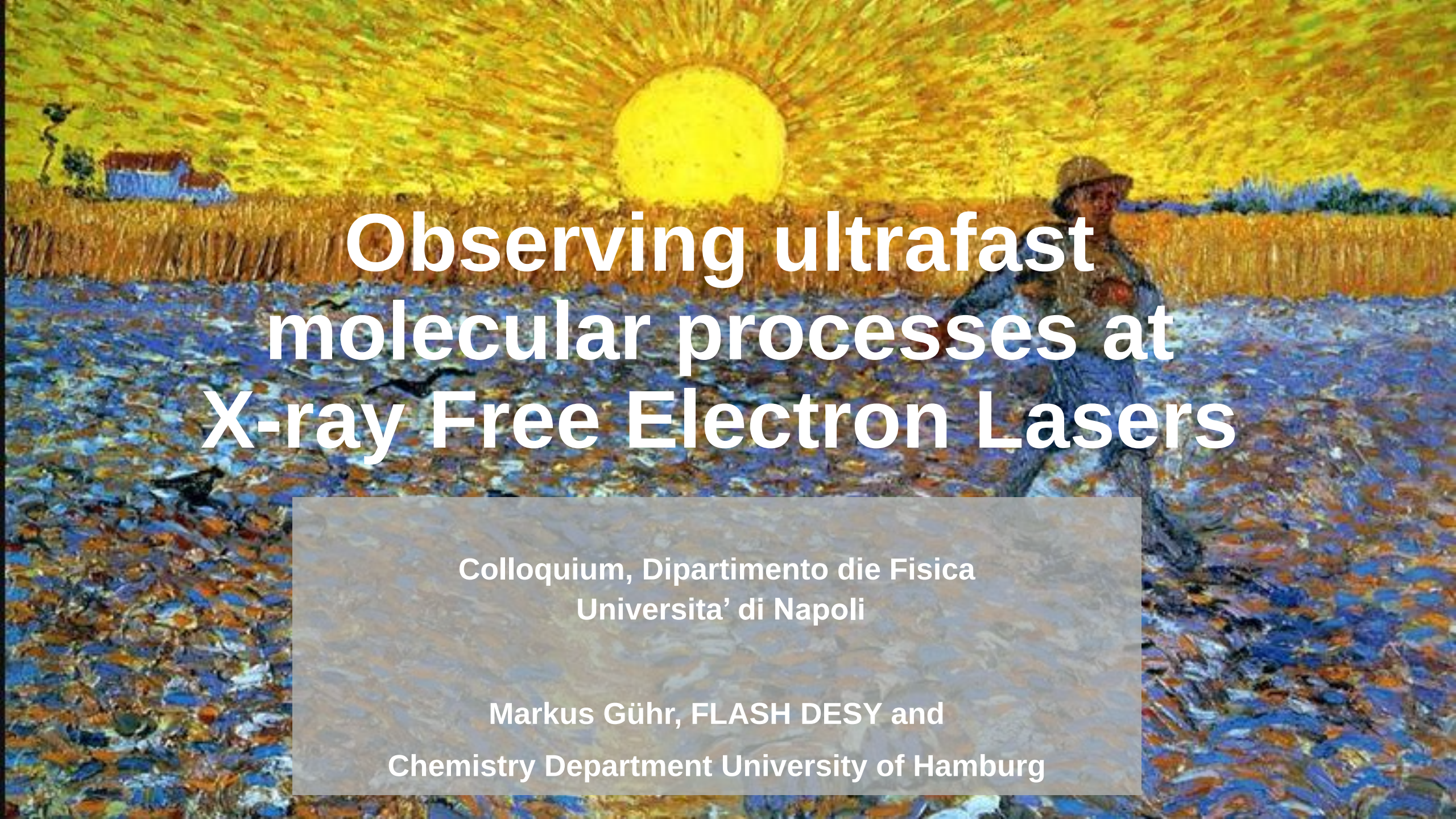
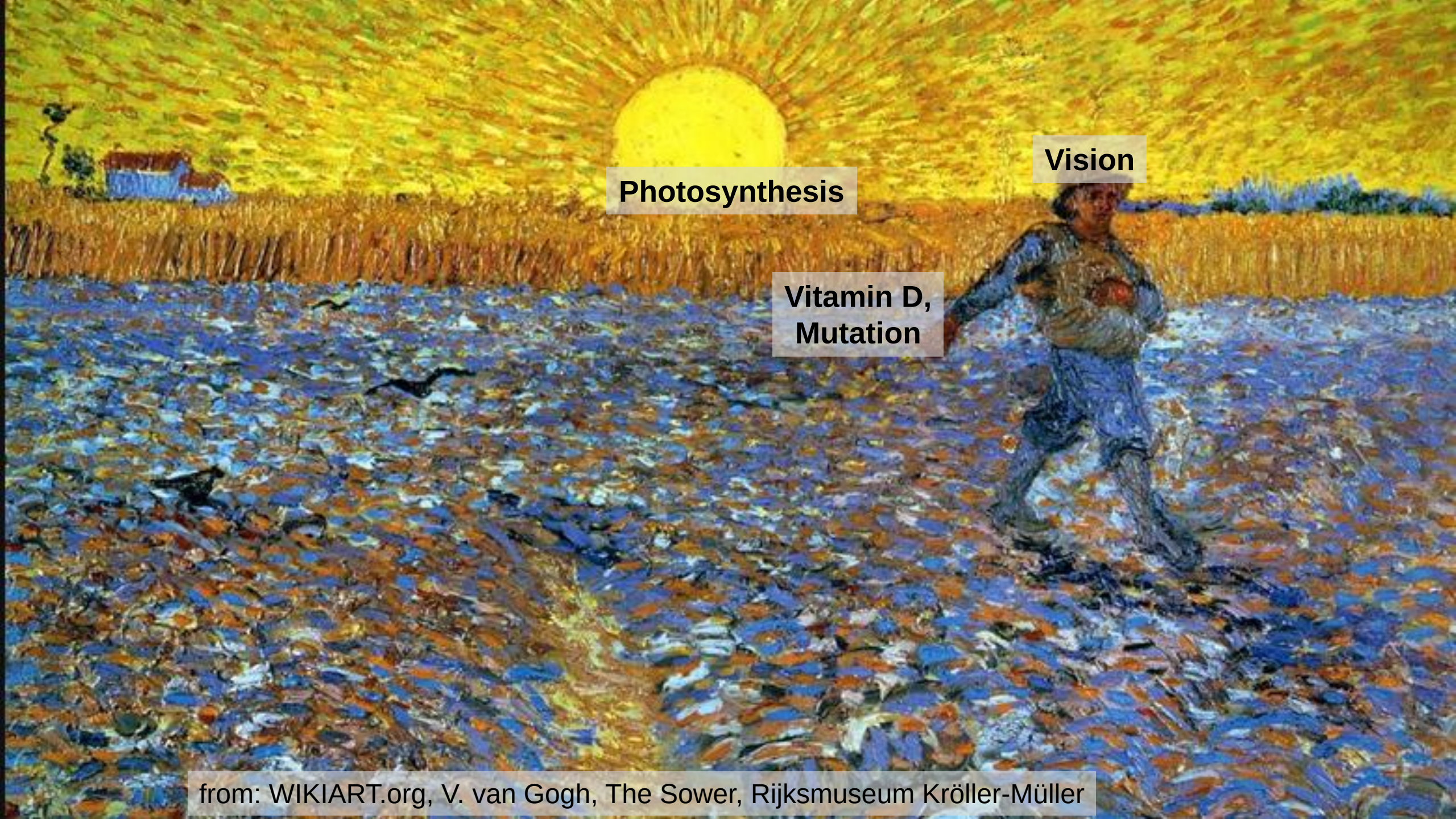


Observing ultrafast molecular processes at X-ray Free Electron Lasers

Colloquium, Dipartimento die Fisica
Universita' di Napoli

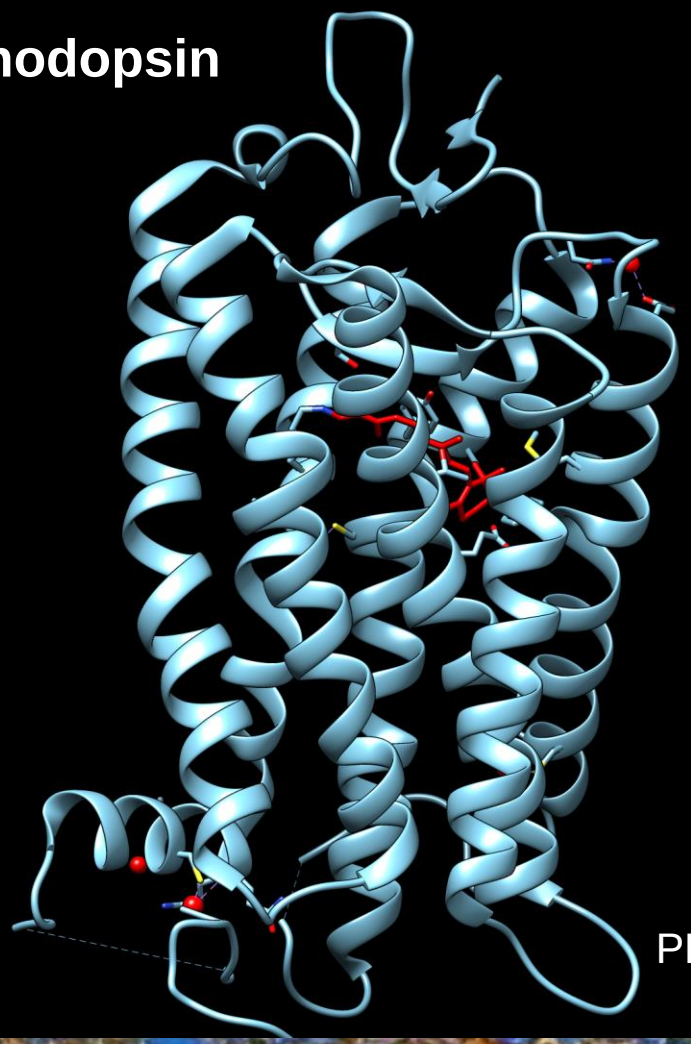
Markus Gühr, FLASH DESY and

Chemistry Department University of Hamburg



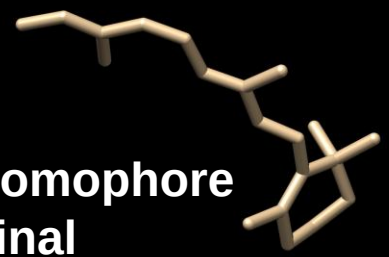
from: WIKIART.org, V. van Gogh, The Sower, Rijksmuseum Kröller-Müller

Rhodopsin



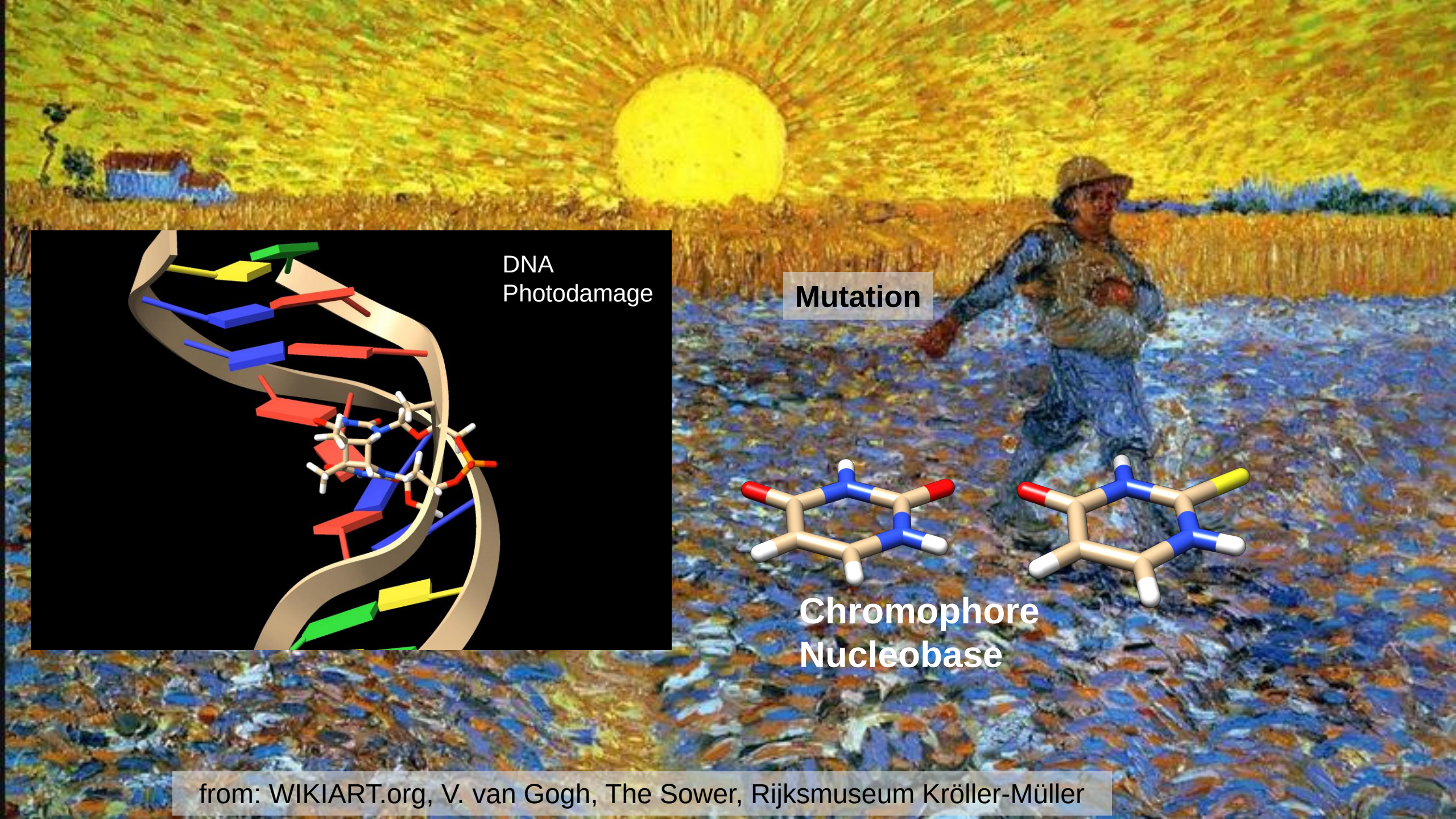
PDB 1F88

Vision



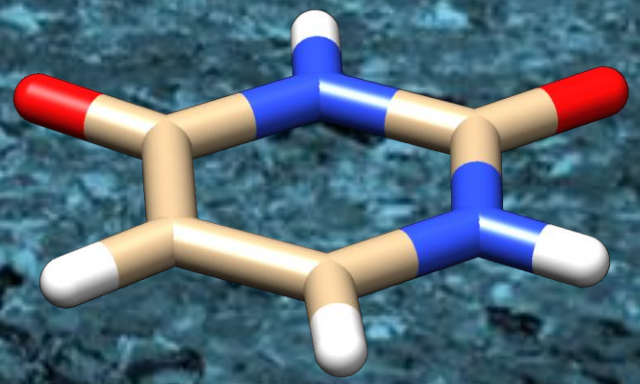
Chromophore
Retinal

from: WIKIART.org, V. van Gogh, The Sower, Rijksmuseum Kröller-Müller

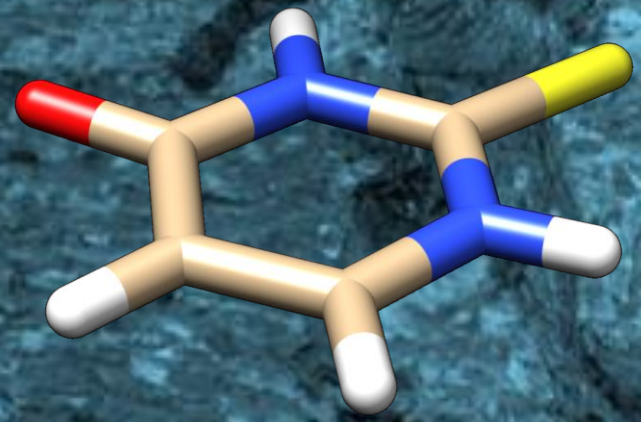


from: WIKIART.org, V. van Gogh, The Sower, Rijksmuseum Kröller-Müller

Heat production



Change in spin

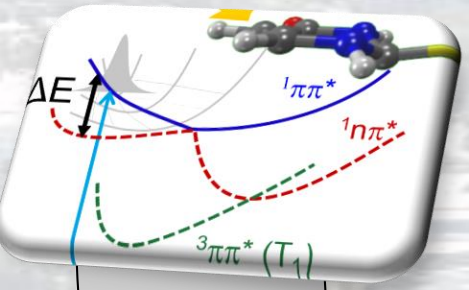


How does this selectivity arise?

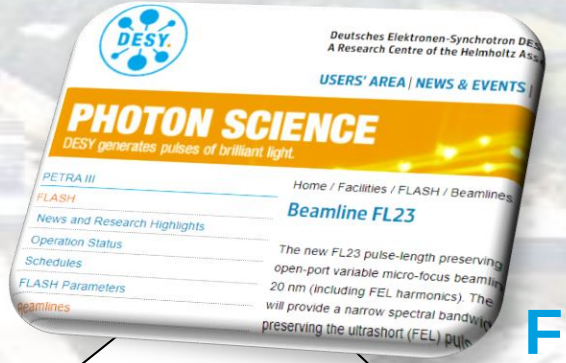
Coupled, ultrafast electron-nuclear dynamics

