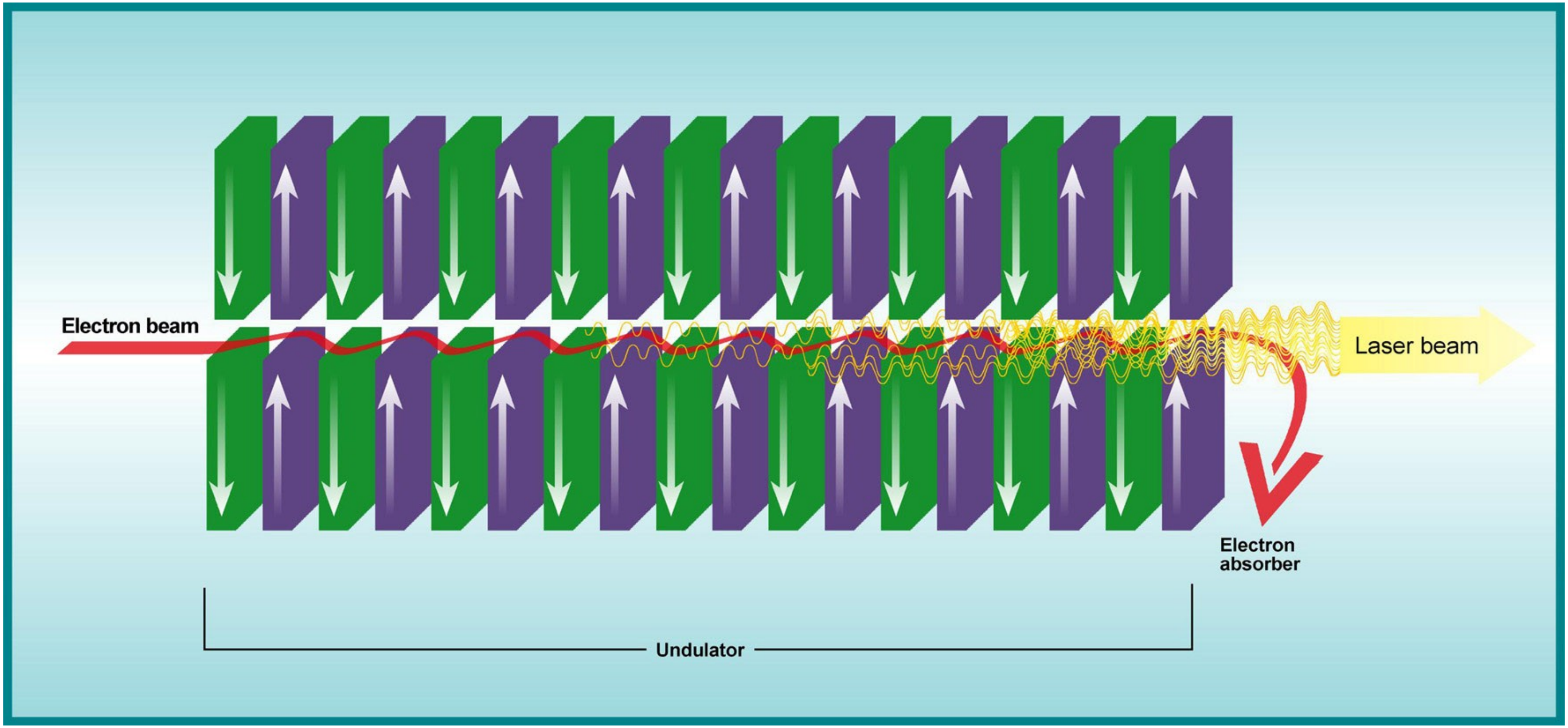


Yesterday's Synchrotrons
Third-Generation Synchrotrons
Technology
Circular electron motion
e−
Continuous circular trajectory
Photons
Photons
e−
• Many straight sections containing periodic magnetic structures
• Tightly controlled electron beam
Bend Magnet Radiation
Undulator Radiation
Spectral Distribution
X-ray light bulb
Photon flux
Photon energy
Photons/s
• Laser-like
• Tunable
500 eV
Photon energy