from: WIKIART.org, V. van Gogh, The Sower, Rijksmuseum Kröller-Müller

Outline

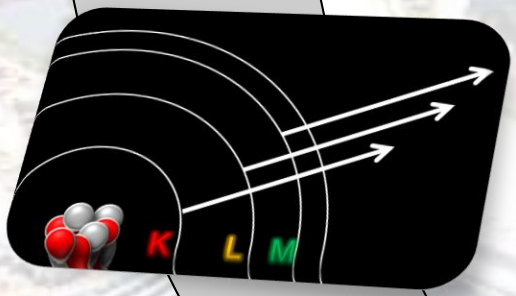


Molecular Photoenergy Conversion

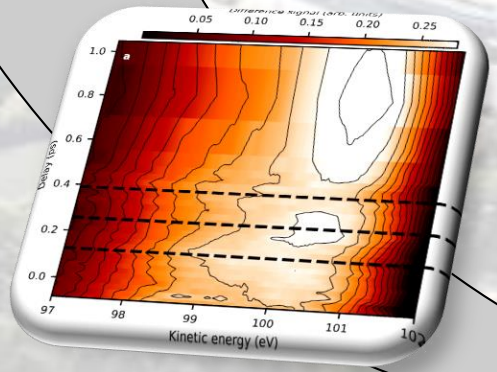


FLASH Beamtime

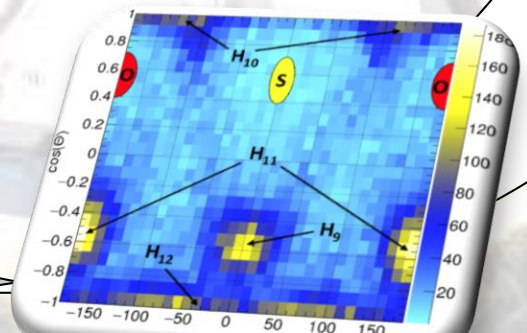
X-ray Probing

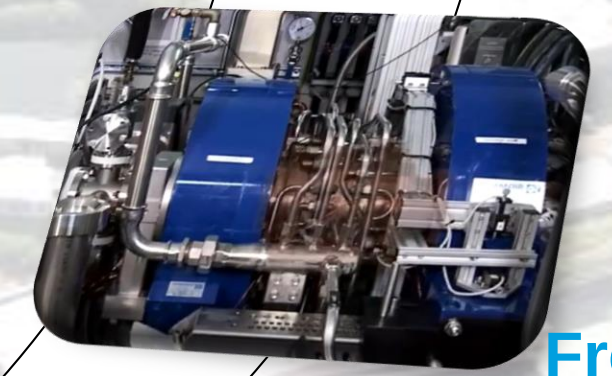


Electronic Movie



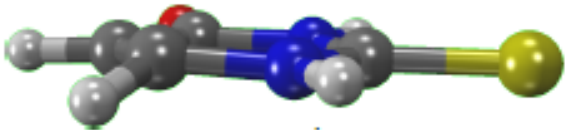
Geometry Movie

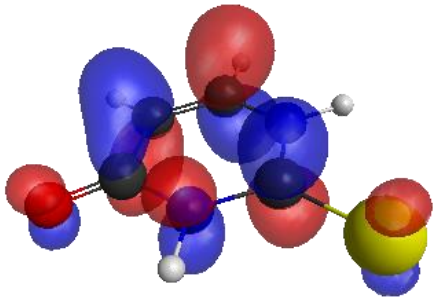


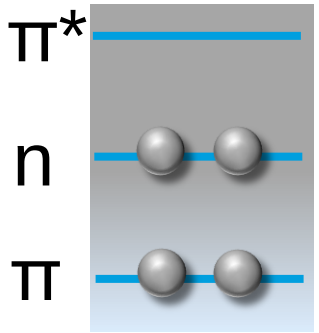


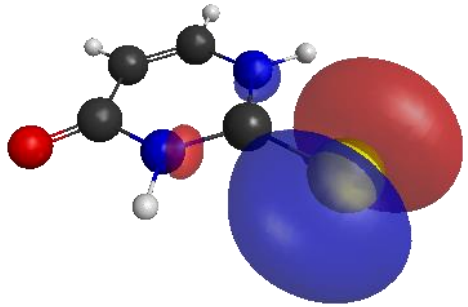
Free-electron laser physics

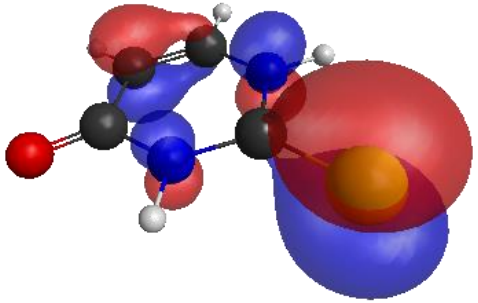
Light couples to electrons



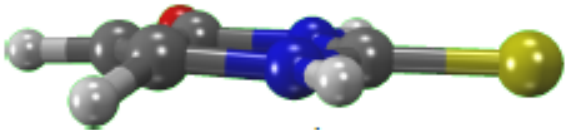


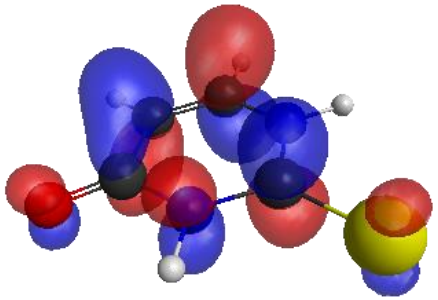


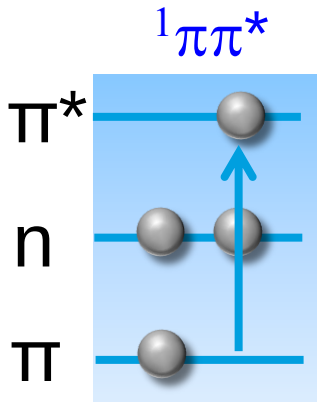


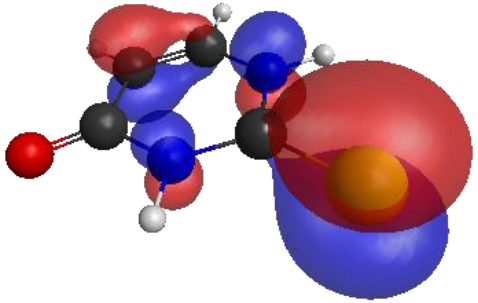


Light couples to electrons

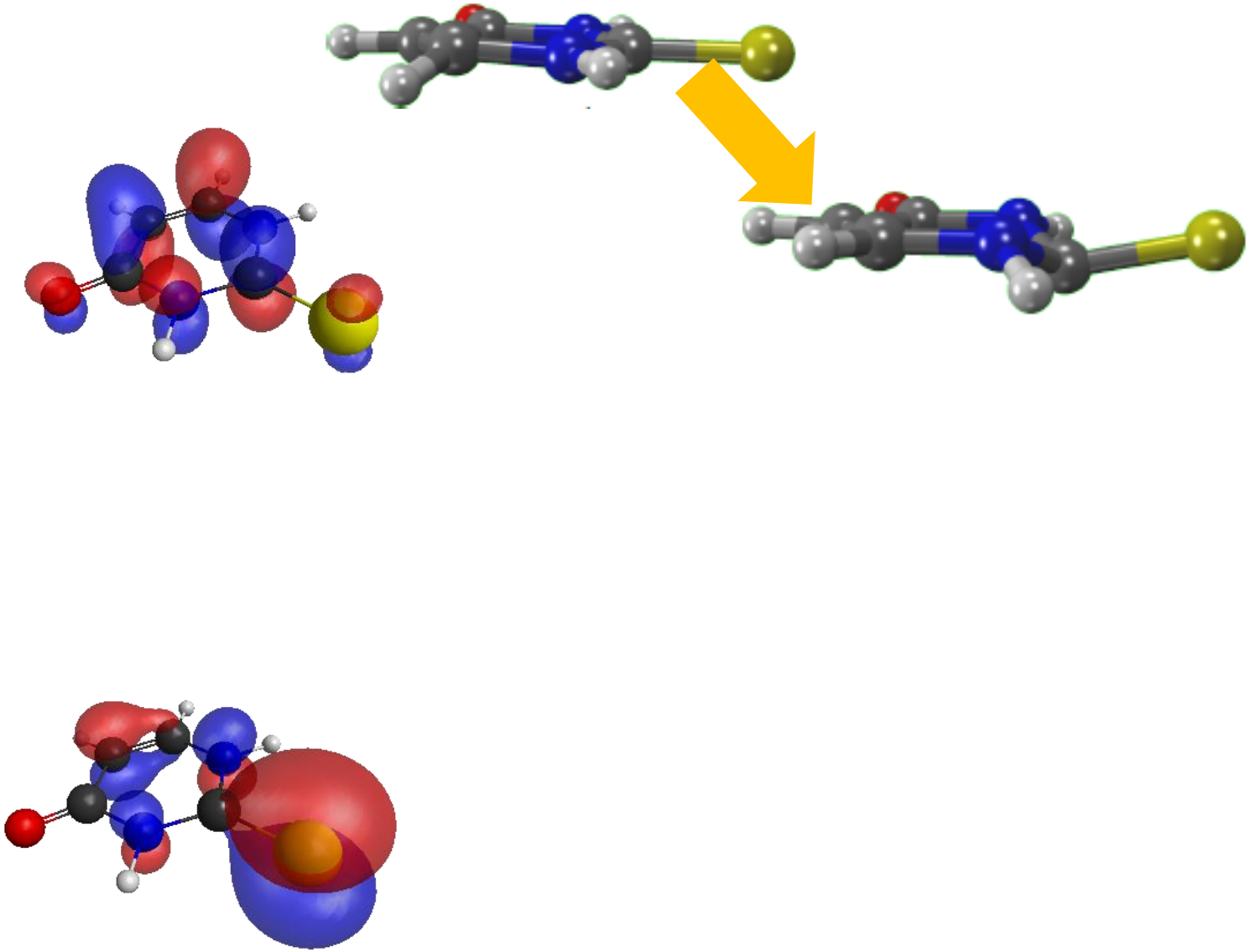




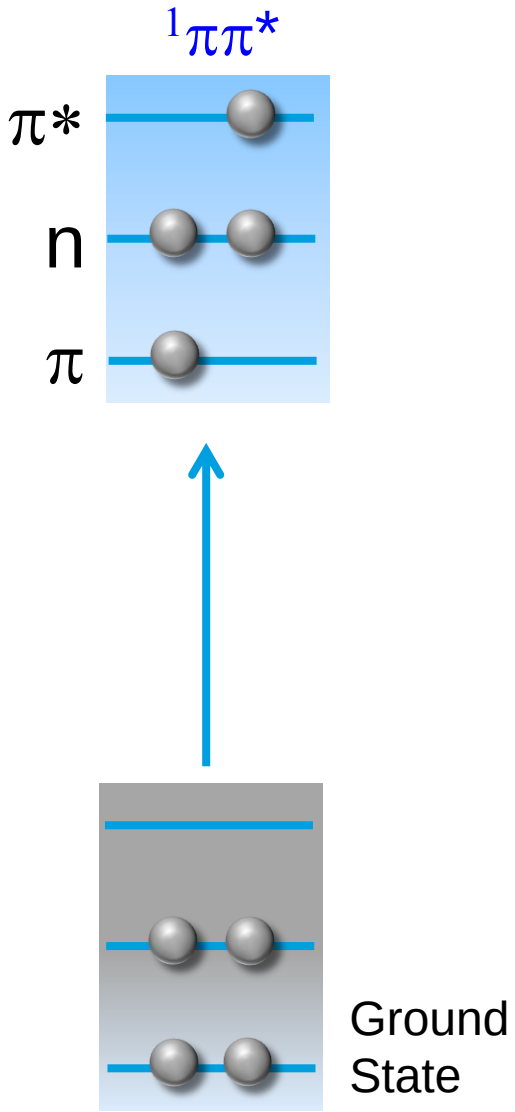


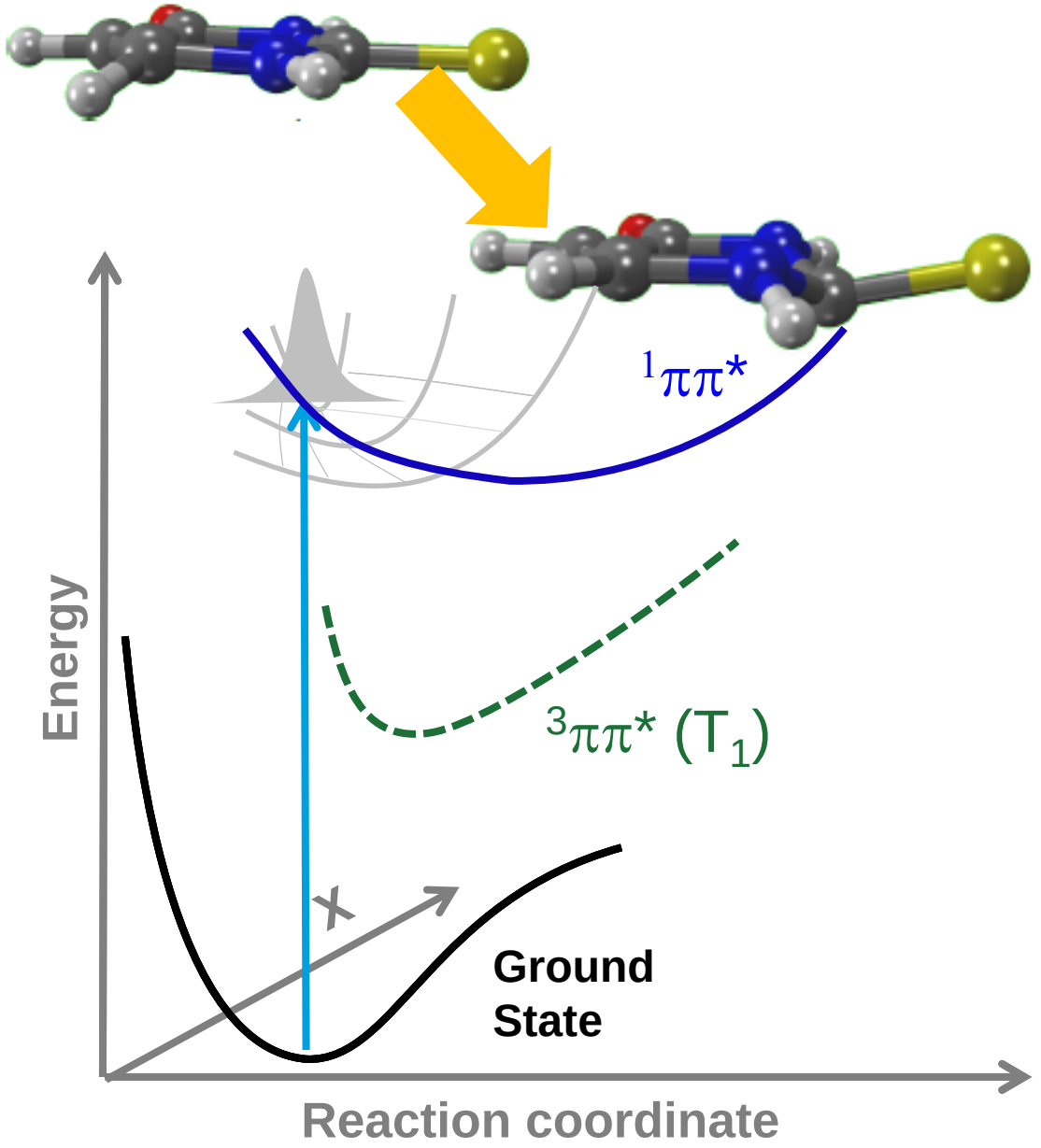


Electrons couple to nuclei

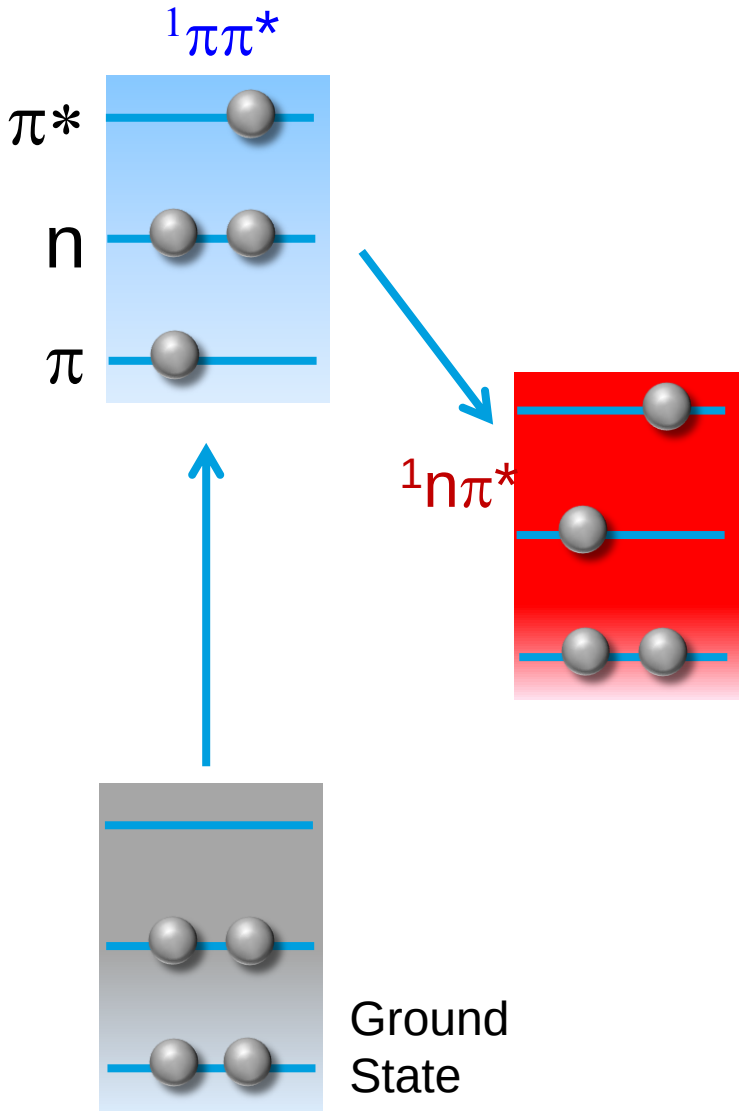


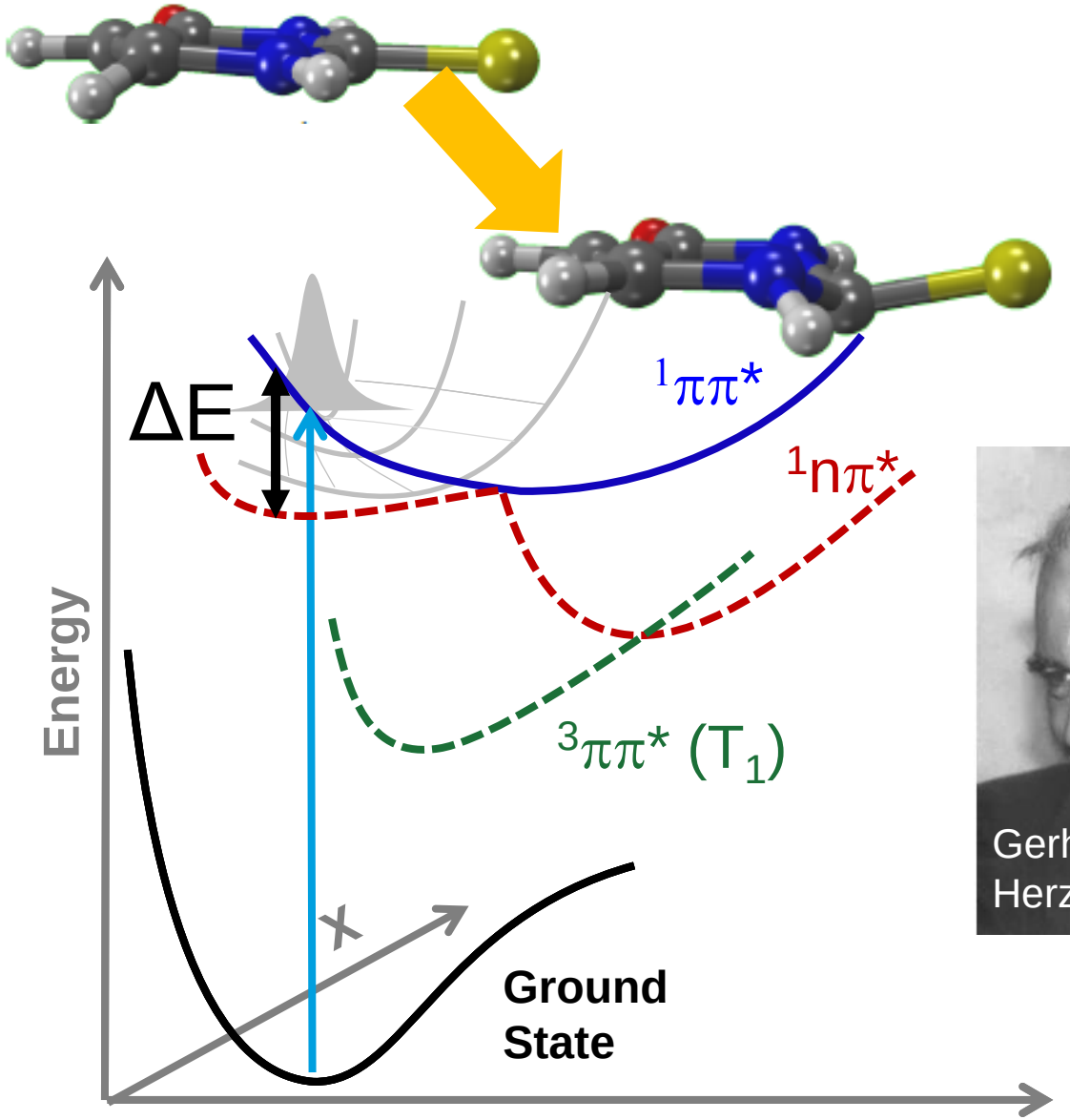
Electrons couple to nuclei

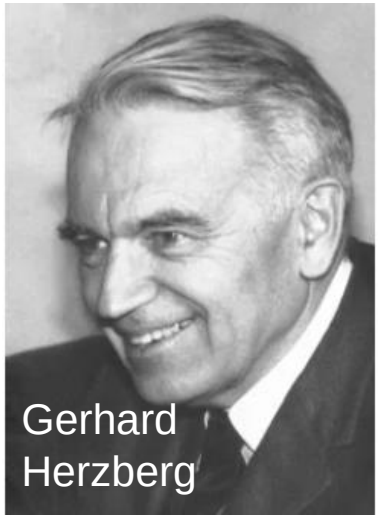




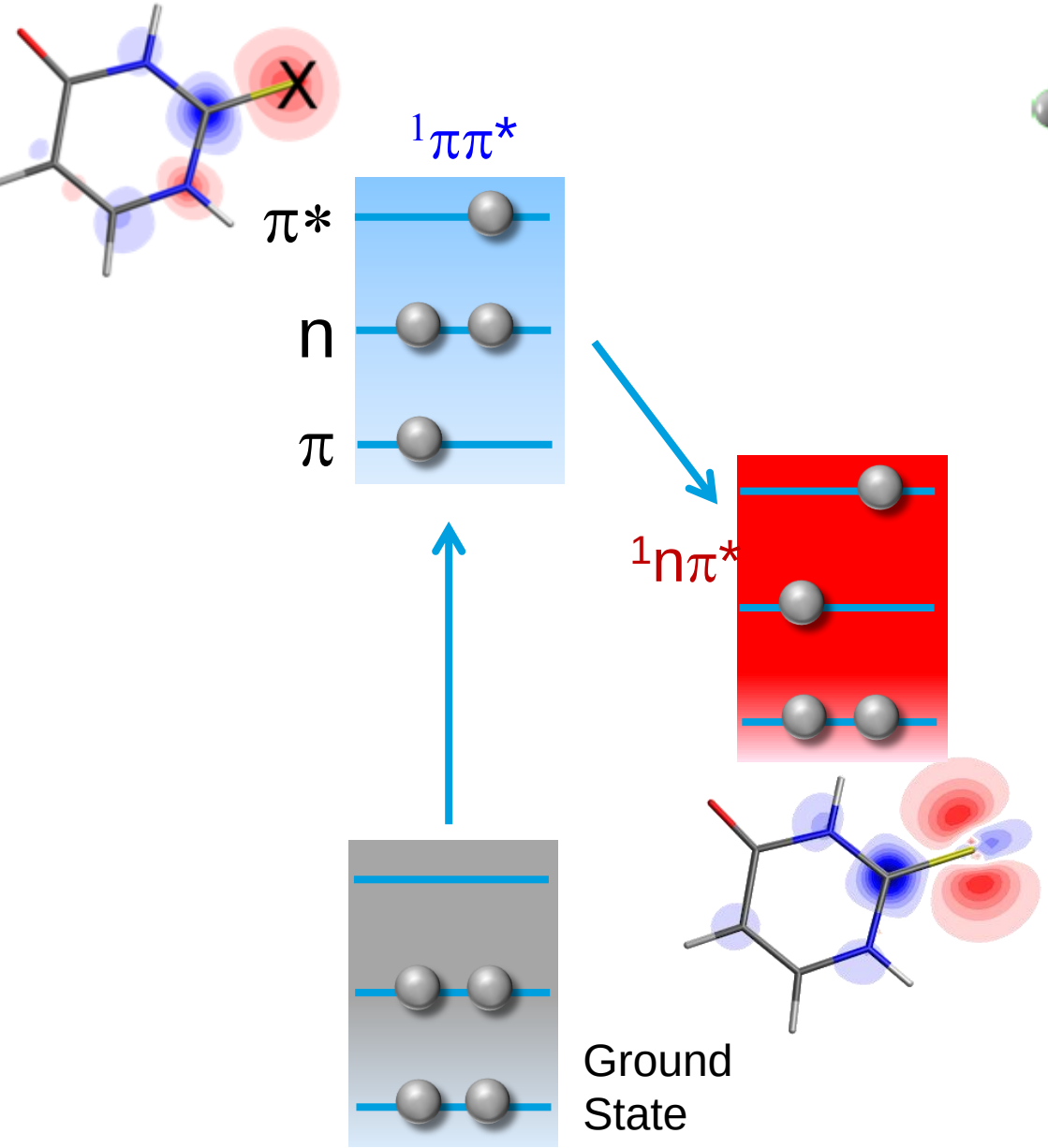
Nuclei couple to electrons

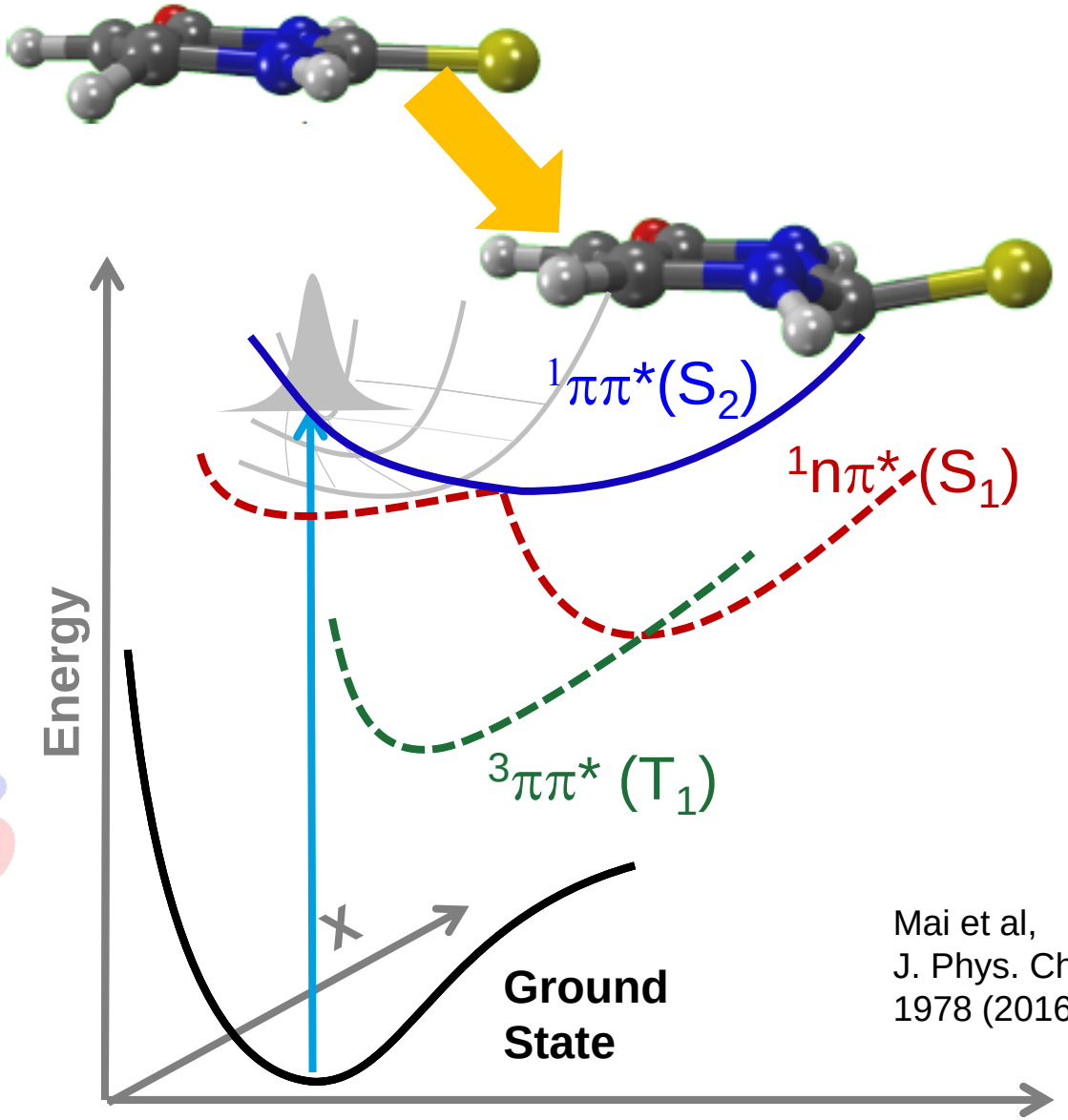






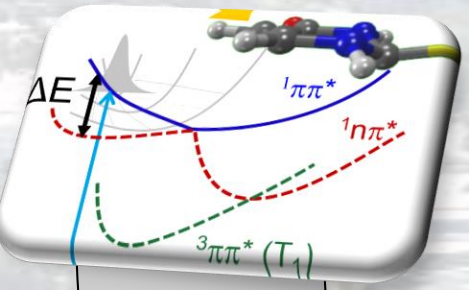
Nuclei couple to electrons and their spin



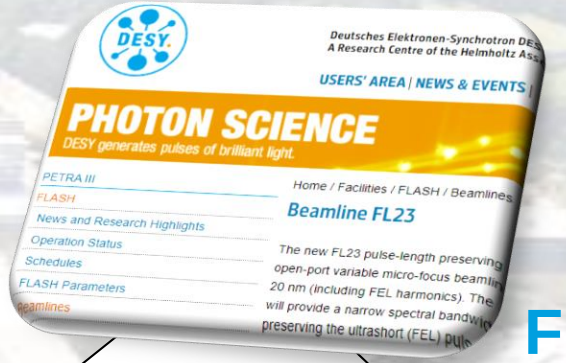


Mai et al,
J. Phys. Chem. Lett. **7**, 1978 (2016)

Outline

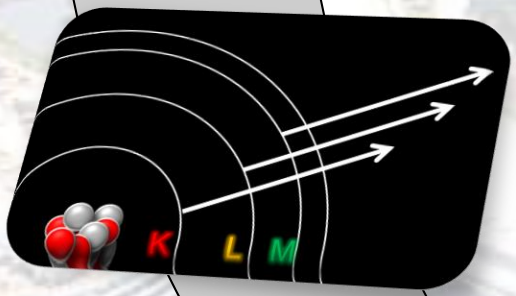


Molecular Photoenergy Conversion

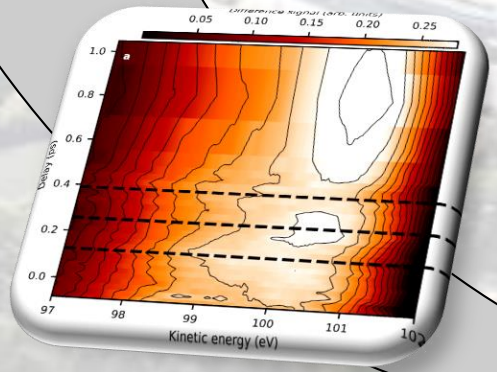


FLASH Beamtime

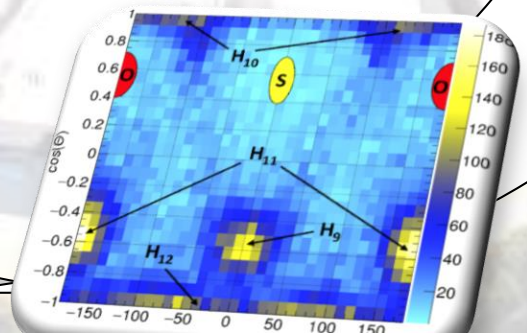
X-ray Probing

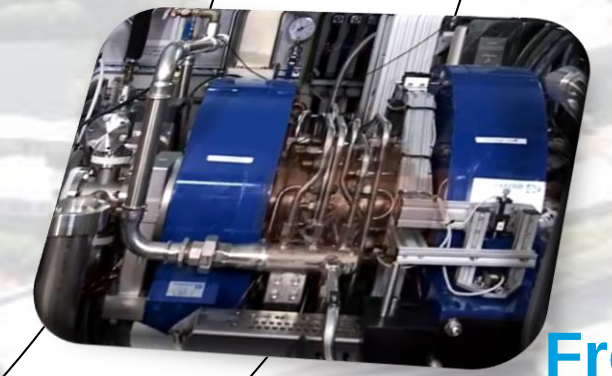


Electronic Movie



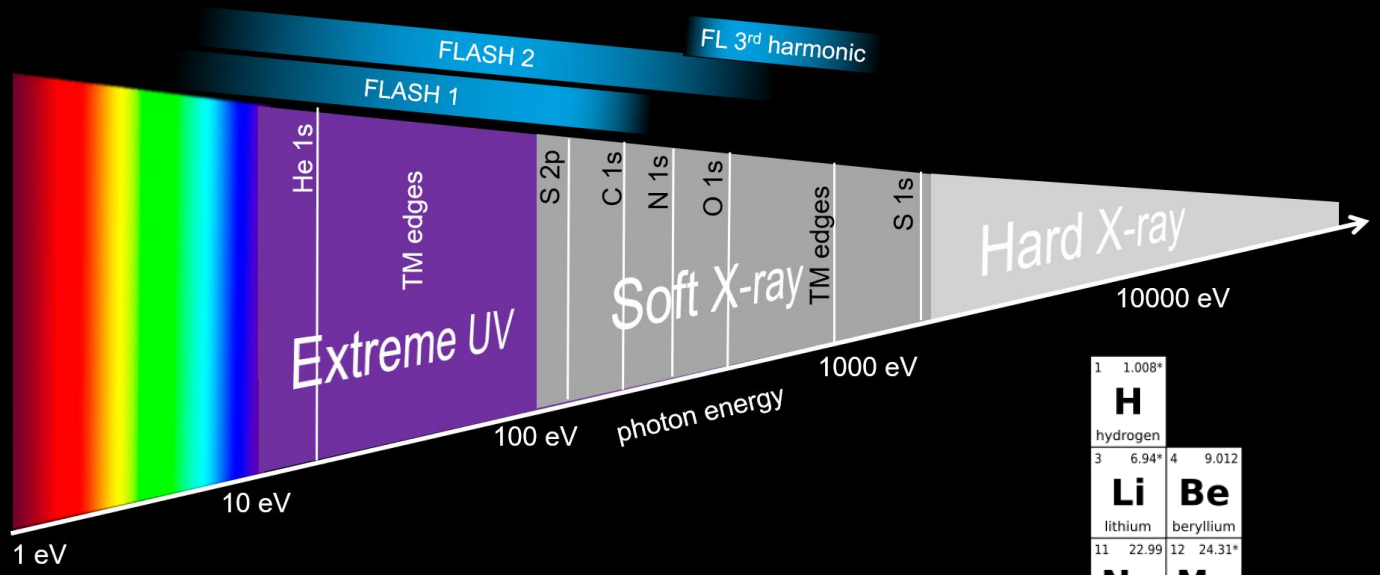
Geometry Movie

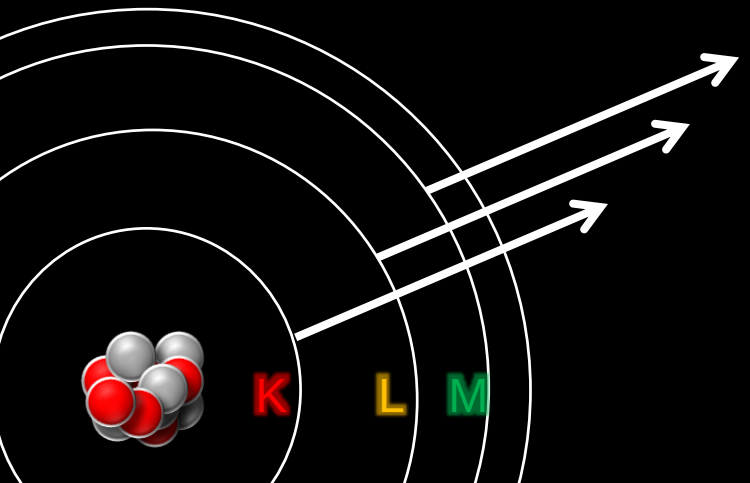




Free-electron laser physics

FLASH allows element and site spefific electronic probing

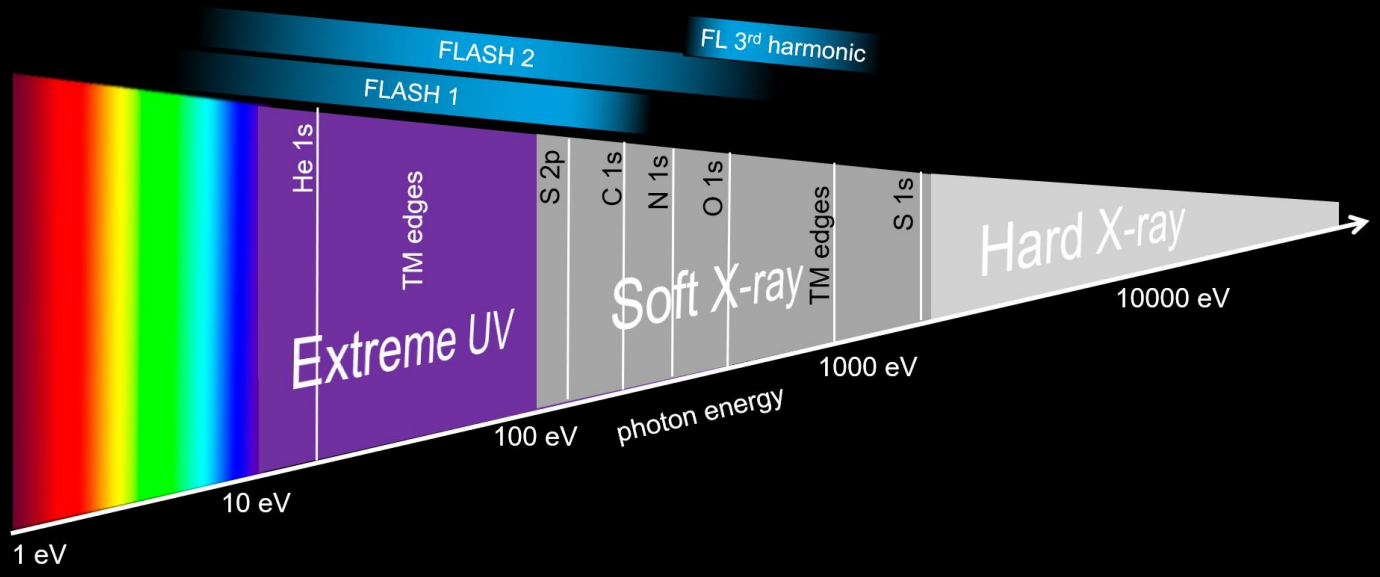


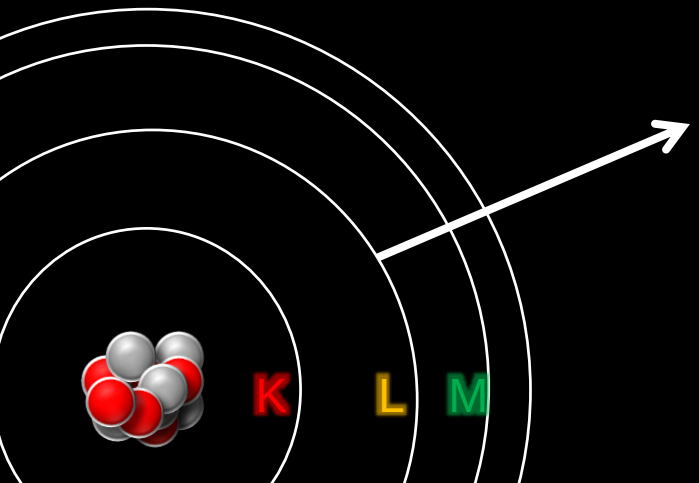


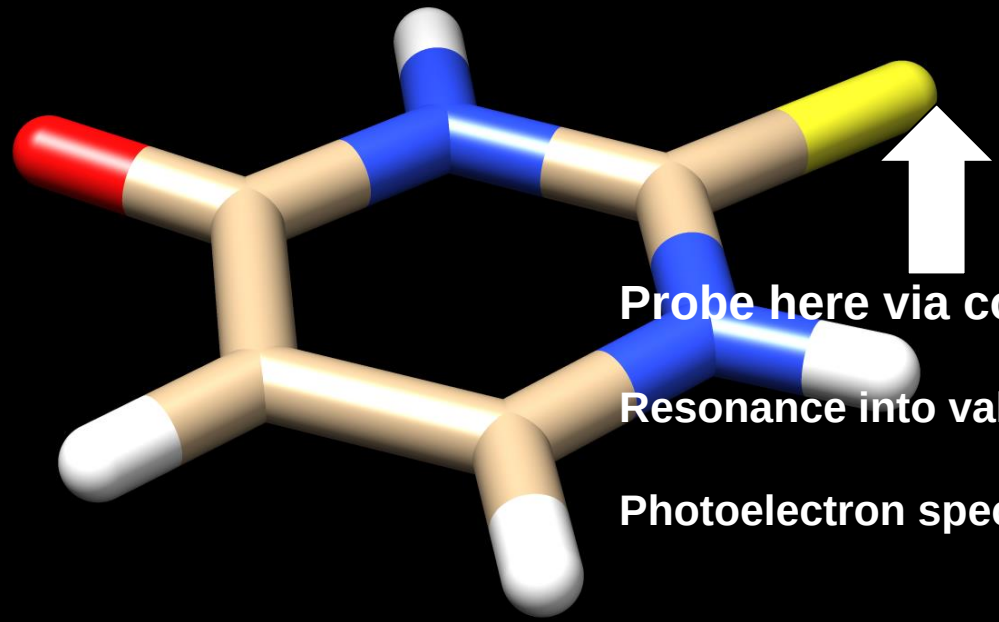
1 1.008* H hydrogen																	2 4.003 He helium
3 6.94* Li lithium	4 9.012 Be beryllium											5 10.81* B boron	6 12.01* C carbon	7 14.01* N nitrogen	8 16.00* O oxygen	9 19.00 F fluorine	10 20.18 Ne
11 22.99 Na sodium	12 24.31* Mg magnesium											13 26.98 Al aluminium	14 28.09* Si silicon	15 30.97 P phosphorus	16 32.06* S sulfur	17 35.45* Cl chlorine	18 39.95 Ar argon
19 39.10 K potassium	20 40.08 Ca calcium	21 44.96 Sc scandium	22 47.87 Ti titanium	23 50.94 V vanadium	24 52.00 Cr chromium	25 54.94 Mn manganese	26 55.85 Fe iron	27 58.93 Co cobalt	28 58.69 Ni nickel	29 63.55 Cu copper	30 65.38* Zn zinc	31 69.72 Ga gallium	32 72.63 Ge germanium	33 74.92 As arsenic	34 78.97* Se selenium	35 79.90* Br bromine	36 83.80 Kr krypton
37 85.47 Rb rubidium	38 87.62 Sr strontium	39 88.91 Y yttrium	40 91.22 Zr zirconium	41 92.91 Nb niobium	42 95.95* Mo molybdenum	43 [98] Tc technetium	44 101.1 Ru ruthenium	45 102.9 Rh rhodium	46 106.4 Pd palladium	47 107.9 Ag silver	48 112.4 Cd cadmium	49 114.8 In indium	50 118.7 Sn tin	51 121.8 Sb antimony	52 127.6 Te tellurium	53 126.9 I iodine	54 131.3 Xe xenon
55 132.9 Cs caesium	56 137.3 Ba barium	72 178.5 Hf hafnium	73 180.9 Ta tantalum	74 183.8 W tungsten	75 186.2 Re rhenium	76 190.2 Os osmium	77 192.2 Ir iridium	78 195.1 Pt platinum	79 197.0 Au gold	80 200.6 Hg mercury	81 204.4* Tl thallium	82 207.2 Pb lead	83 209.0 Bi bismuth	84 [209] Po polonium	85 [210] At astatine	86 [222] Rn radon	
87 [223] Fr francium	88 [226] Ra radium	104 [267] Rf rutherfordium	105 [268] Db dubnium	106 [269] Sg seaborgium	107 [270] Bh bohrium	108 [277] Hs hassium	109 [278] Mt meitnerium	110 [281] Ds darmstadtium	111 [282] Rg roentgenium	112 [285] Cn copernicium	113 [286] Nh nihonium	114 [289] Fl flerovium	115 [290] Mc moscovium	116 [293] Lv livermorium	117 [294] Ts tennessine	118 [294] Og oganesson	

57 138.9 La lanthanum	58 140.1 Ce cerium	59 140.9 Pr praseodymium	60 144.2 Nd neodymium	61 [145] Pm promethium	62 150.4 Sm samarium	63 152.0 Eu europium	64 157.3 Gd gadolinium	65 158.9 Tb terbium	66 162.5 Dy dysprosium	67 164.9 Ho holmium	68 167.3 Er erbium	69 168.9 Tm thulium	70 173.0 Yb ytterbium	71 175.0 Lu lutetium
89 [227] Ac actinium	90 232.0 Th thorium	91 231.0 Pa protactinium	92 238.0 U uranium	93 [237] Np neptunium	94 [244] Pu plutonium	95 [243] Am americium	96 [247] Cm curium	97 [247] Bk berkelium	98 [251] Cf californium	99 [252] Es einsteinium	100 [257] Fm fermium	101 [258] Md mendelevium	102 [259] No nobelium	103 [266] Lr lawrencium