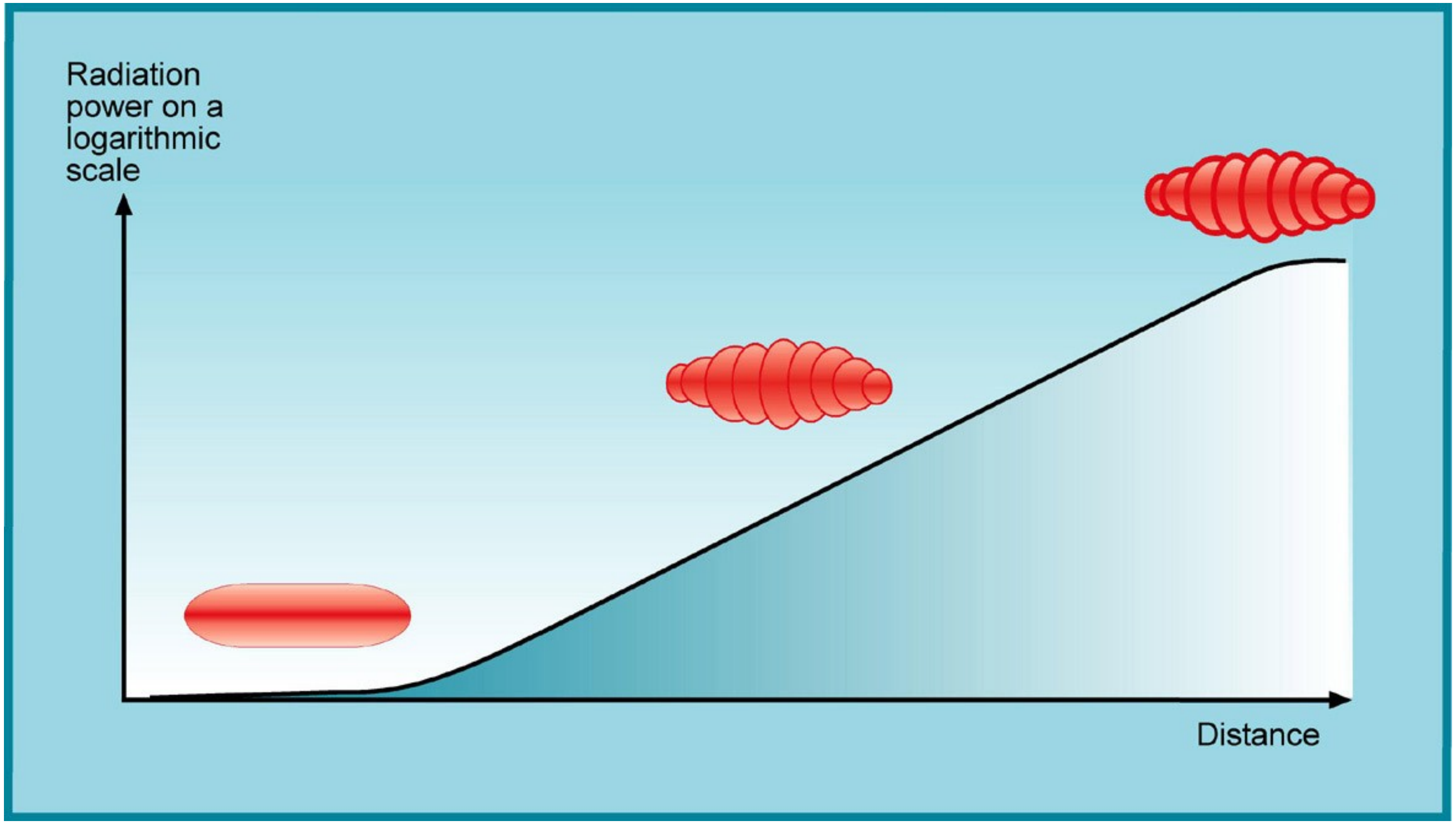
Ablenkmagnet Bending Magnet
Wiggler Wiggler
Undulator Undulator
Freie-Elektronen-Laser Free Electron Laser
Elektronenstrahl Electron beam
Röntgenstrahl X-ray radiation
Magnetstrukturen Magnetic structures

Lasing via self-amplified spontaneous emission (SASE)