FLASH allows element and site spefific electronic probing





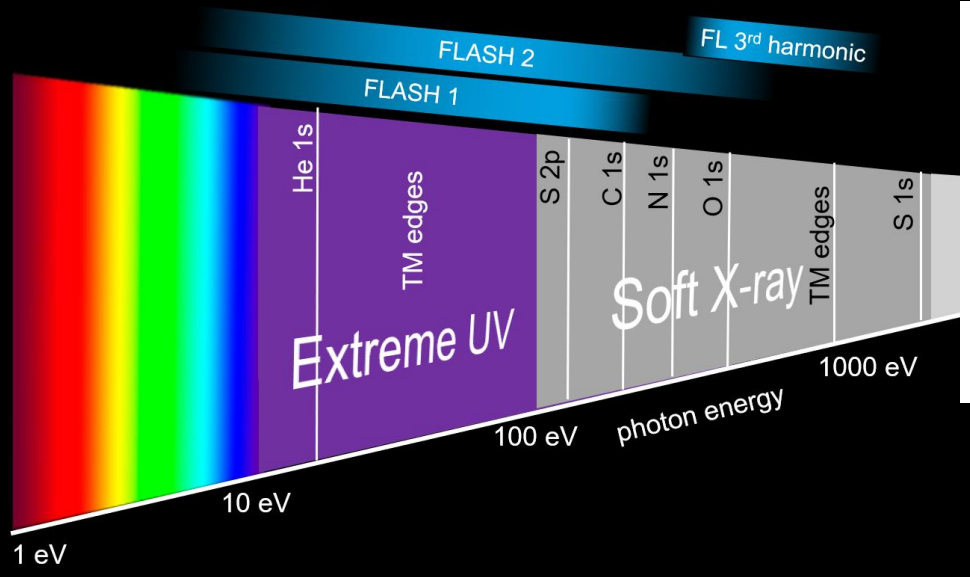


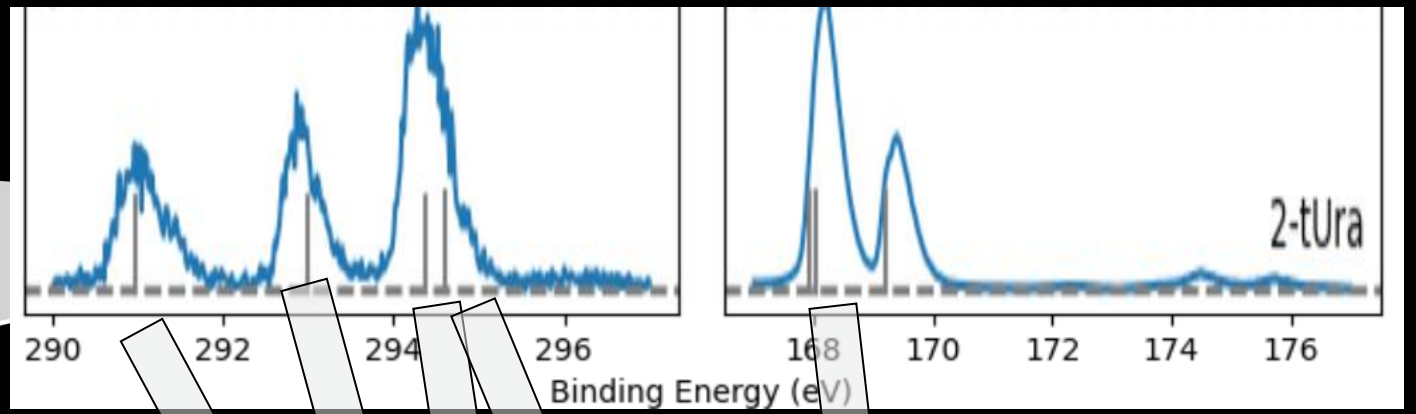
Probe here via core ionization

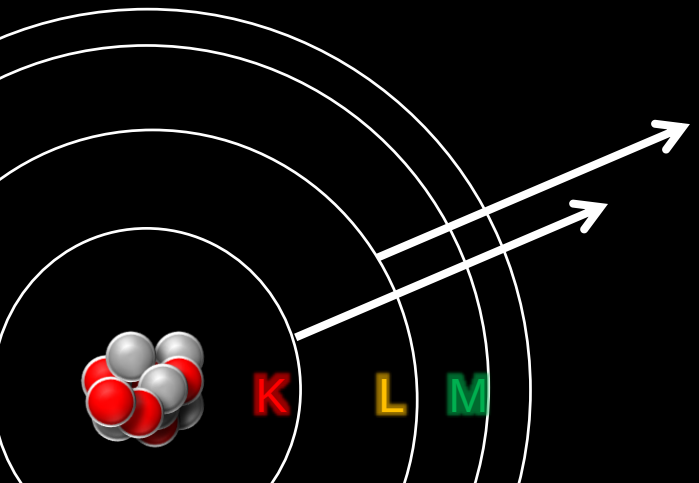
Resonance into valence states

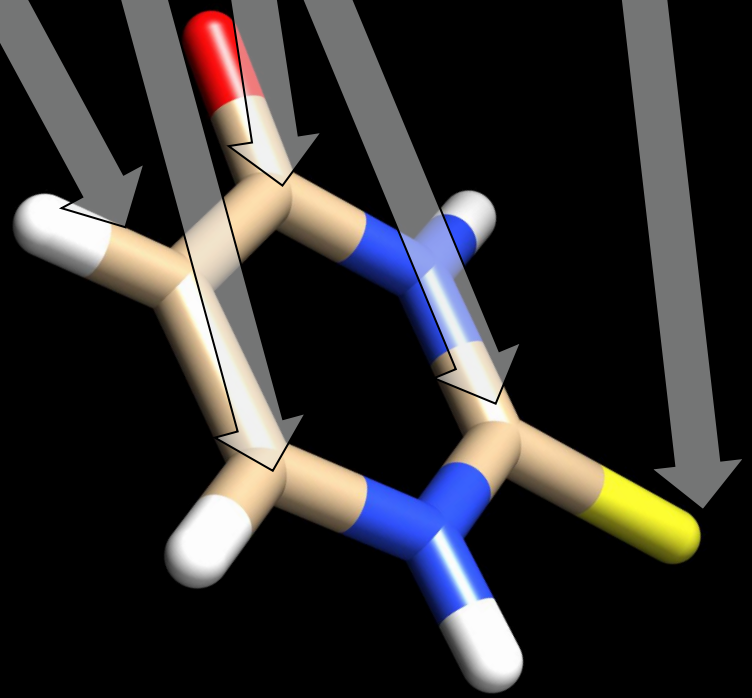
Photoelectron spectroscopy

FLASH allows element and site spefific electronic probing

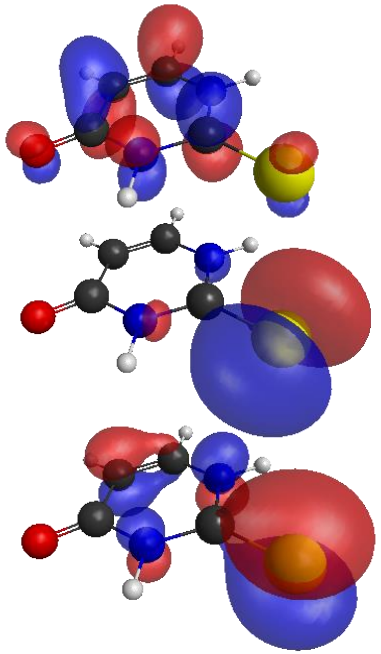




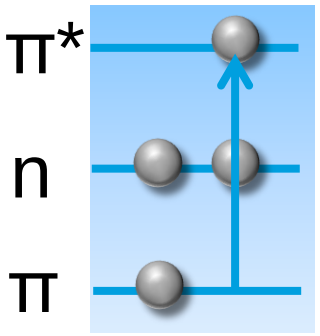


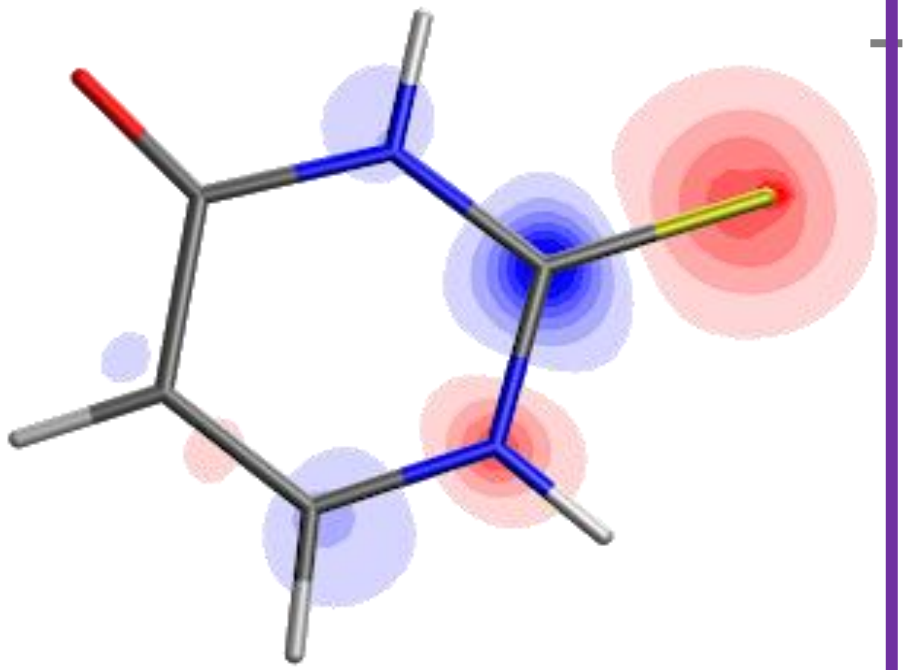


FLASH makes electronic molecular movies

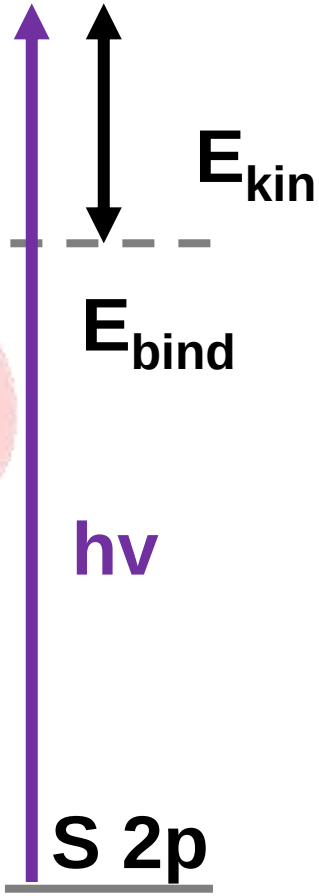


$^1\pi\pi^*(S_2)$





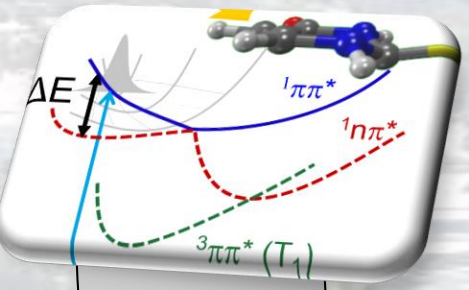
Charge difference plot



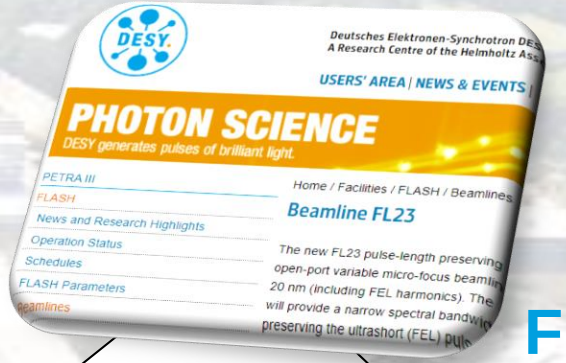
Ground state

$^1\pi\pi^*(S_2)$

Outline

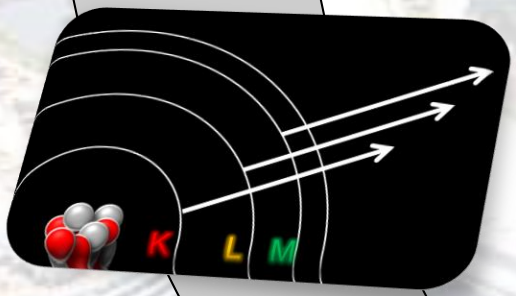


Molecular Photoenergy Conversion



FLASH Beamtime

X-ray Probing



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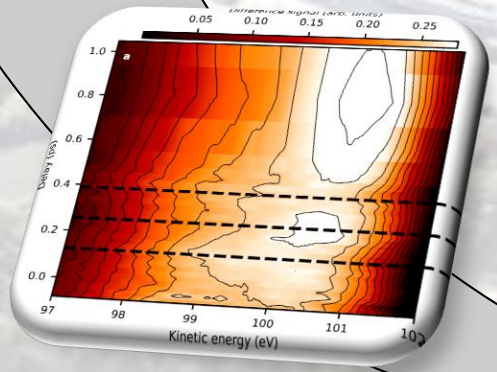
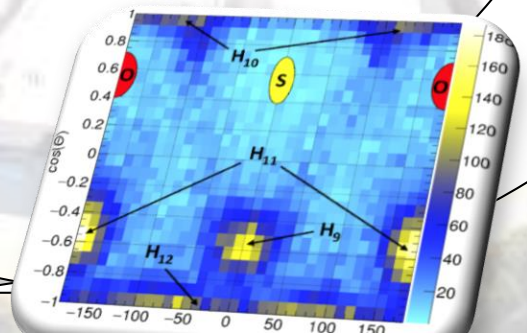
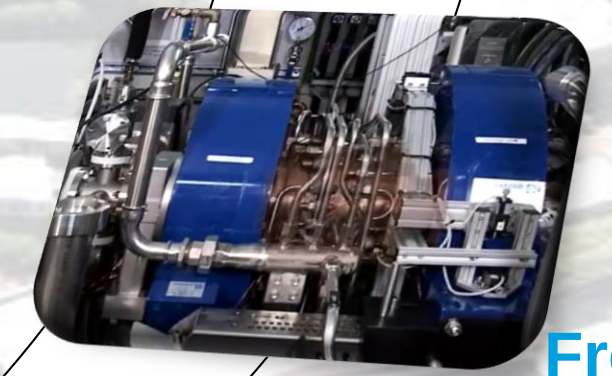


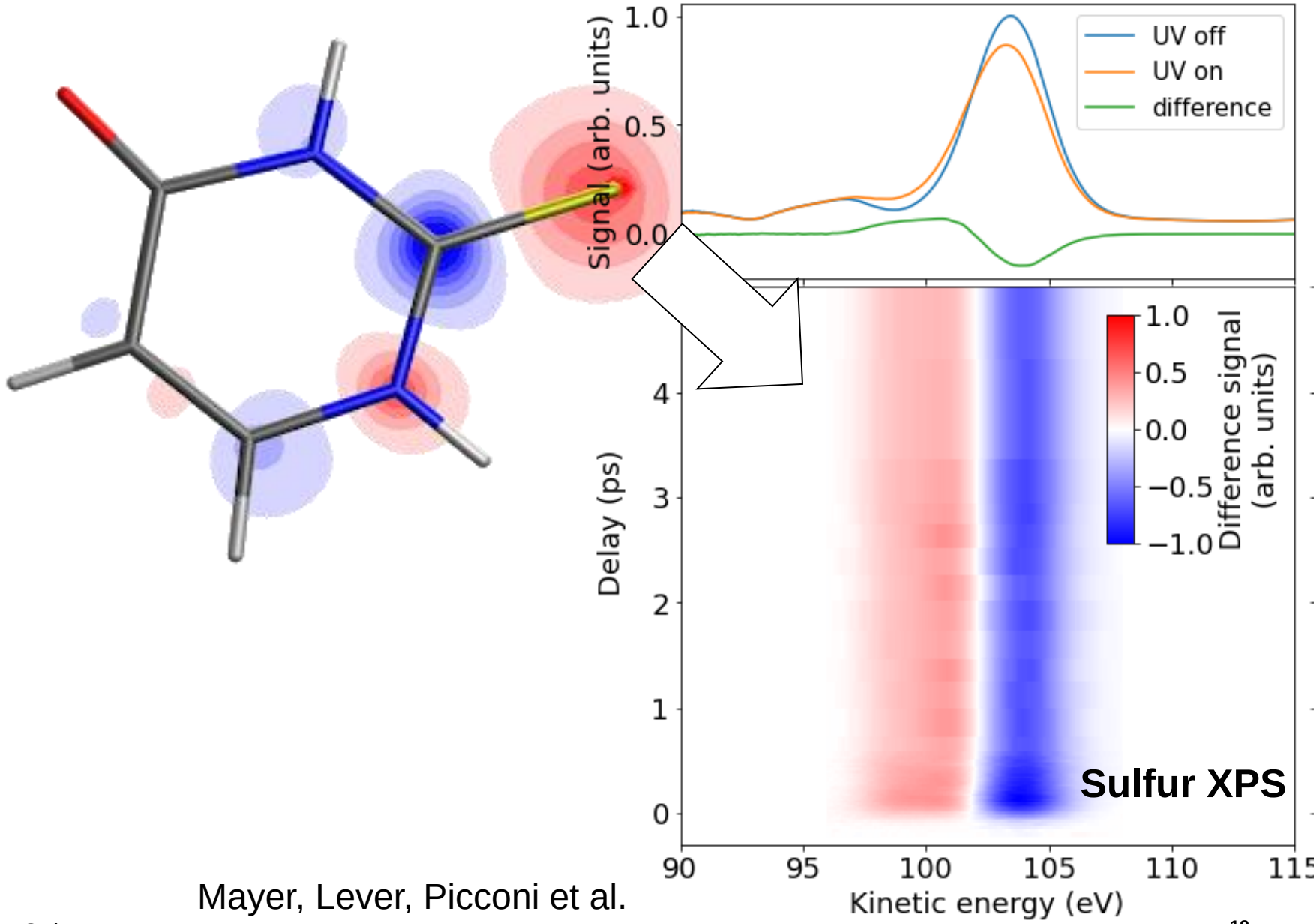
Geometry Movie





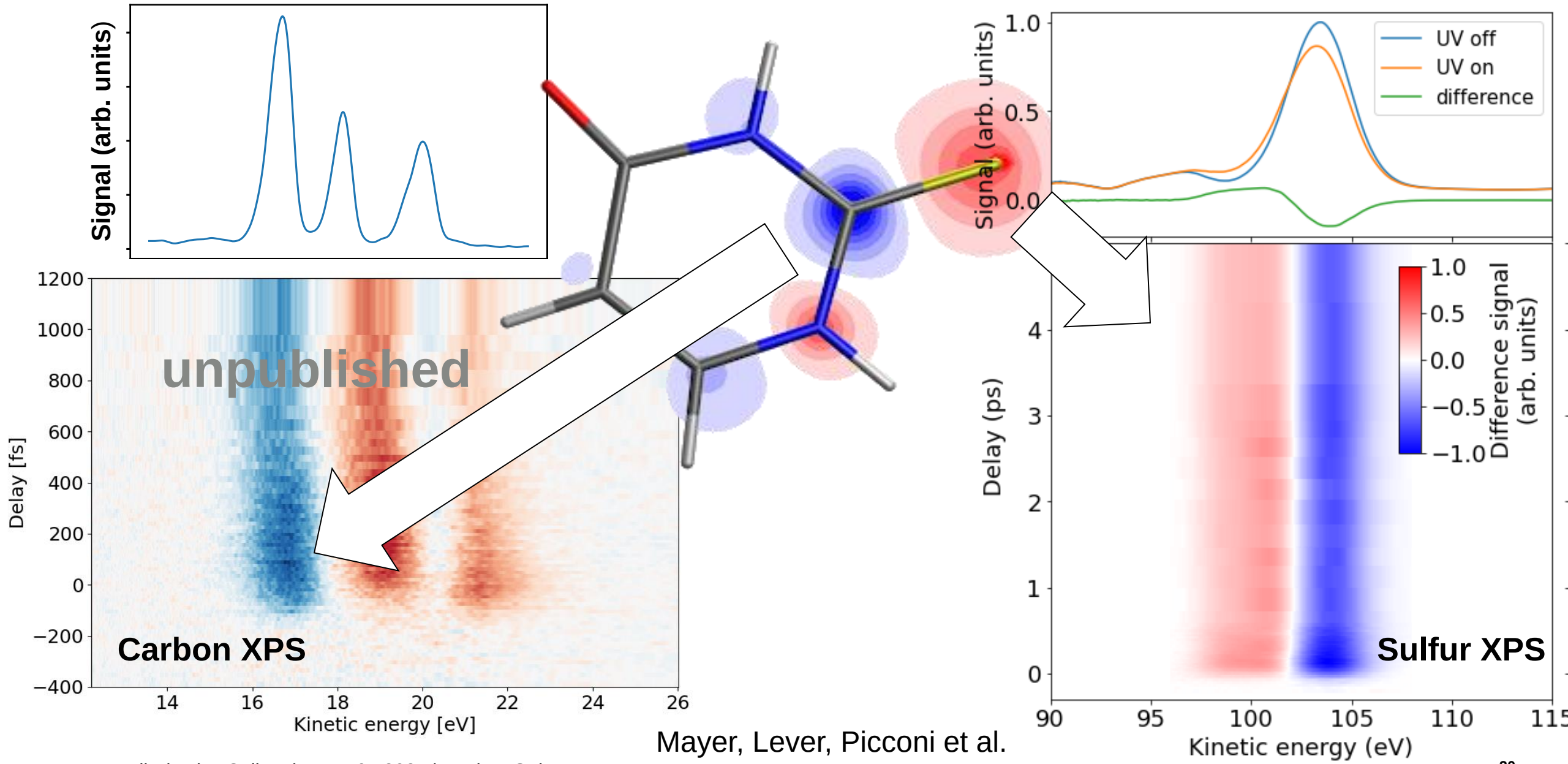
Free-electron laser physics

FLASH makes electronic molecular movies



Mayer, Lever, Picconi et al.
Nature Comm. **13**, 198 (2022)

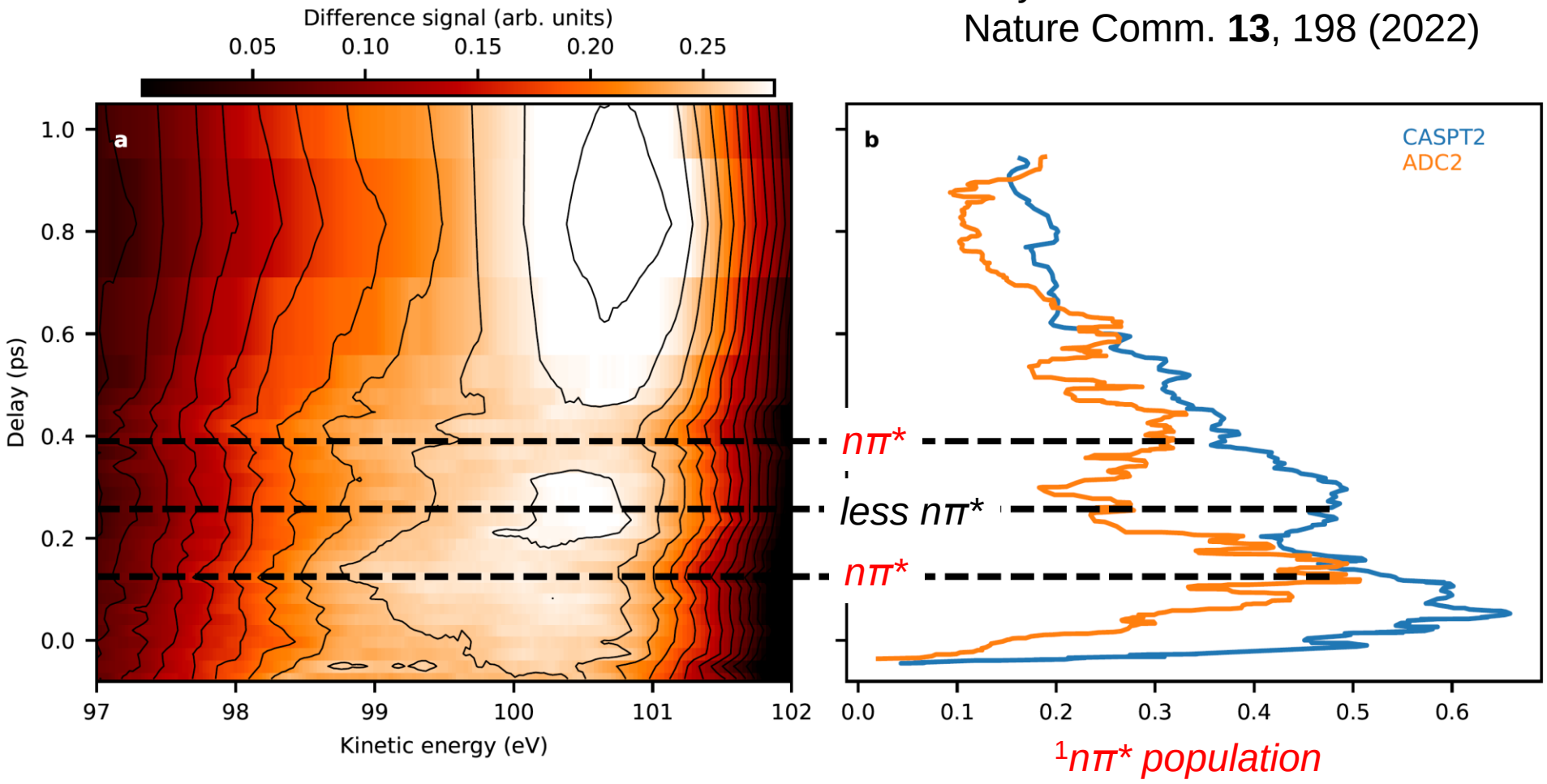
FLASH makes electronic molecular movies



Mayer, Lever, Picconi et al.
Nature Comm. **13**, 198 (2022)