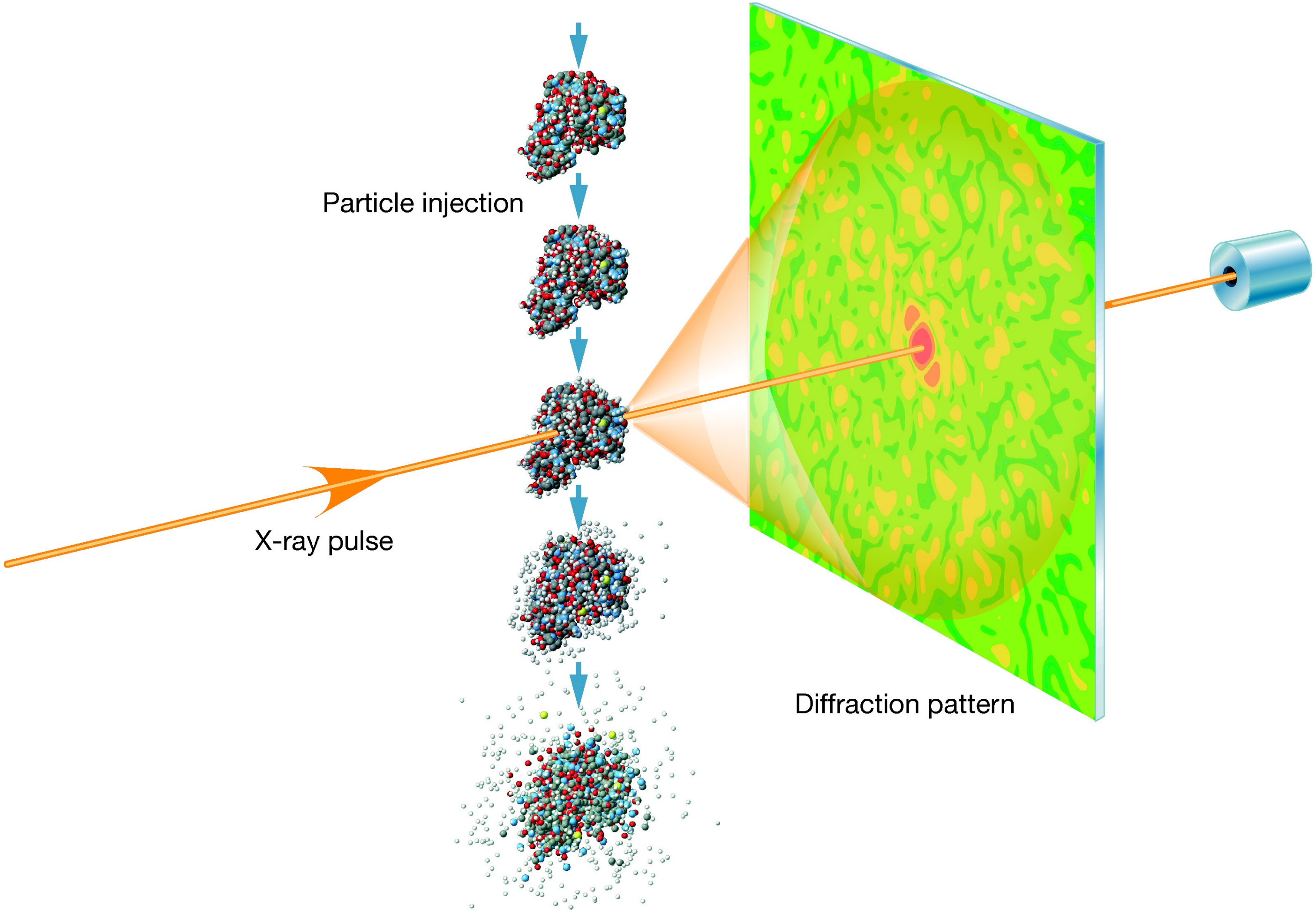


Claudio Pellegrini *et al.*

Microbunching and exponential gain

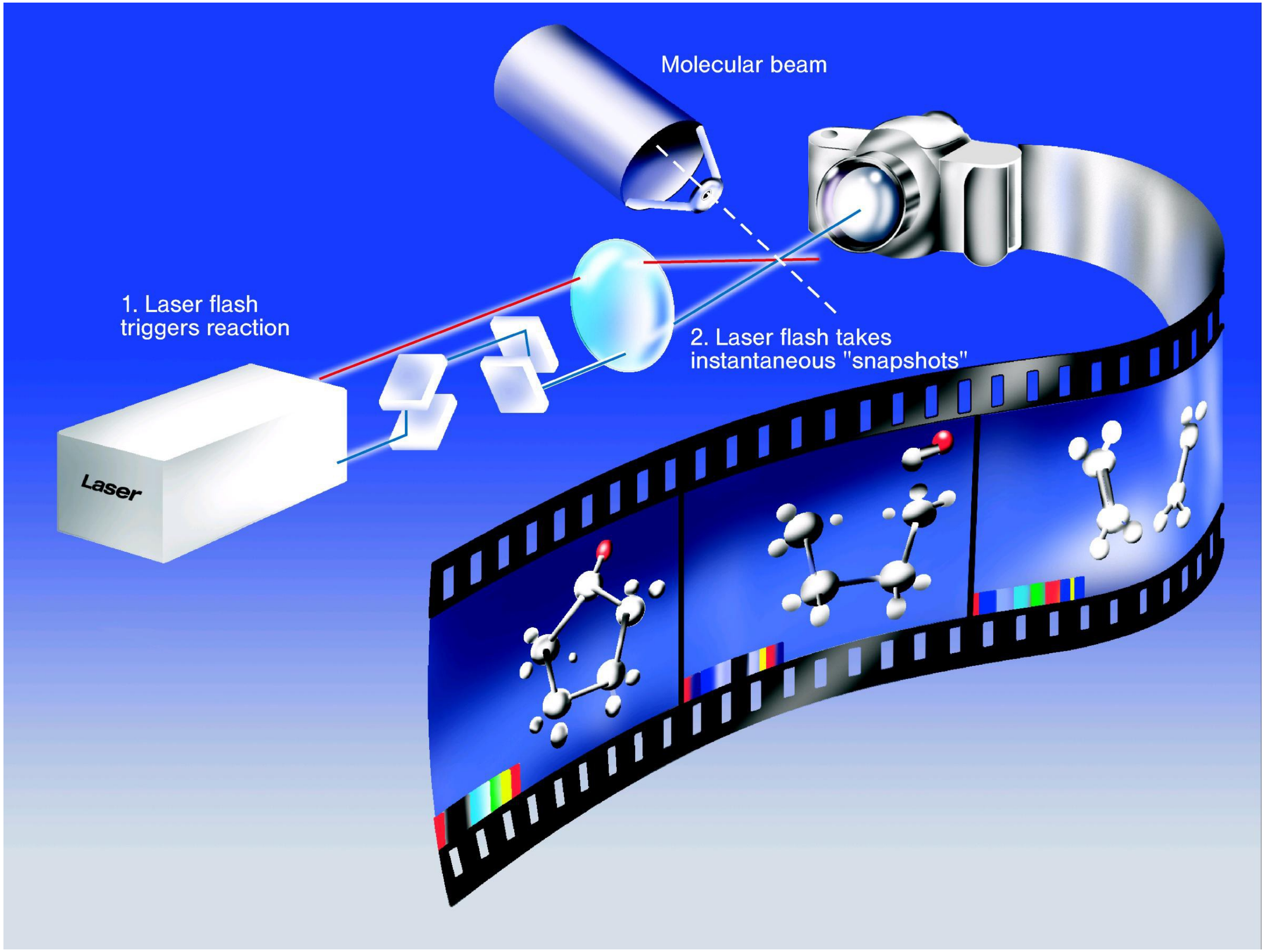


Single-shot structure determination of biomolecules

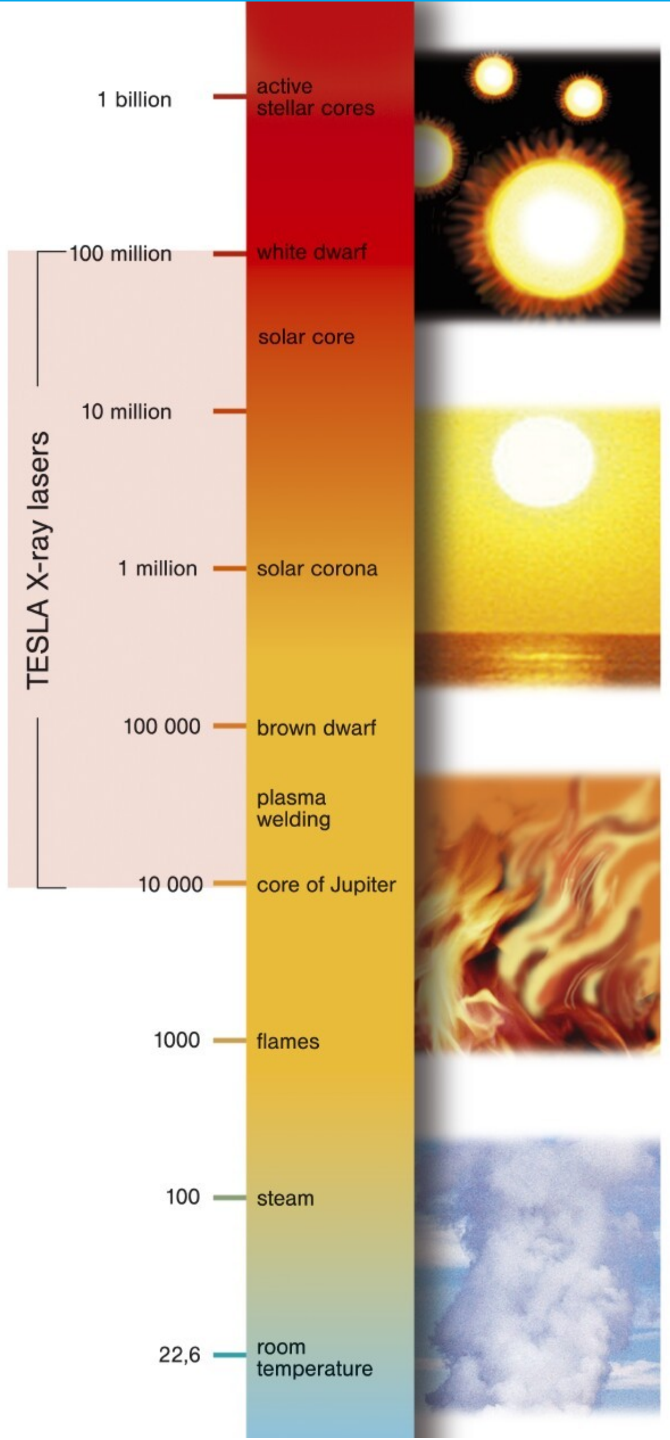


Neutze *et al.*, Nature **406**, 752 (2000).