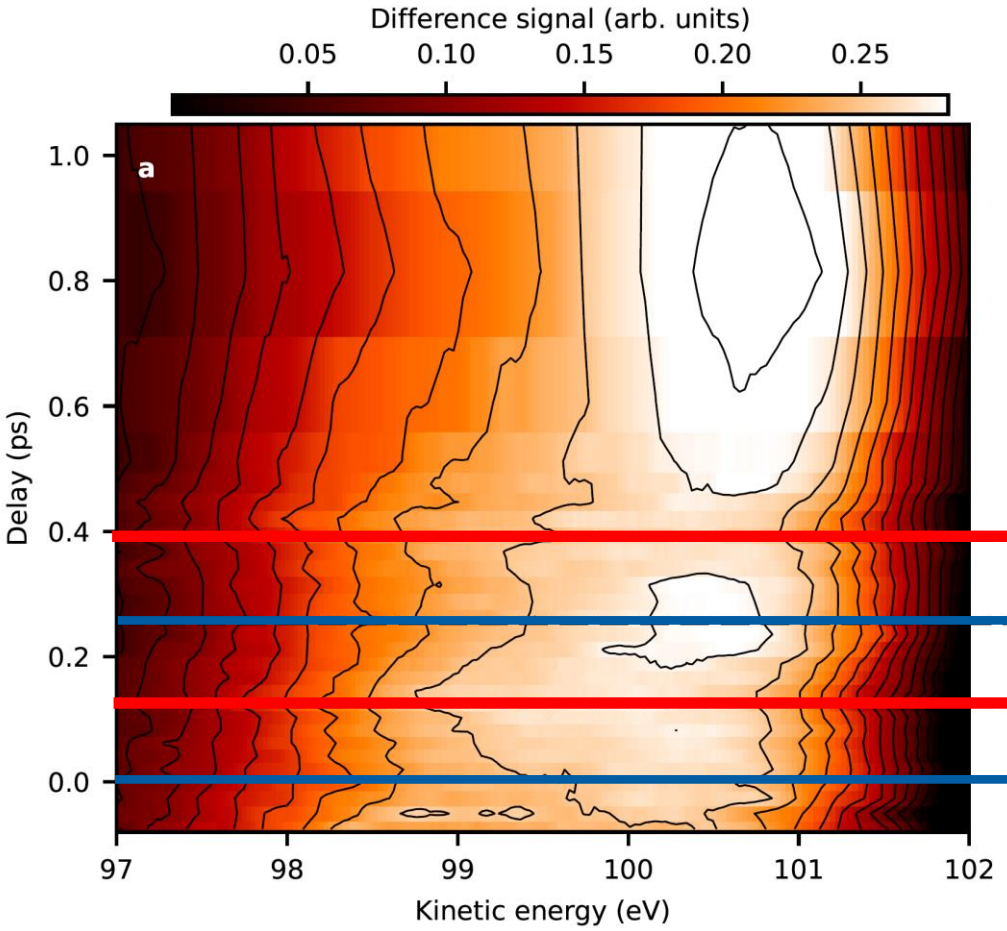
Oscillations exhibit coherent molecular dynamics

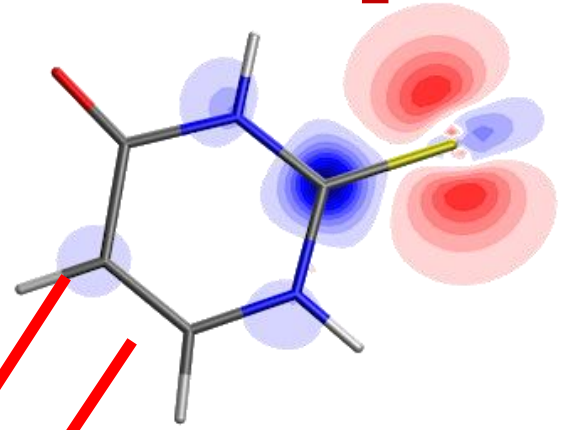
Mayer, Lever, Picconi et al.
Nature Comm. **13**, 198 (2022)

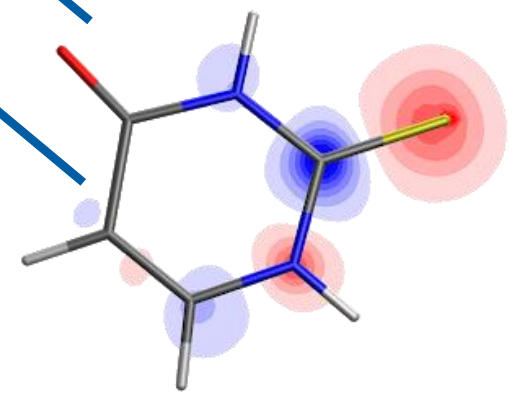


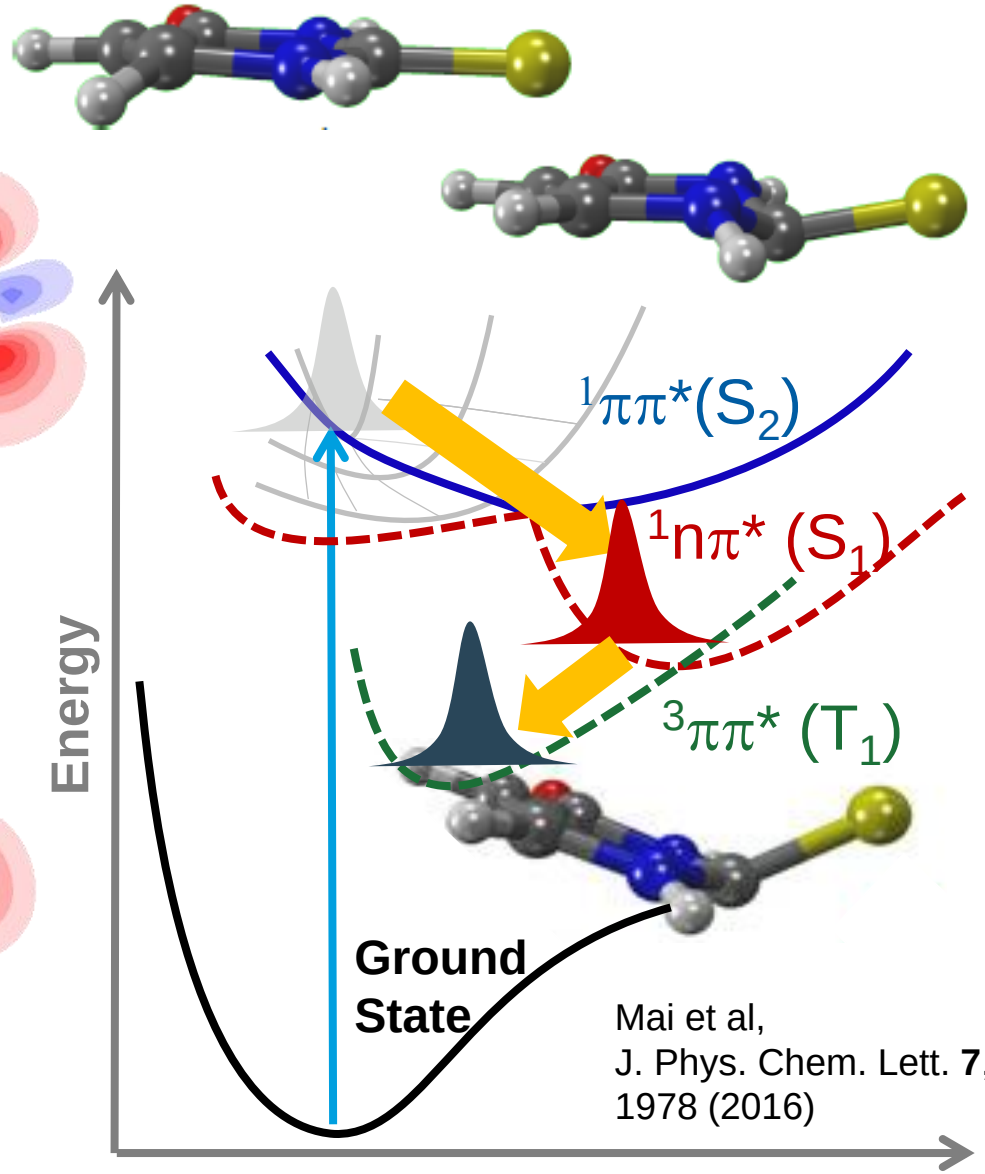
Simulations:
Mai, Marquetand, González, J. Phys. Chem. Lett. **7**, 1978–1983 (2016)
Mai *et al.* J. Chem. Phys. **147**, 184109 (2017)

Coupling of electrons and nuclei determines photochemistry









Mayer, Lever, Picconi et al.
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Mai et al,
J. Phys. Chem. Lett. **7**, 1978 (2016)

DESY
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Huseyin Cankaya
Marion Kuhlmann
Giovanni Cirmi
Sebastian Schulz
Ulrike Frühling
Atia Tul Noor
Francesca Calegari
Andrea Trabattoni
Ingmar Hartl
Agata Azzolin
Atia Tul Noor
Steffen Paluttke
Fabiano Lever
Dennis Mayer
Markus Gühr
Gesa Goetzke

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Peter Saalfrank
Christopher Ehlert (Heidelberg)
Evegenii Titov

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Mans Wallner

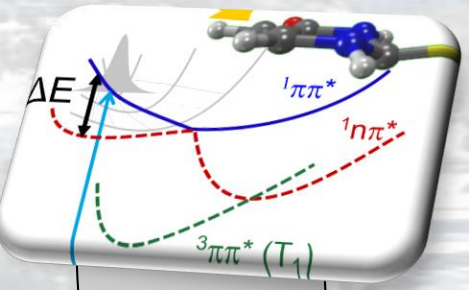
UCL:
Rebecca Ingle

SOLEIL:
John Bozek
Christophe Nicolas

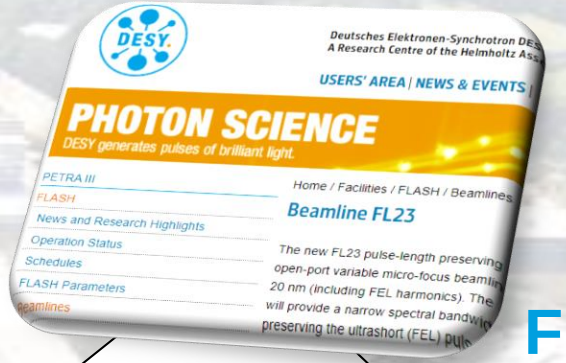


Dennis Mayer, Fabiano Lever, David Picconi et al.
Nature Comm. **13**, 198 (2022)

Outline



Molecular Photoenergy Conversion



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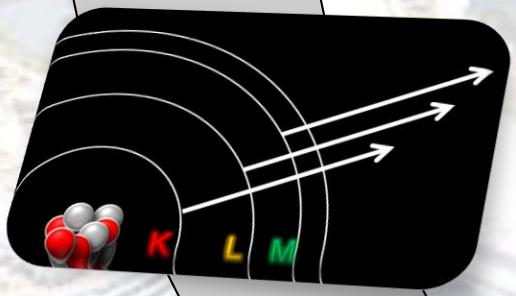

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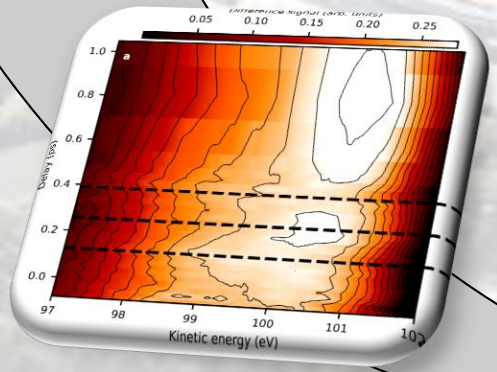

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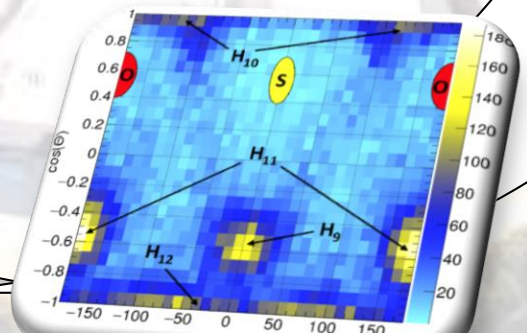
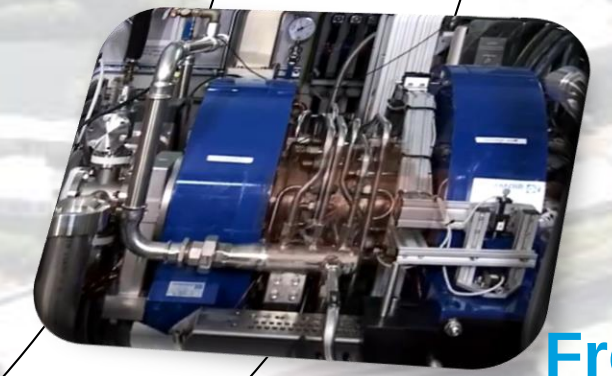
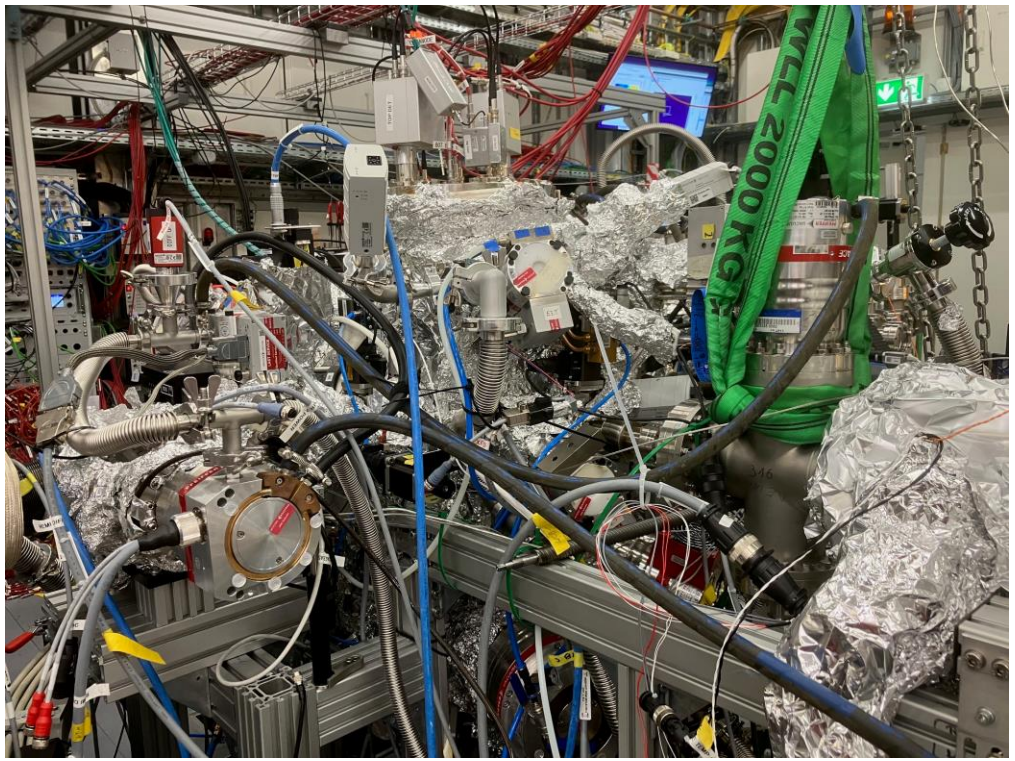


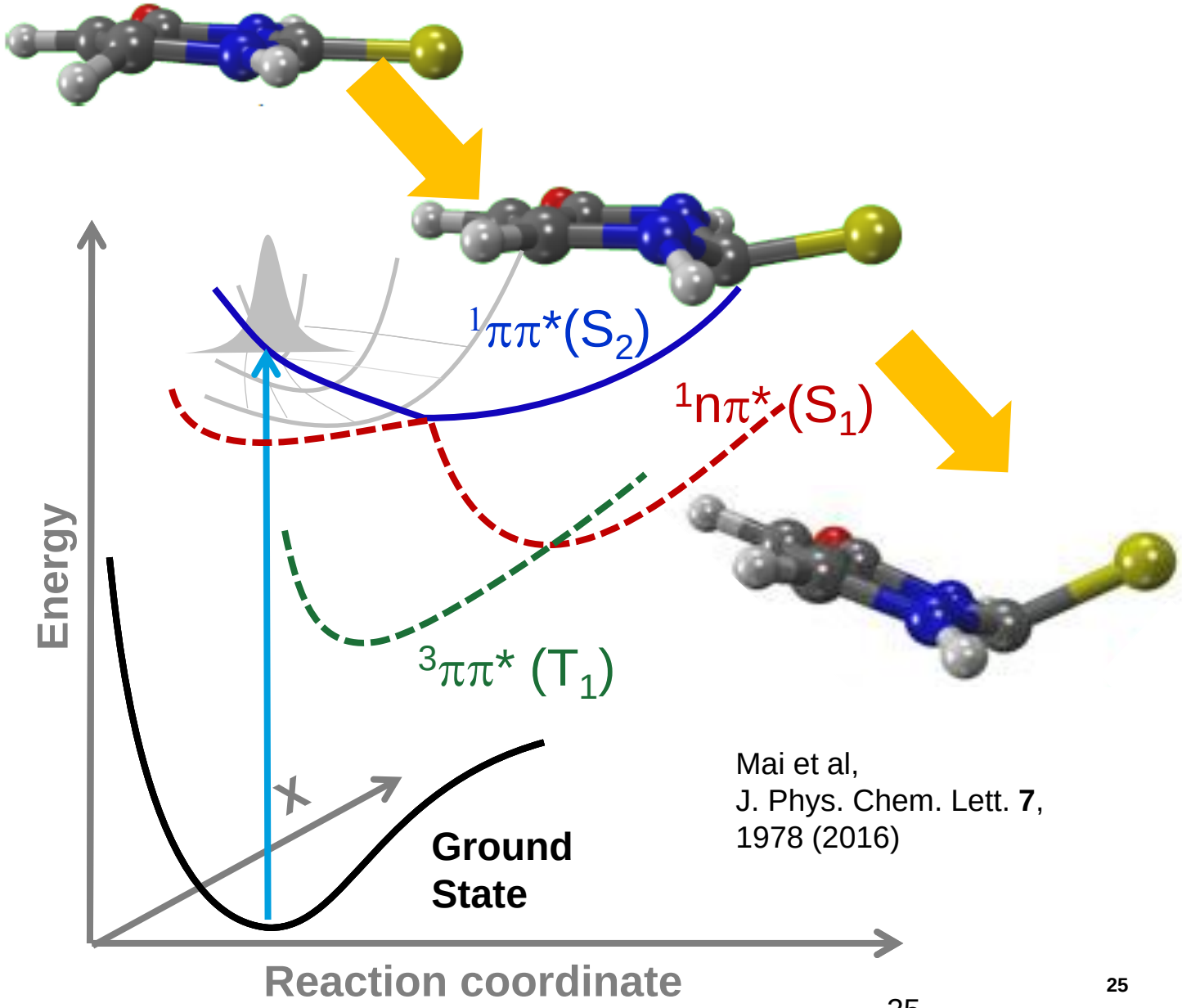


Free-electron laser physics

Looking at the same dynamics via nuclear geometry



R. Boll, ….T. Jahnke, Nat. Phys. **18** 423 (2022)



Mai et al,
J. Phys. Chem. Lett. **7**, 1978 (2016)

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Till Jahnke
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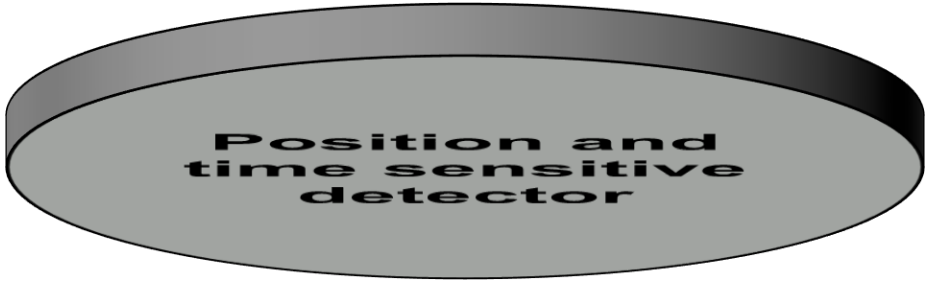
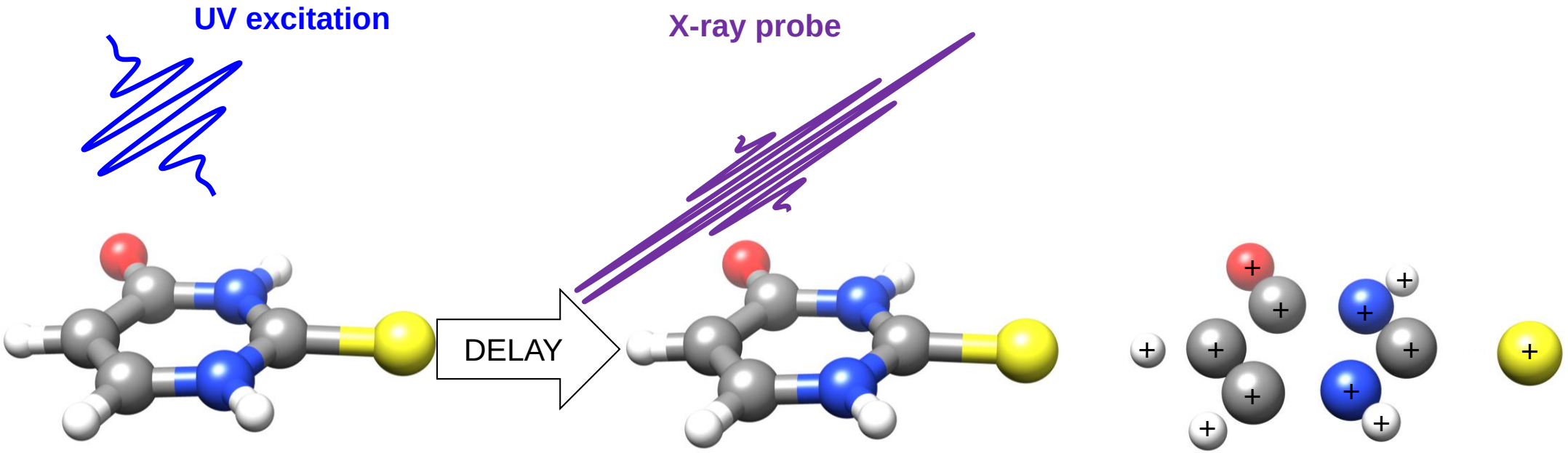
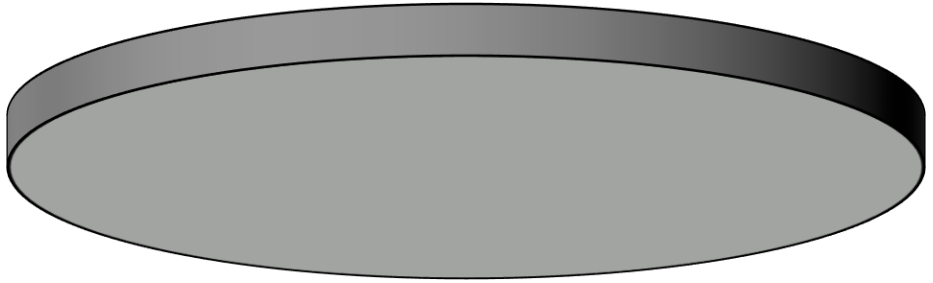
Coulomb Explosion Imaging