Making molecular movies: a new tool for femtochemistry



Generating and probing extreme states of matter



The Linac Coherent Light Source (LCLS) at SLAC

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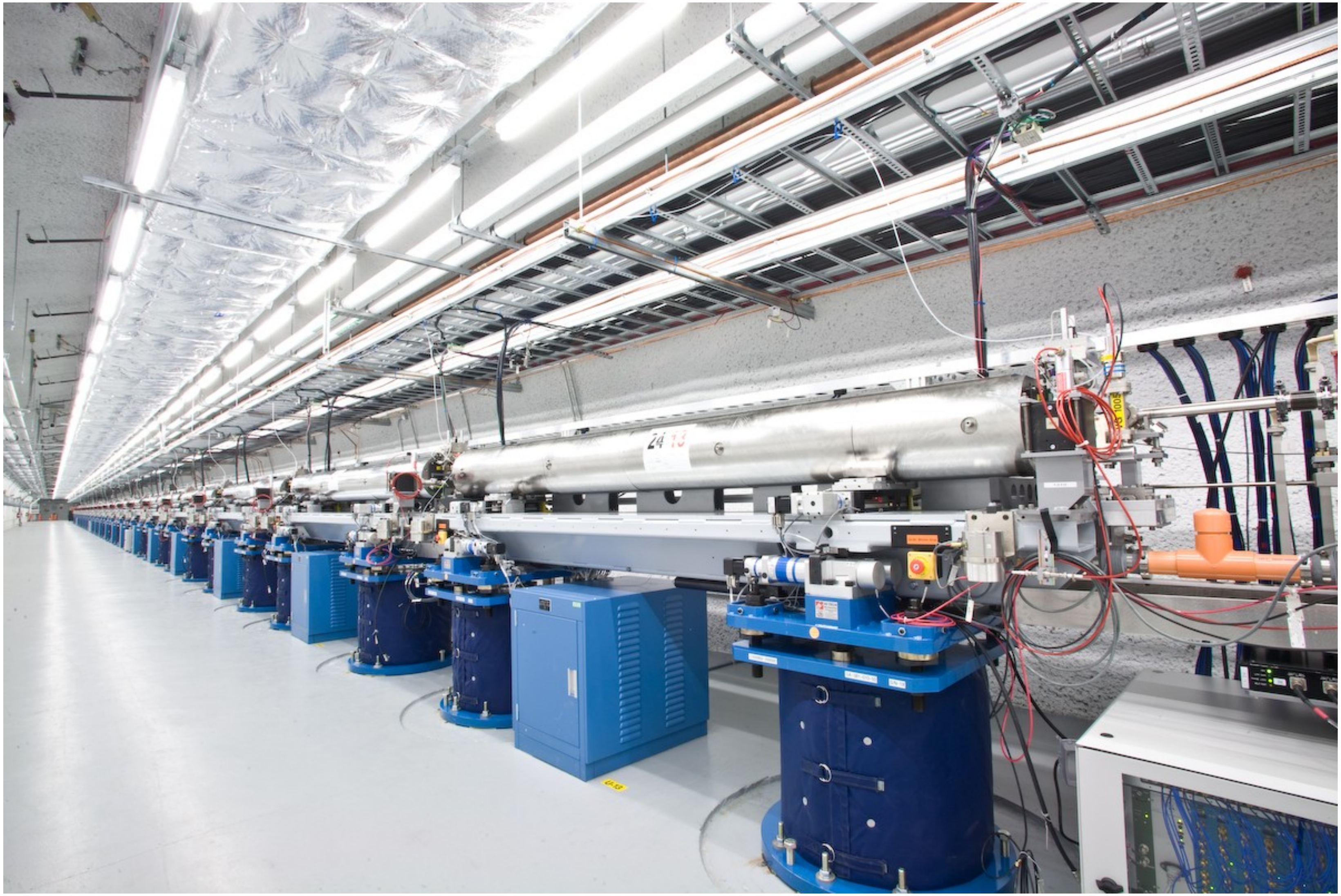
A look down the LCLS undulator hall



The first user experiment at the LCLS

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

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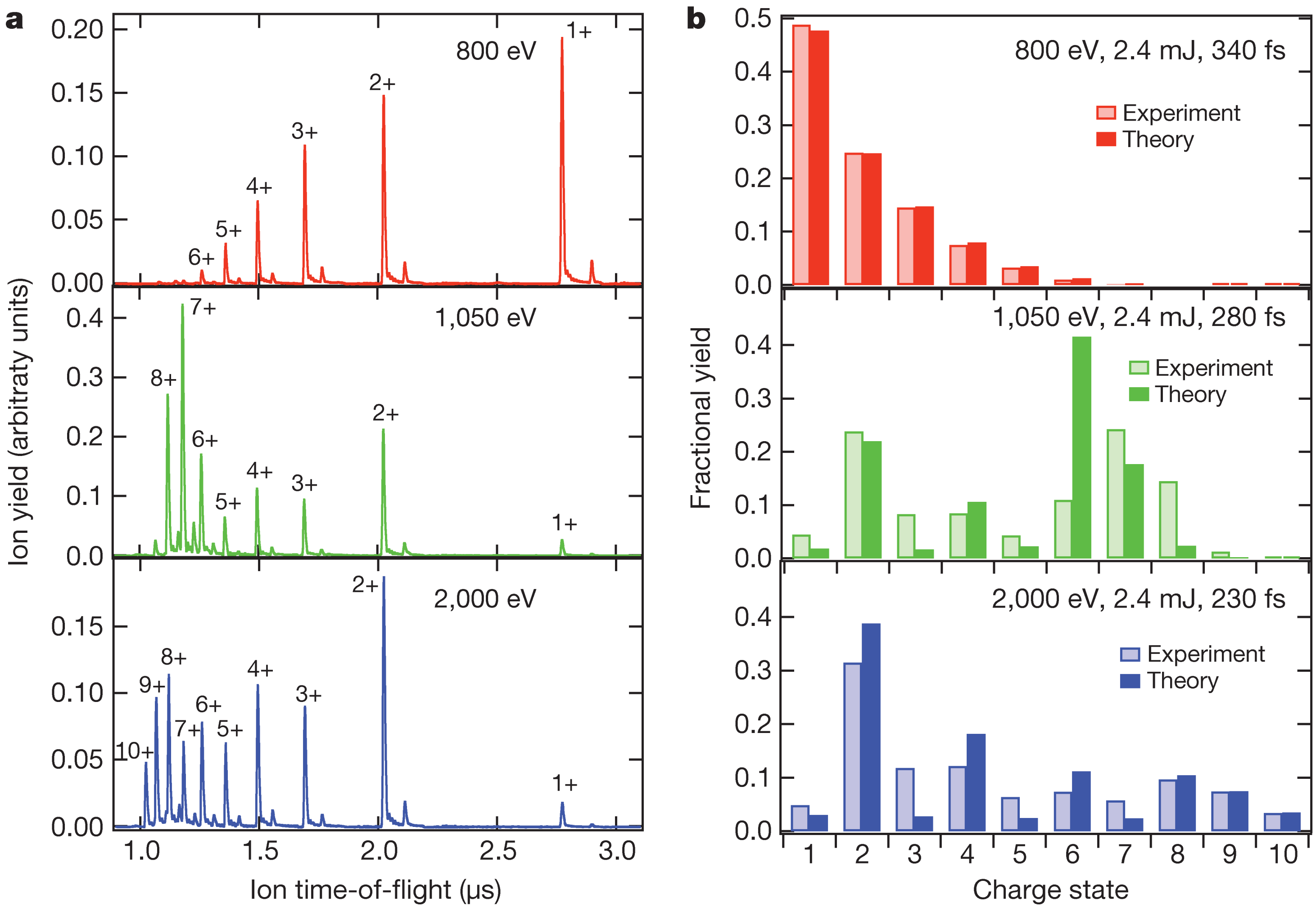
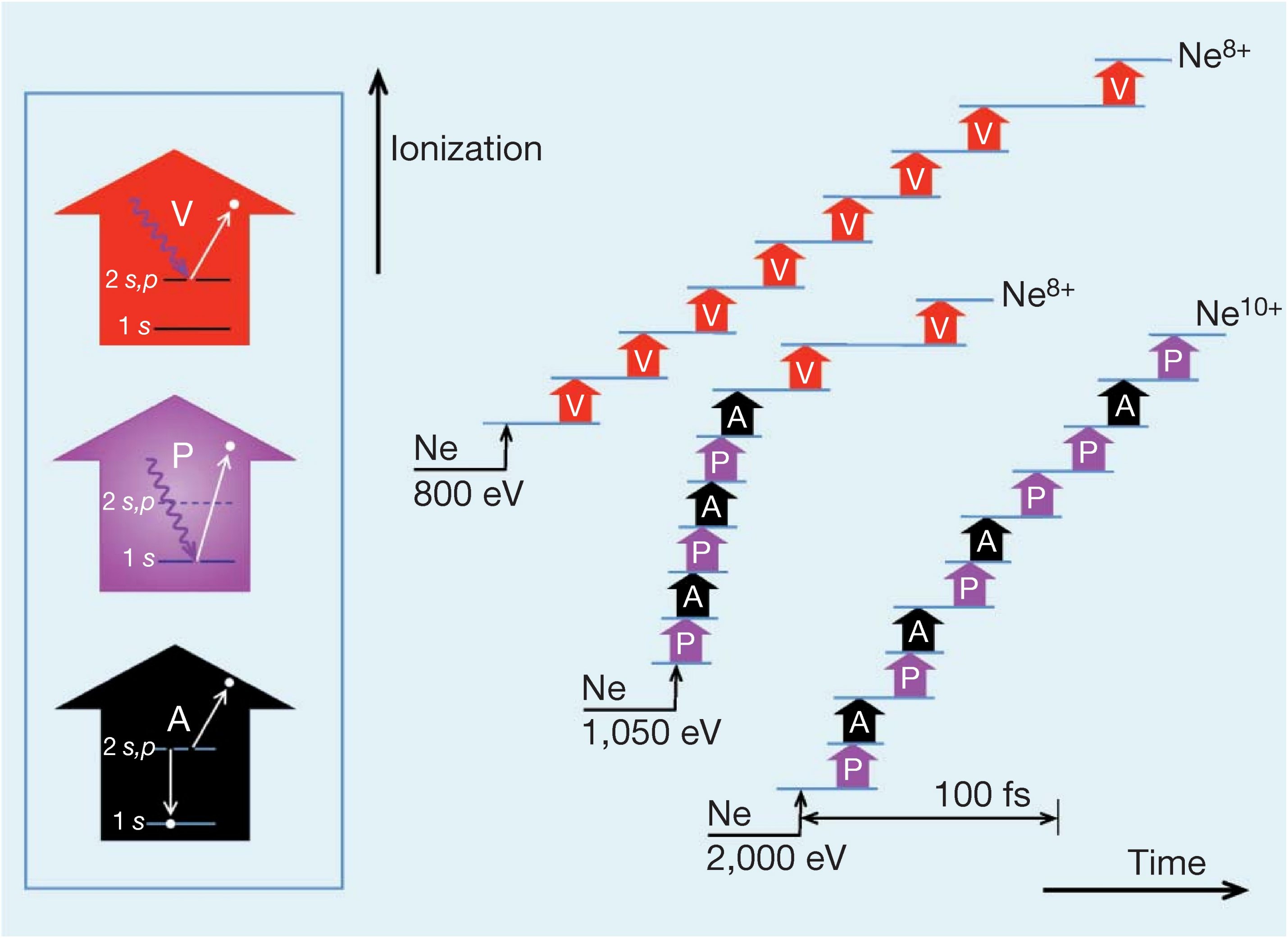
Neon charge states as a function of the photon energy