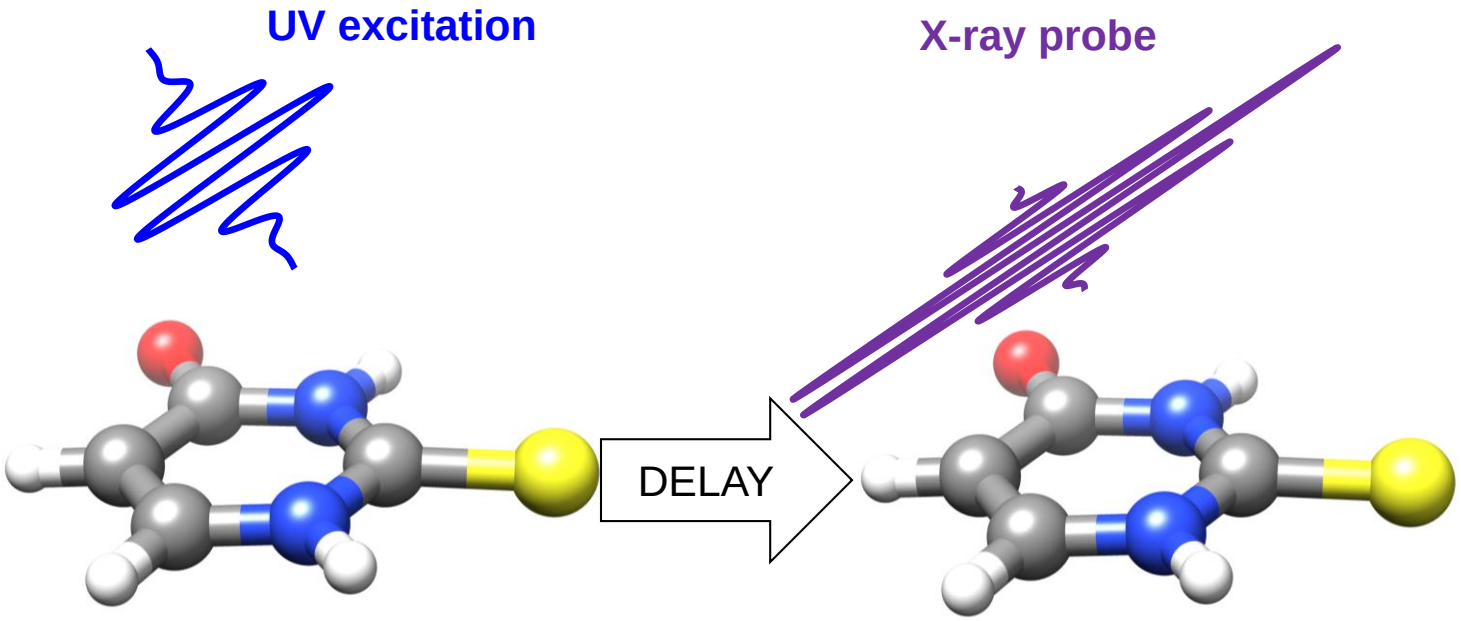




one molecule in focus

Coulomb Explosion Imaging





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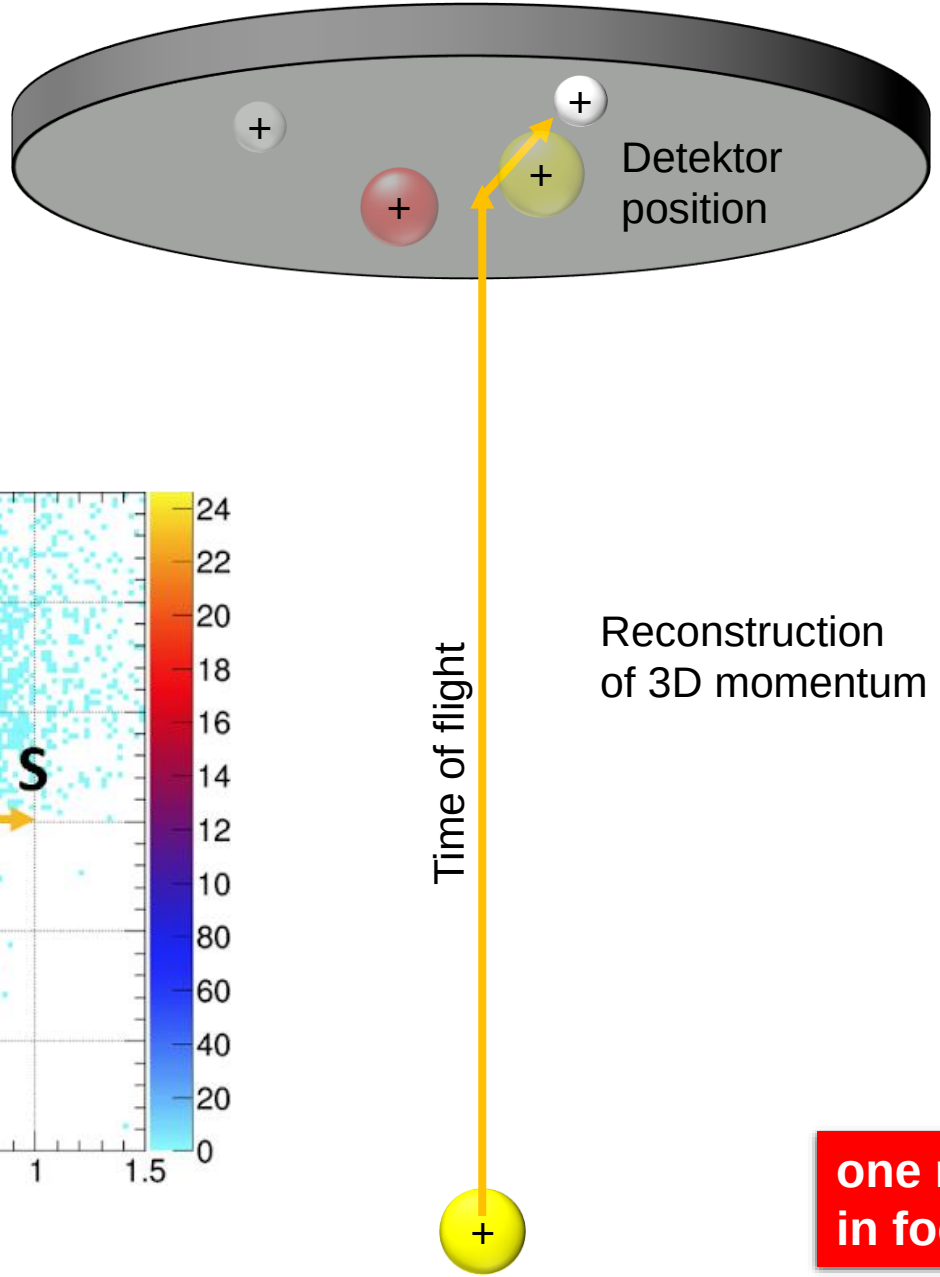
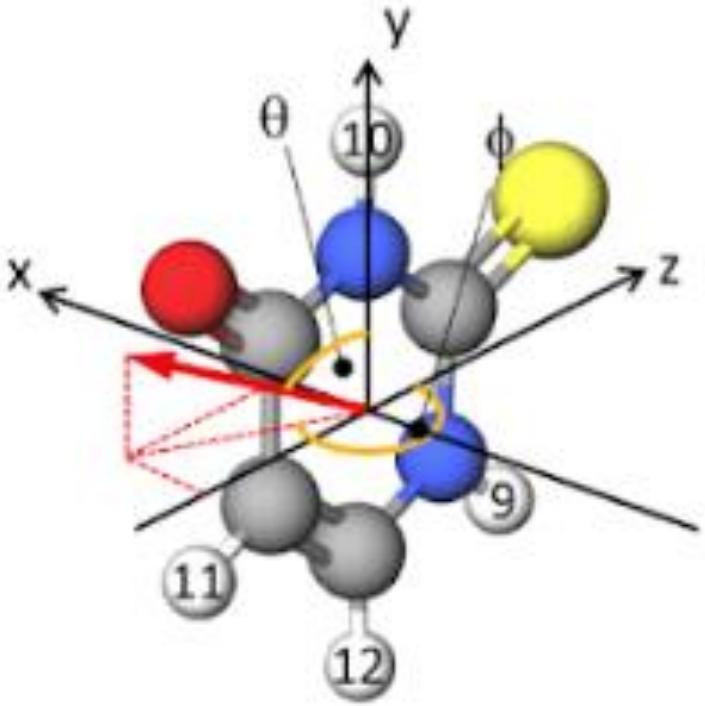
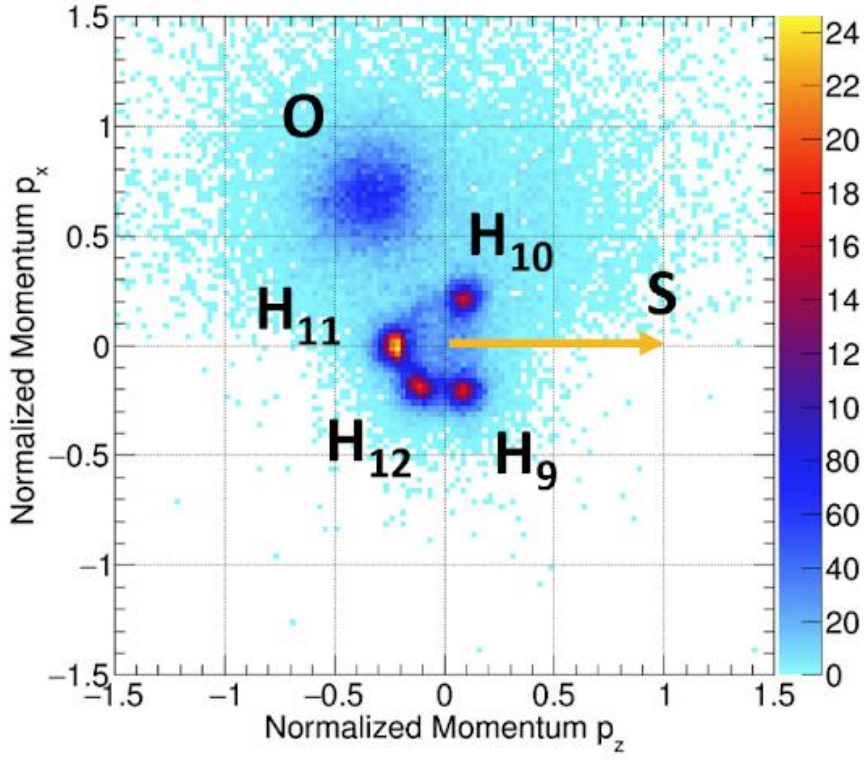


Reconstruction
of 3D momentum

Courtesy
Till Jahnke

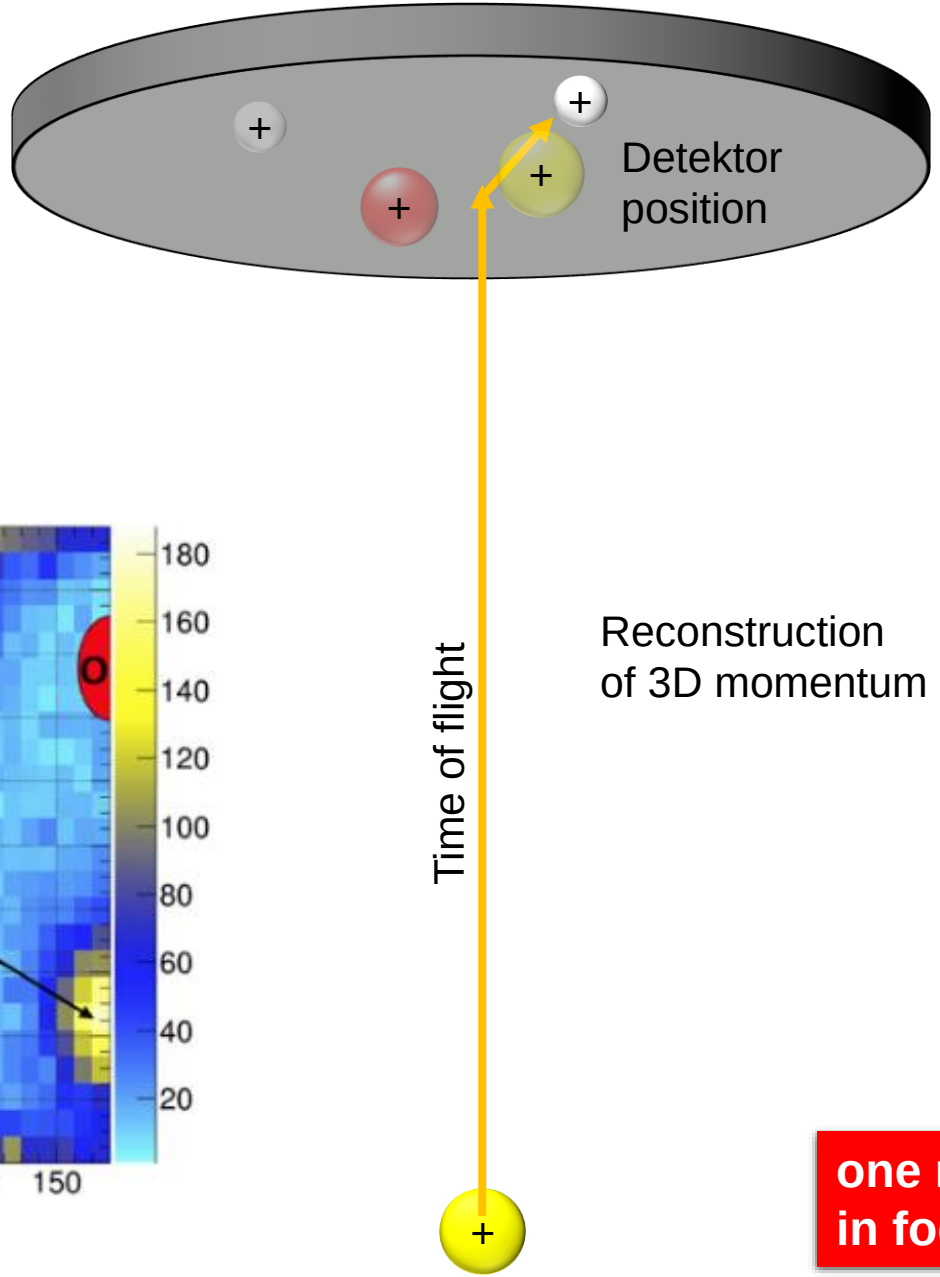




unpublished

one molecule in focus

Coulomb Explosion Imaging



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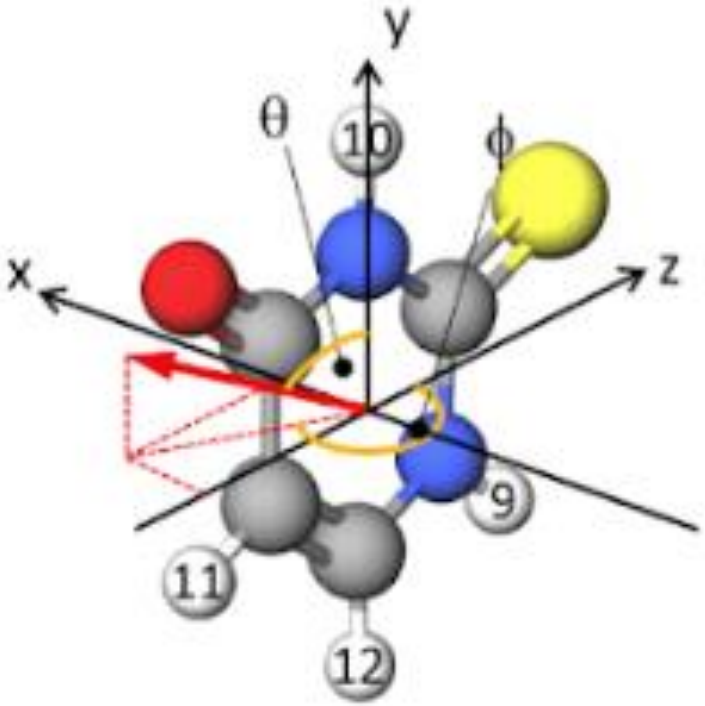
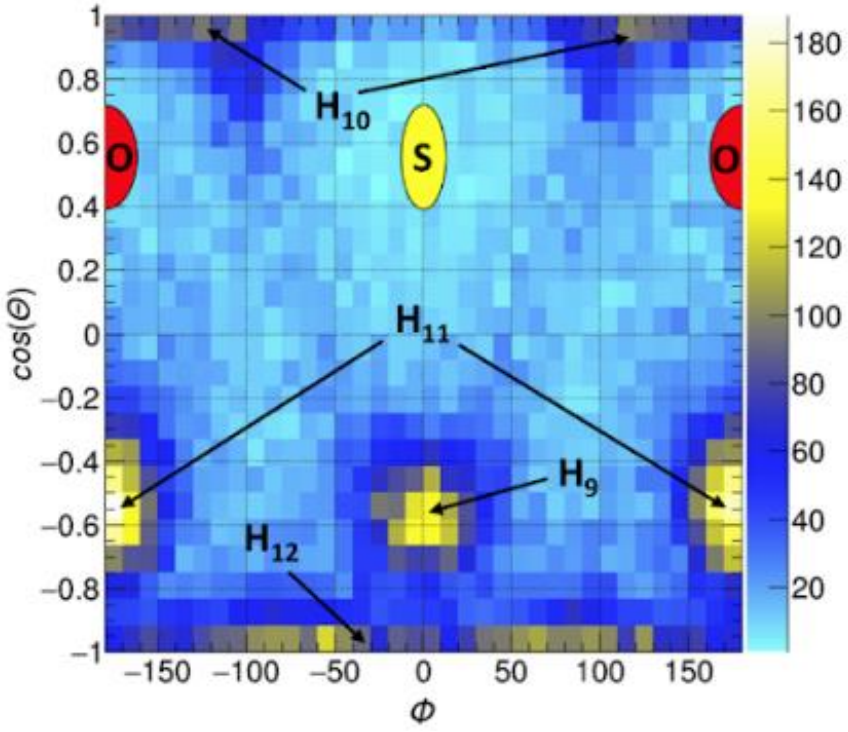


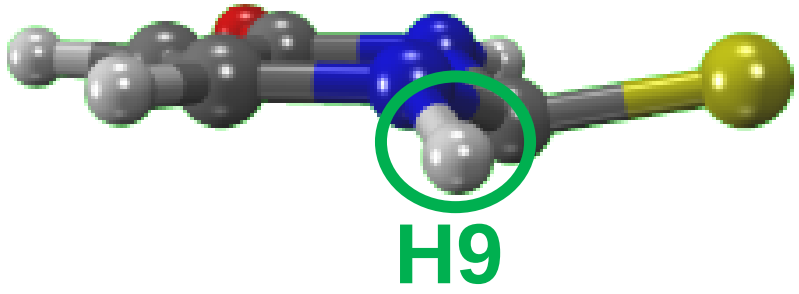


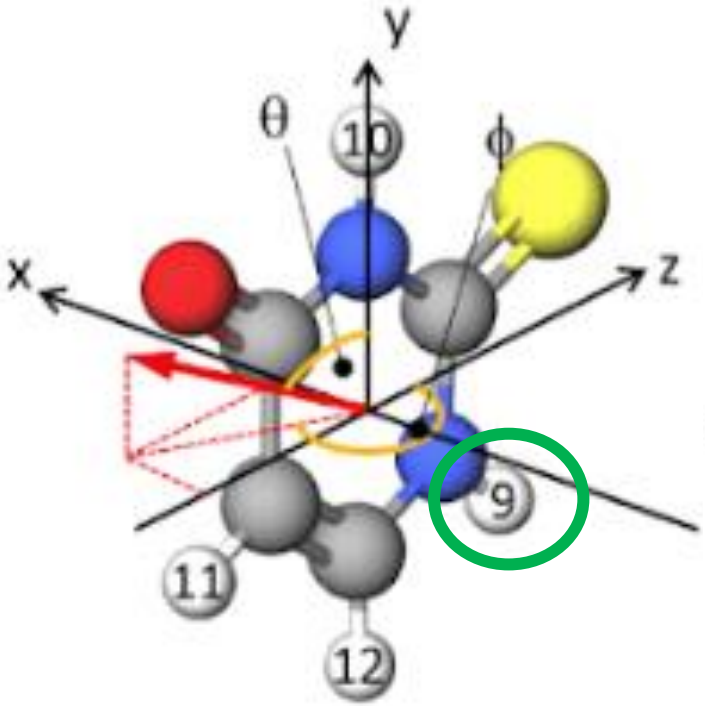
one molecule in focus

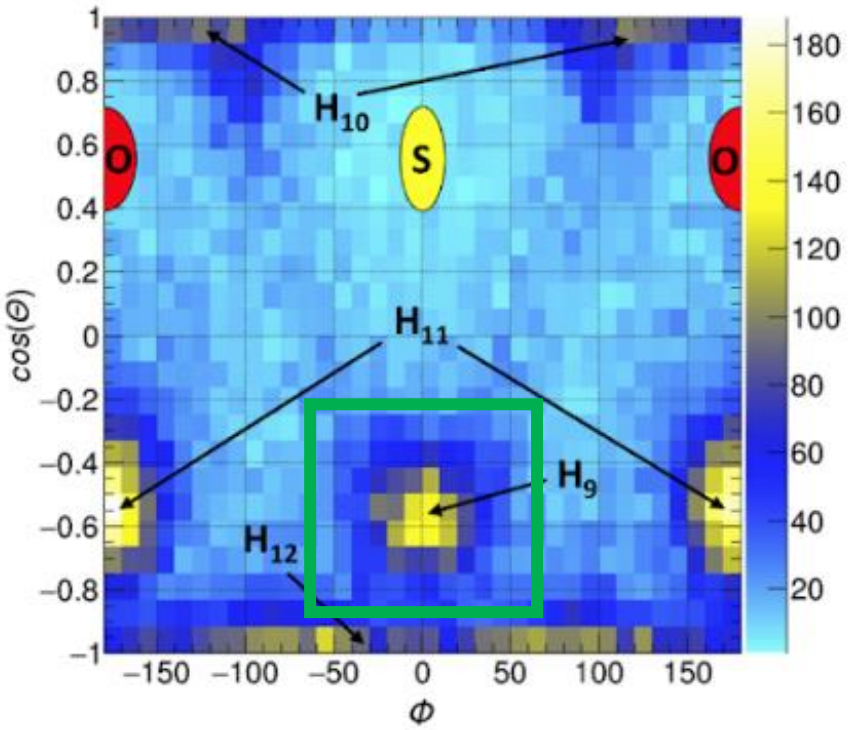
Jahnke et al. https://arxiv.org/pdf/2405.15367 (2024)