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

Photon energy-dependent ionization pathways



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

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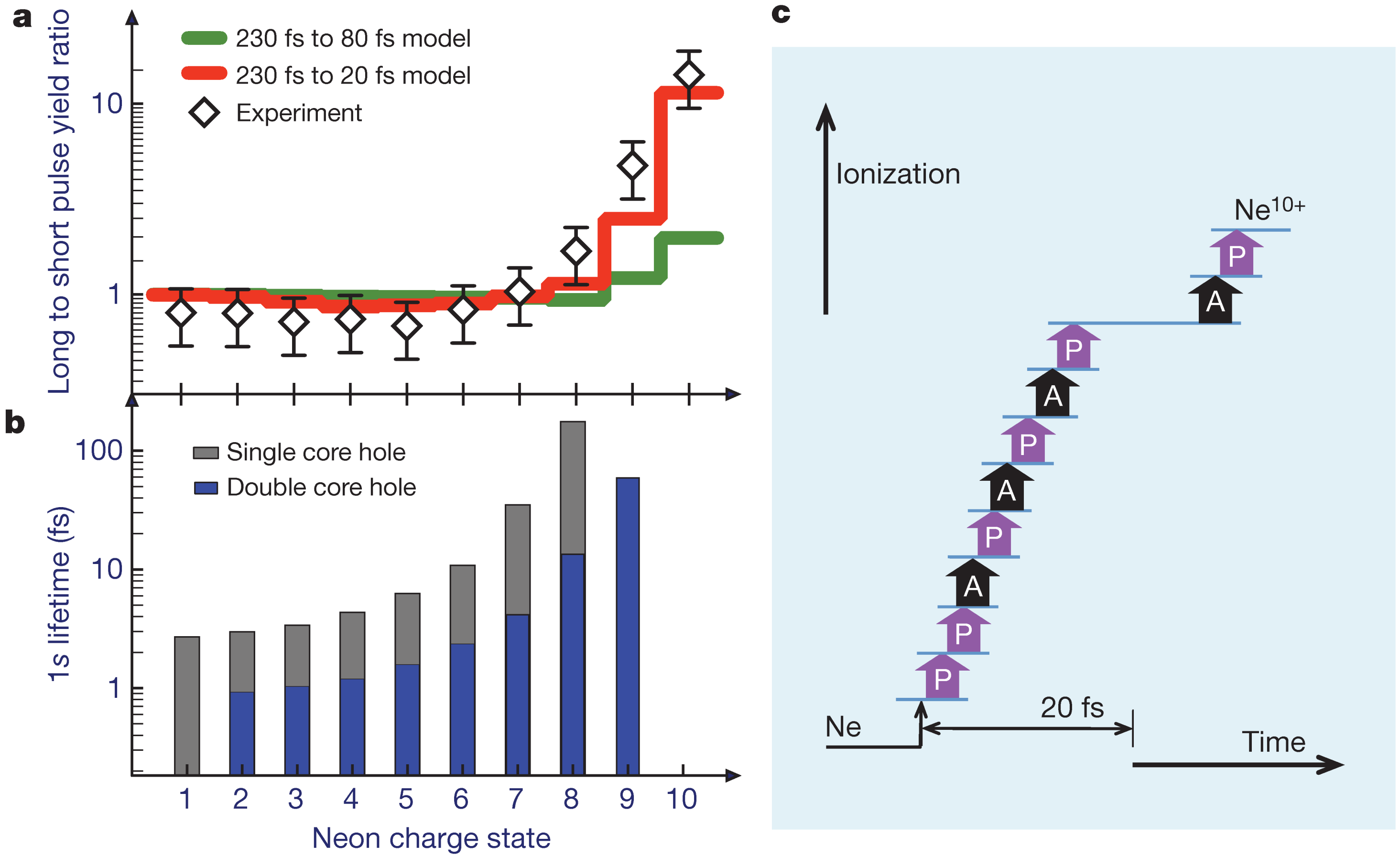
Counterintuitive impact of pulse duration

photon energy 2 keV, pulse energy 2 mJ



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

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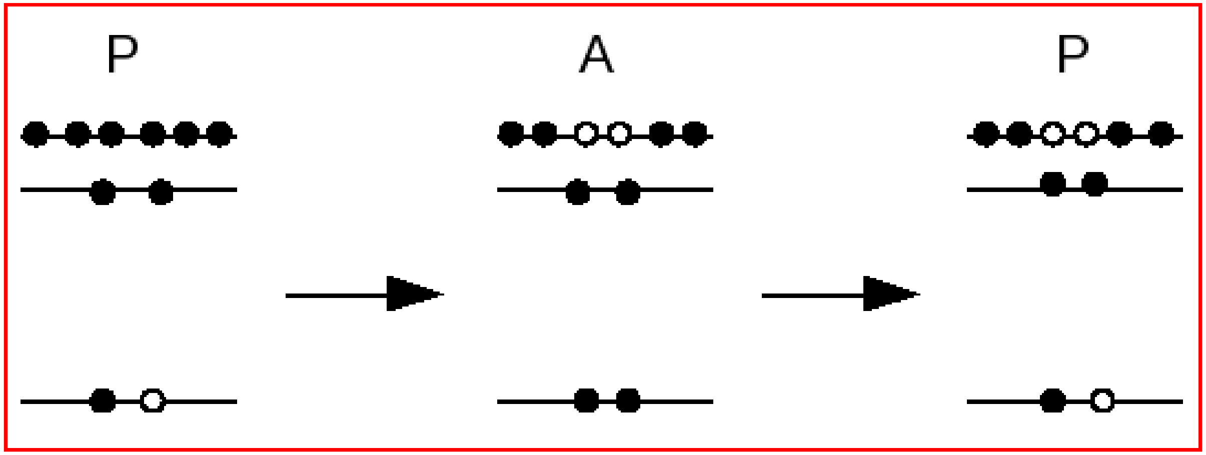
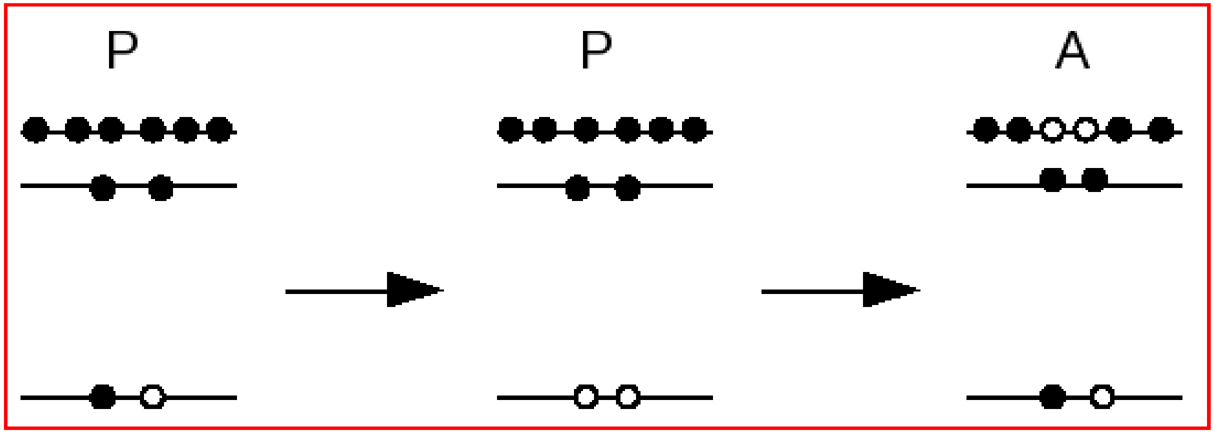
Beating the Auger clock: observe the formation of double-core-hole states via Auger electron spectroscopy





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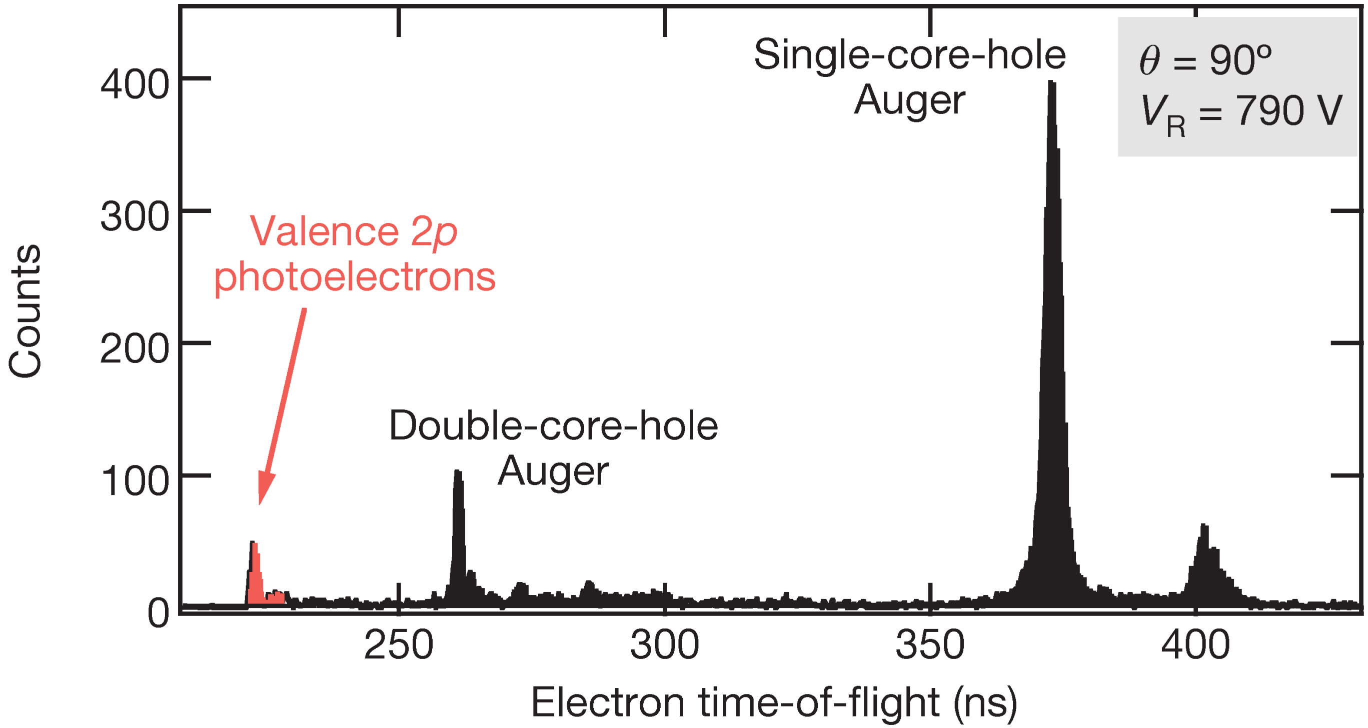
Observation of double-core-hole formation

photon energy 1050 eV, pulse energy 2 mJ, nominal pulse duration 80 fs, electrons emitted perpendicular to x-ray polarization axis



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

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Conclusions

- Multiphoton absorption is central for experiments using intense x-ray FEL radiation.
- Multiphoton absorption in the x-ray regime is predominantly sequential.
- Sequential multiphoton absorption can display nonlinearities.
- Multiphoton absorption in the x-ray regime is quite insensitive to the spiky pulse structure of SASE radiation.
- There is first evidence for a nonsequential process in the x-ray regime.