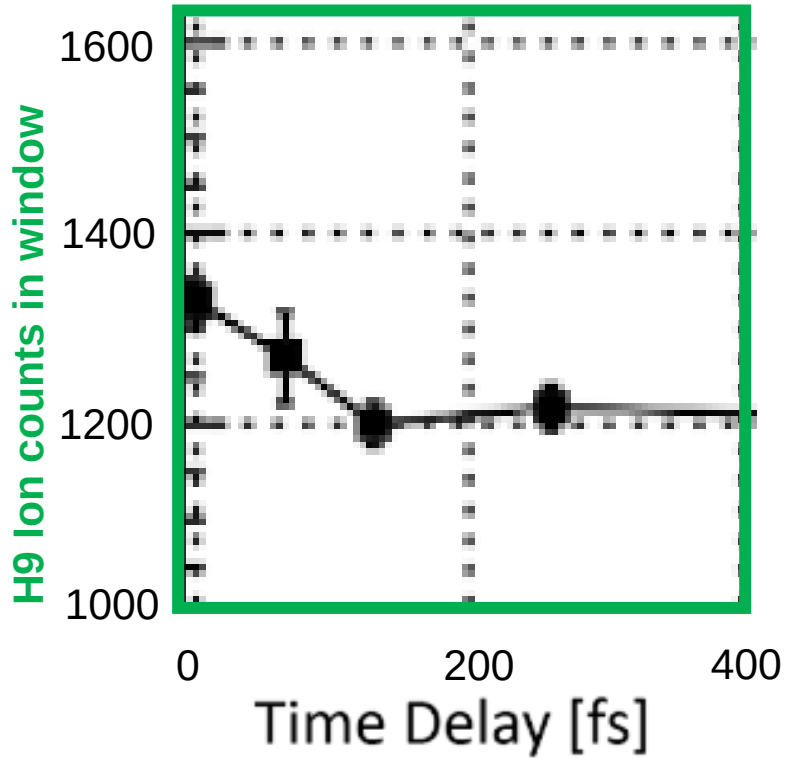
First the ring is puckering to go through the conical intersection…

Courtesy
Till Jahnke



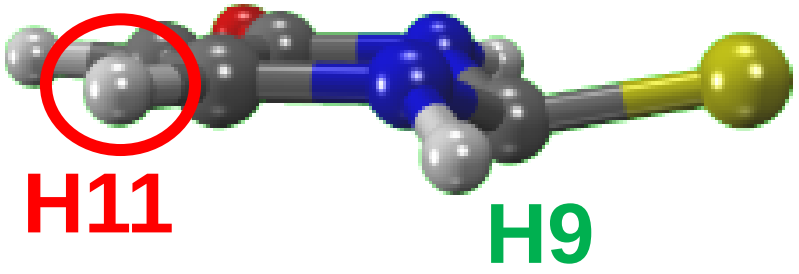


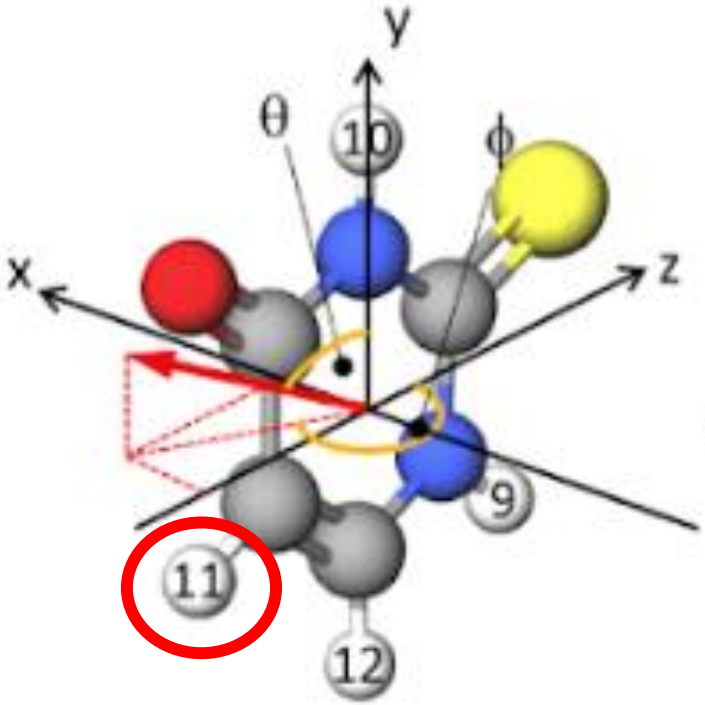


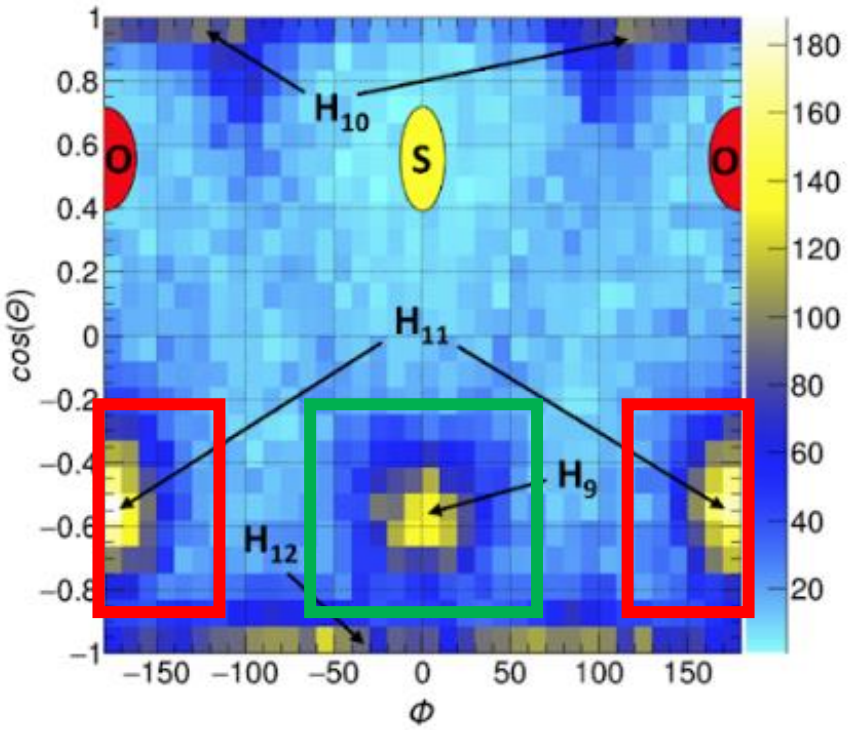


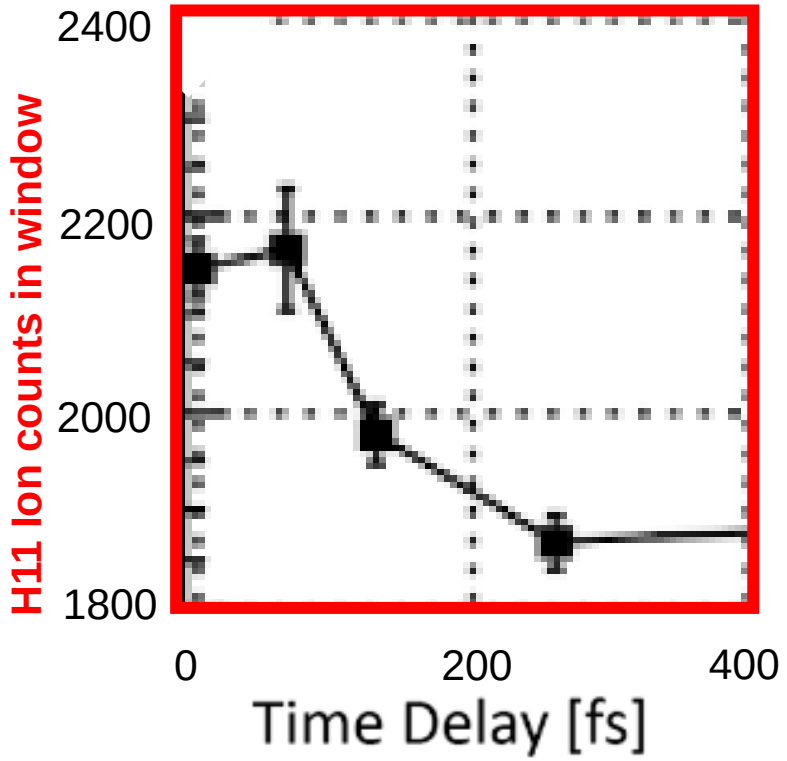
….then the sulfur points up with a delay of 60 fs

Courtesy
Till Jahnke

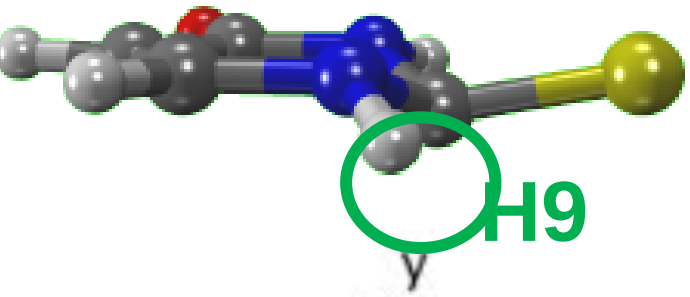


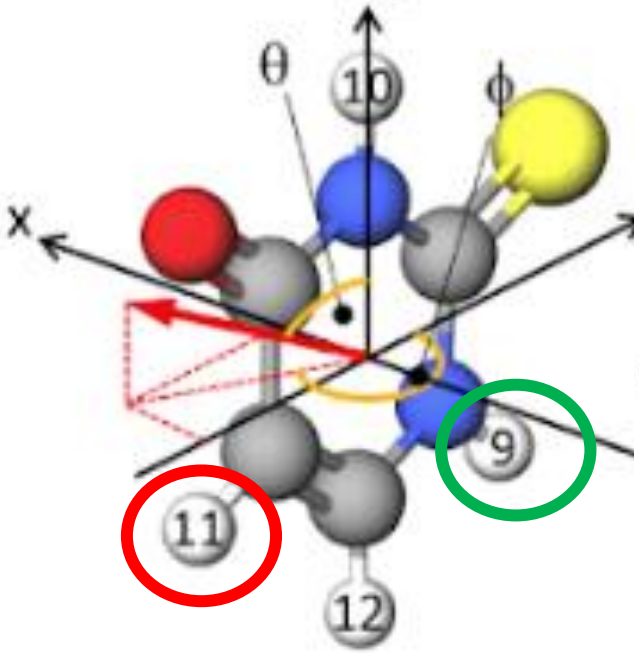


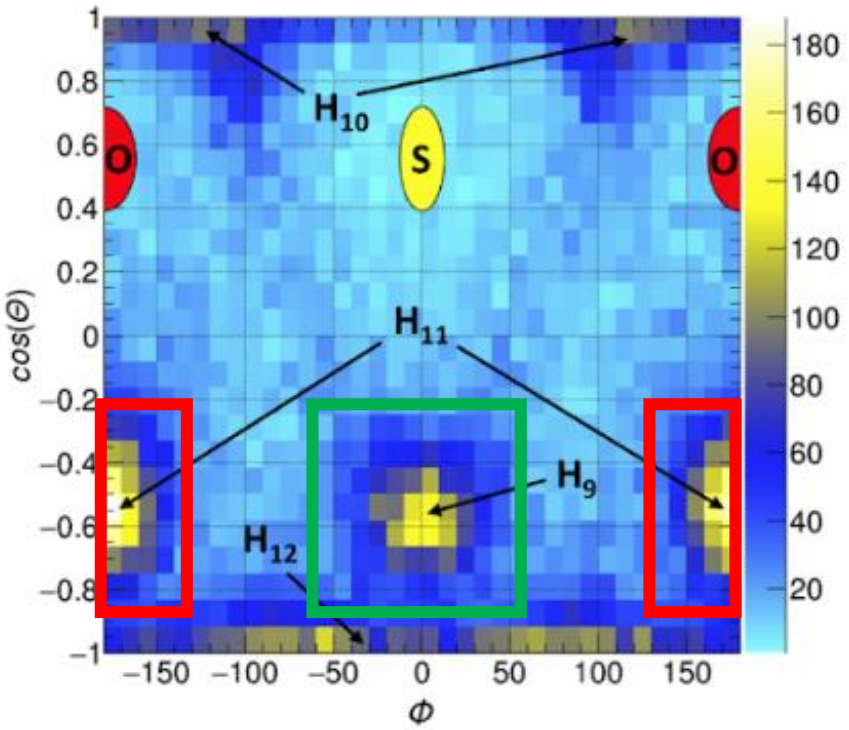


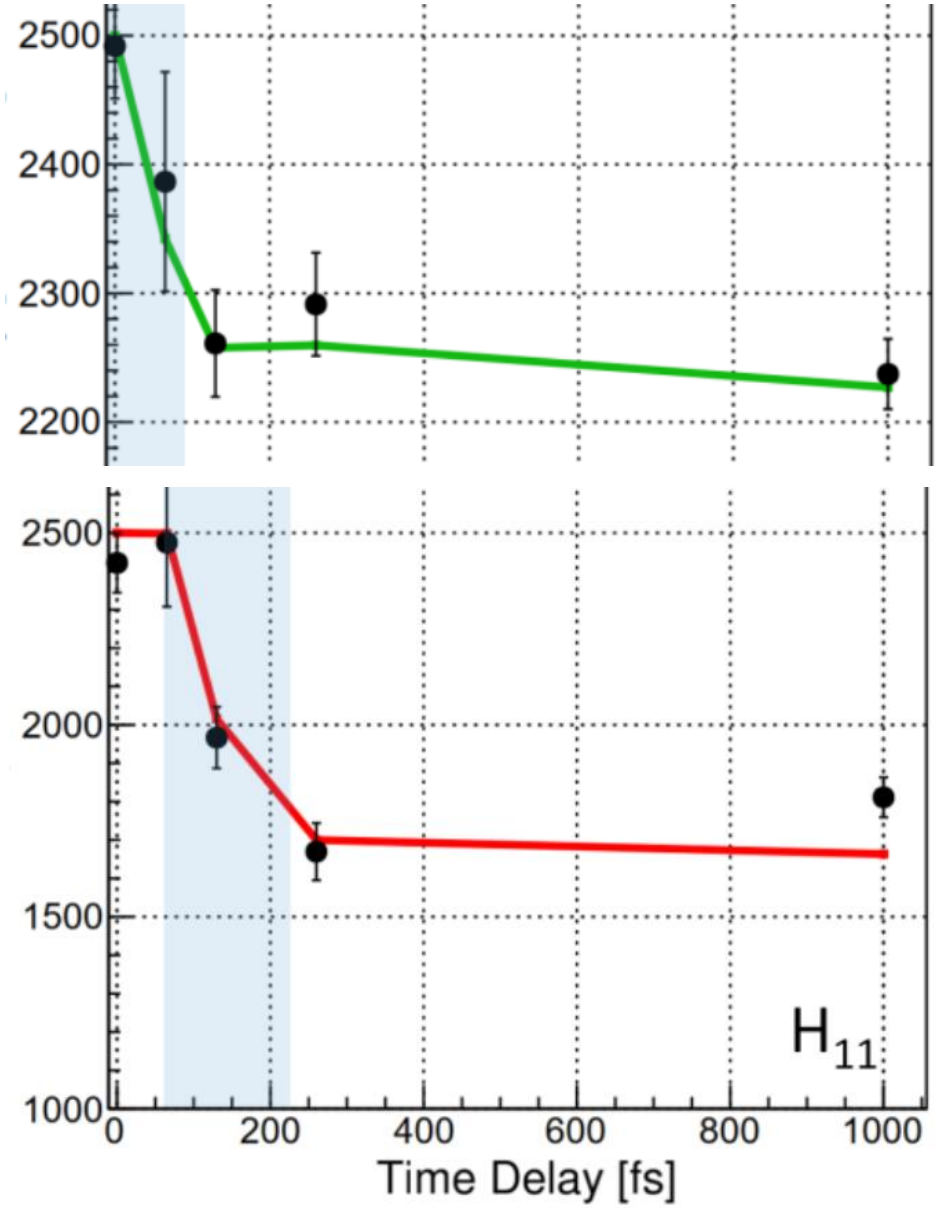


Imaging deplanariztion with CEI



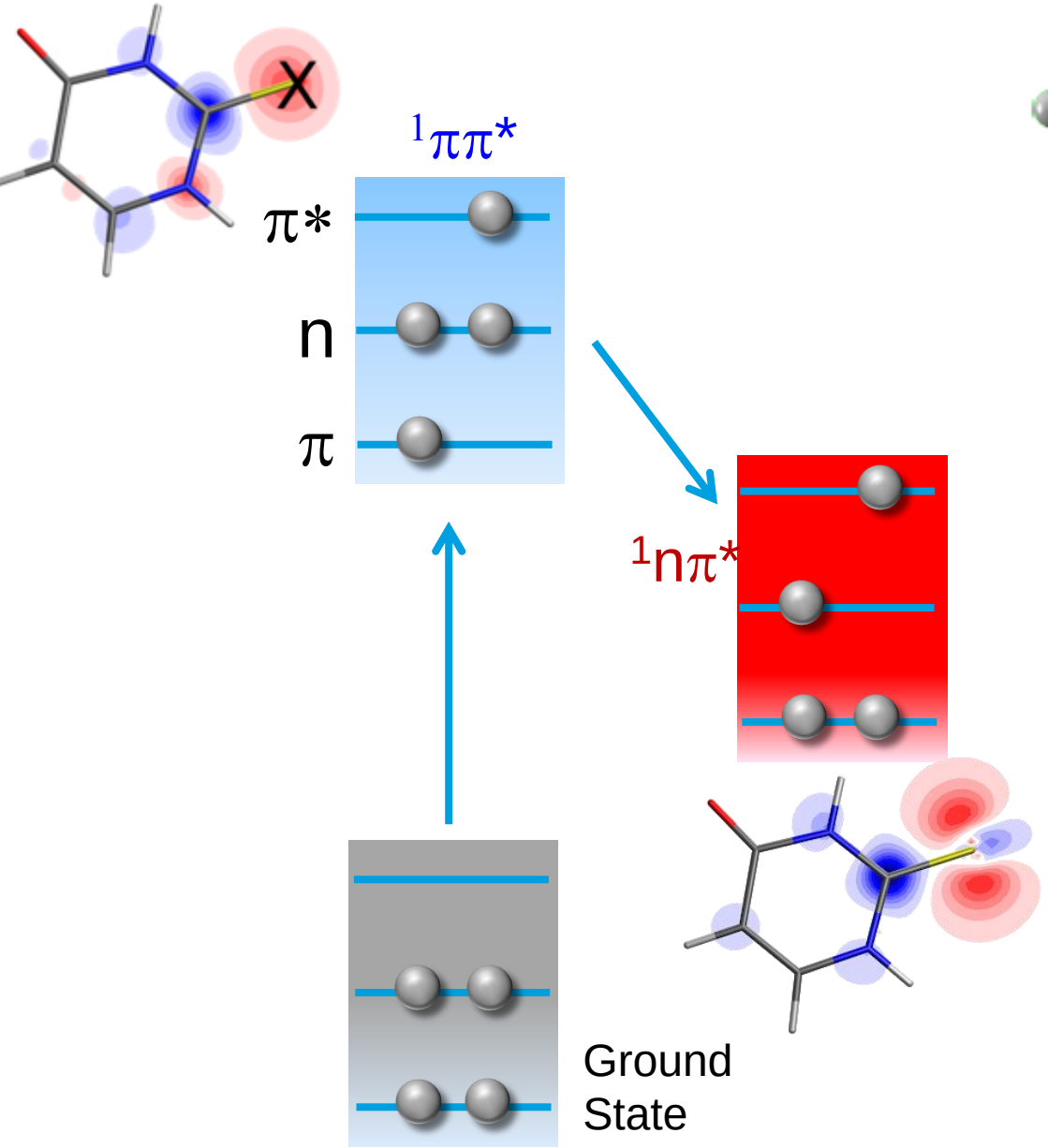


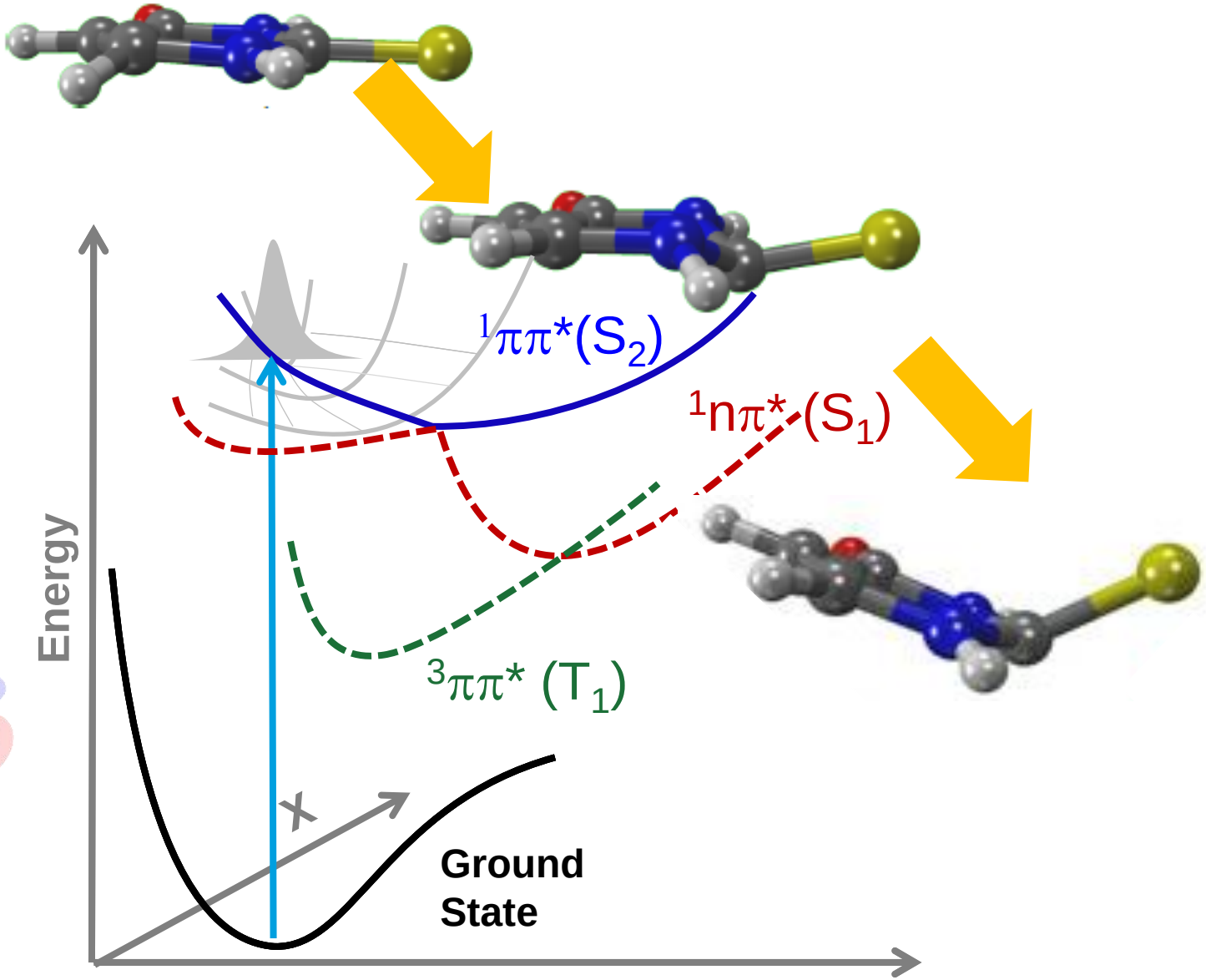




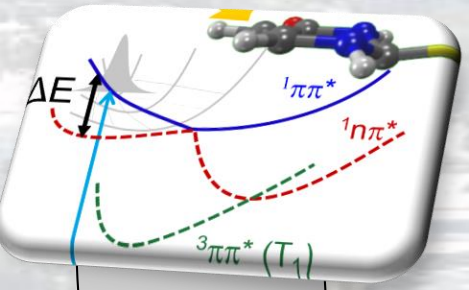
Jahnke et al. https://arxiv.org/pdf/2405.15367 (2024)

Nuclei couple to electrons and their spin

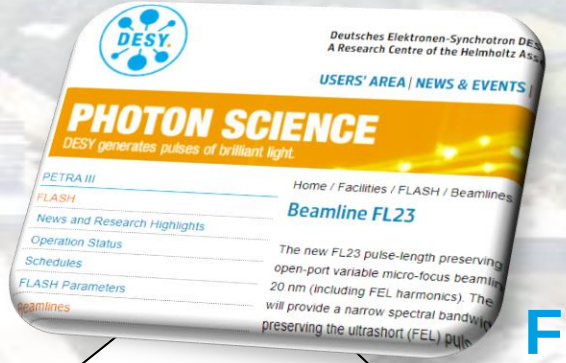




Outline

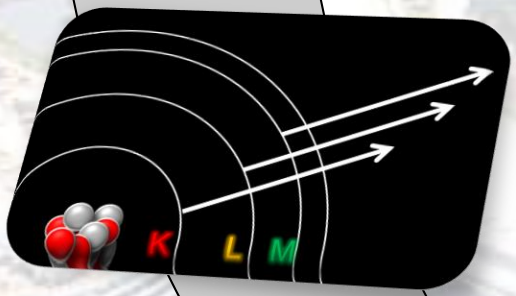


Molecular Photoenergy Conversion

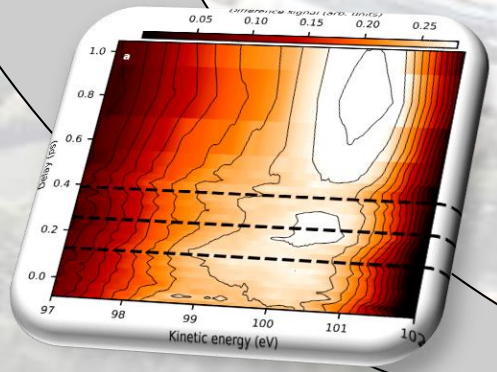


FLASH Beamtime

X-ray Probing



Electronic Movie



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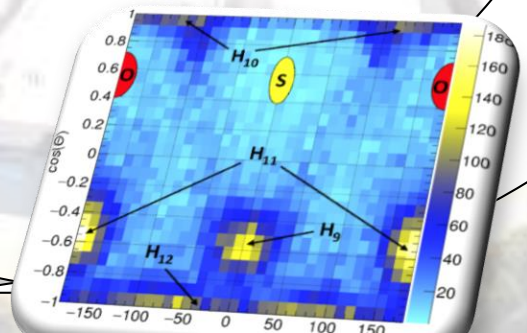
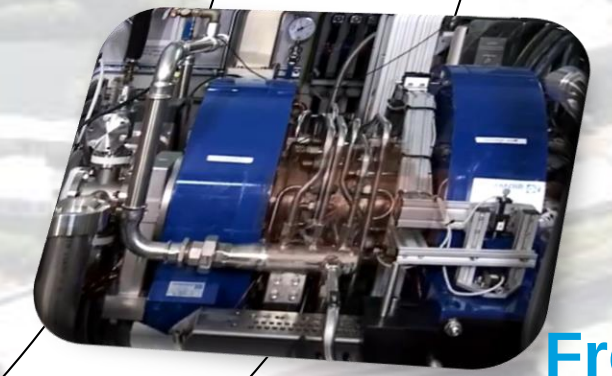
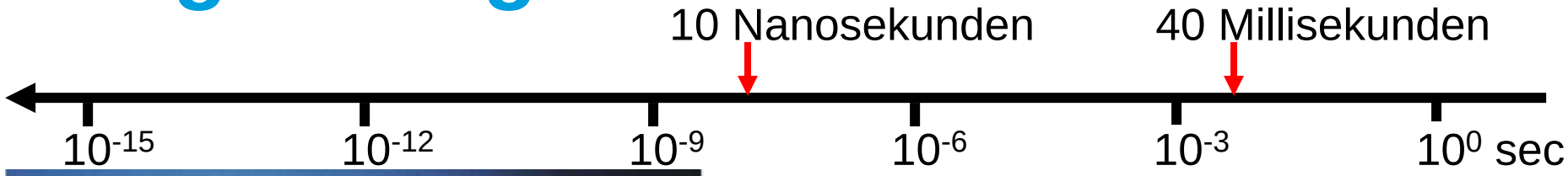


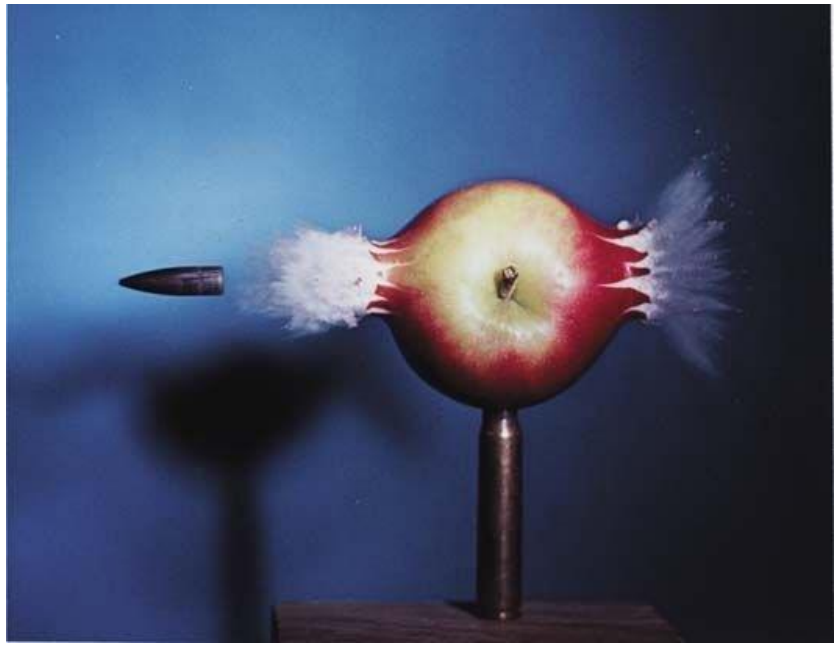


Free-electron laser physics

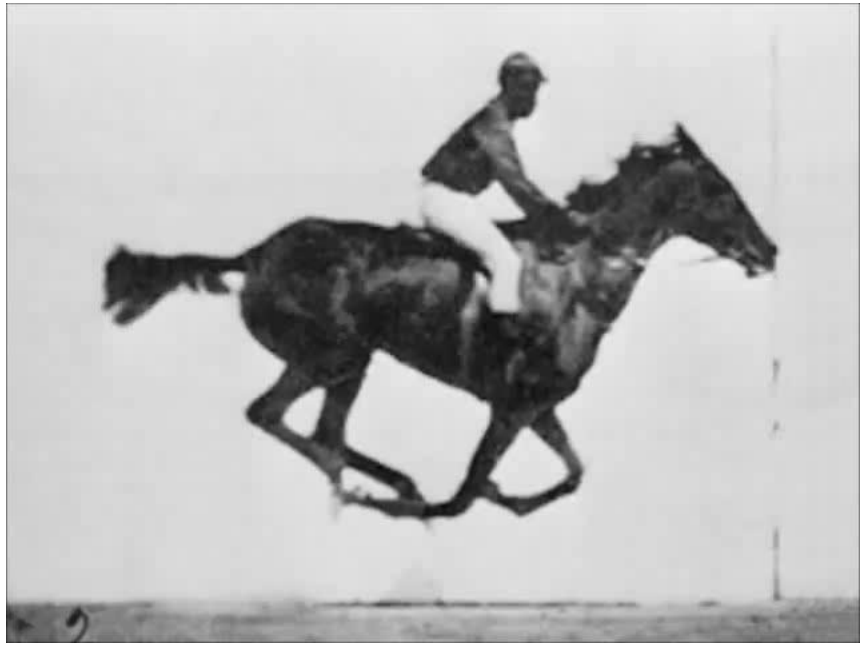
Travelling through timescales

Travelling through timescales



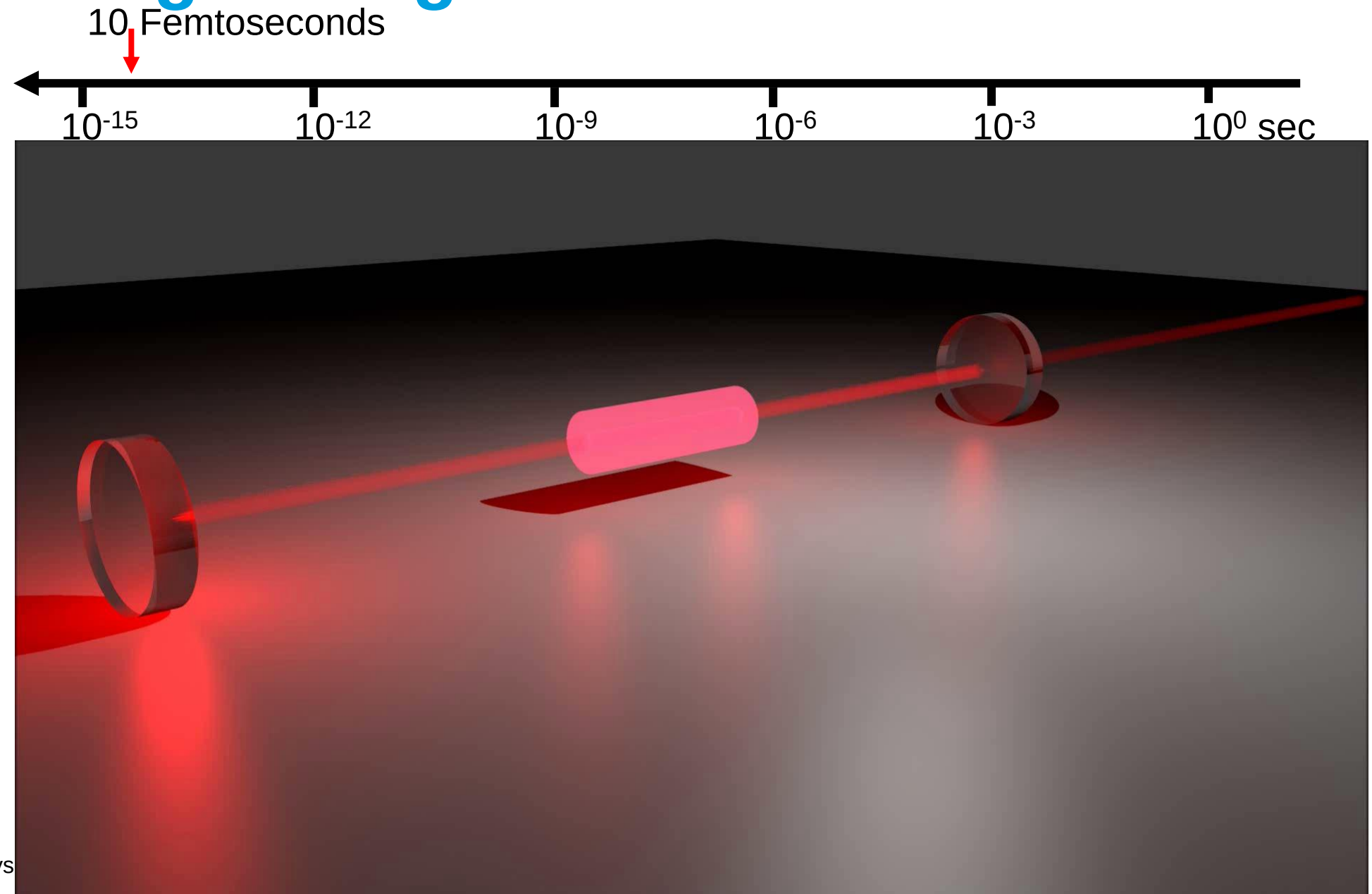


Edgerton, 1964



Muybride und Stanford, 1876

Travelling through timescales



Working principle of a Free Electron Laser

Google Maps

Working principle of a Free Electron Laser

«Pancini era divenuto sostenitore del fatto che gli apparecchi si dovevano costruire completamente in casa, perché... per fare della buona ricerca sperimentale bisogna sapere come gli apparecchi sono fatti e perciò non acquistarli.»

(parole di Giovanni Boato, che fu suo collaboratore a Genova, https://it.wikipedia.org/wiki/Ettore_Pancini)

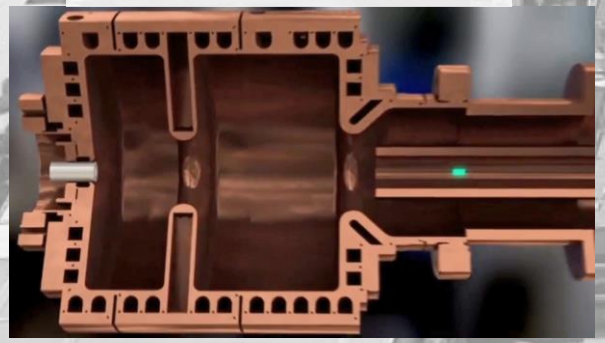
Google Maps

Working principle of a Free Electron Laser

Superconducting accelerator

Undulator

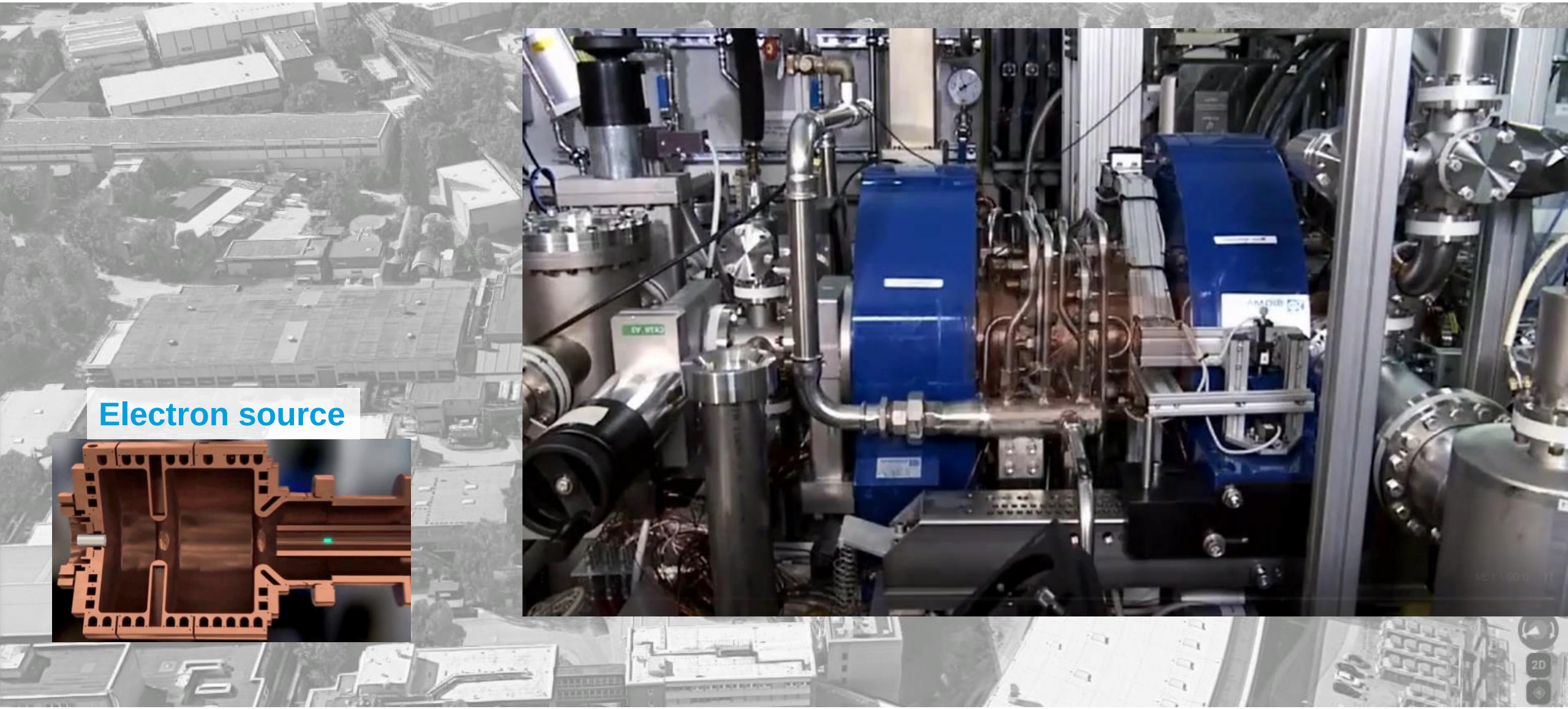
Electron source



Photon diagnostics and instruments

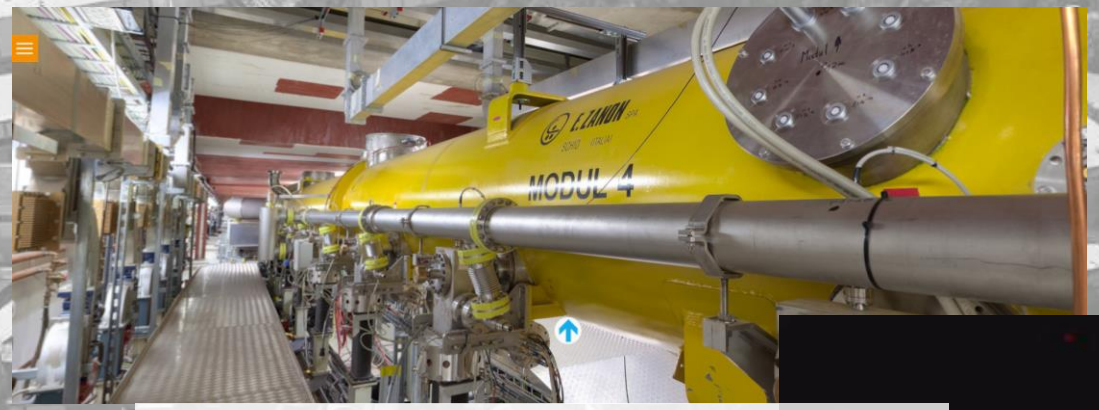
https://vtour.desy.de/desytour/index_de.html#node5

Working principle of a Free Electron Laser



https://vtour.desy.de/desytour/index_de.html#node5

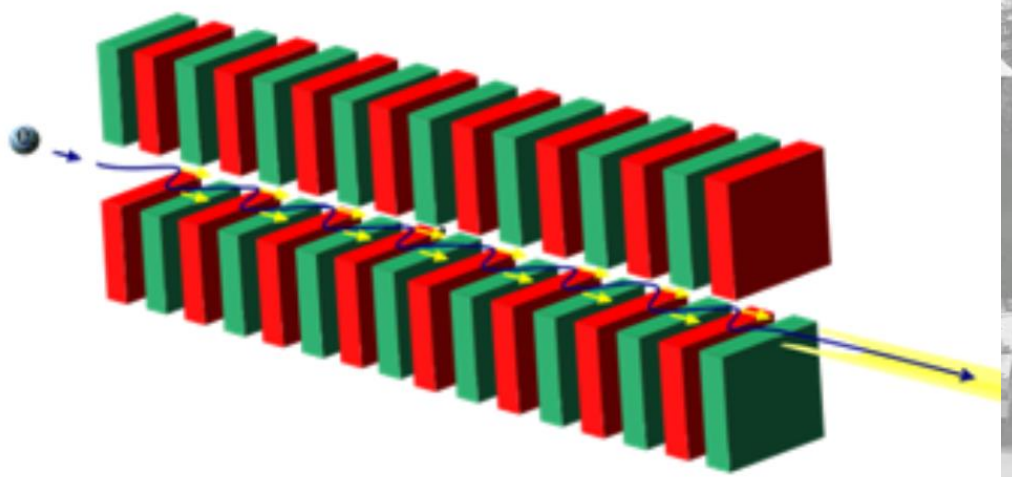
Working principle of a Free Electron Laser



Superconducting accelerator

https://vtour.desy.de/desytour/index_de.html#node5

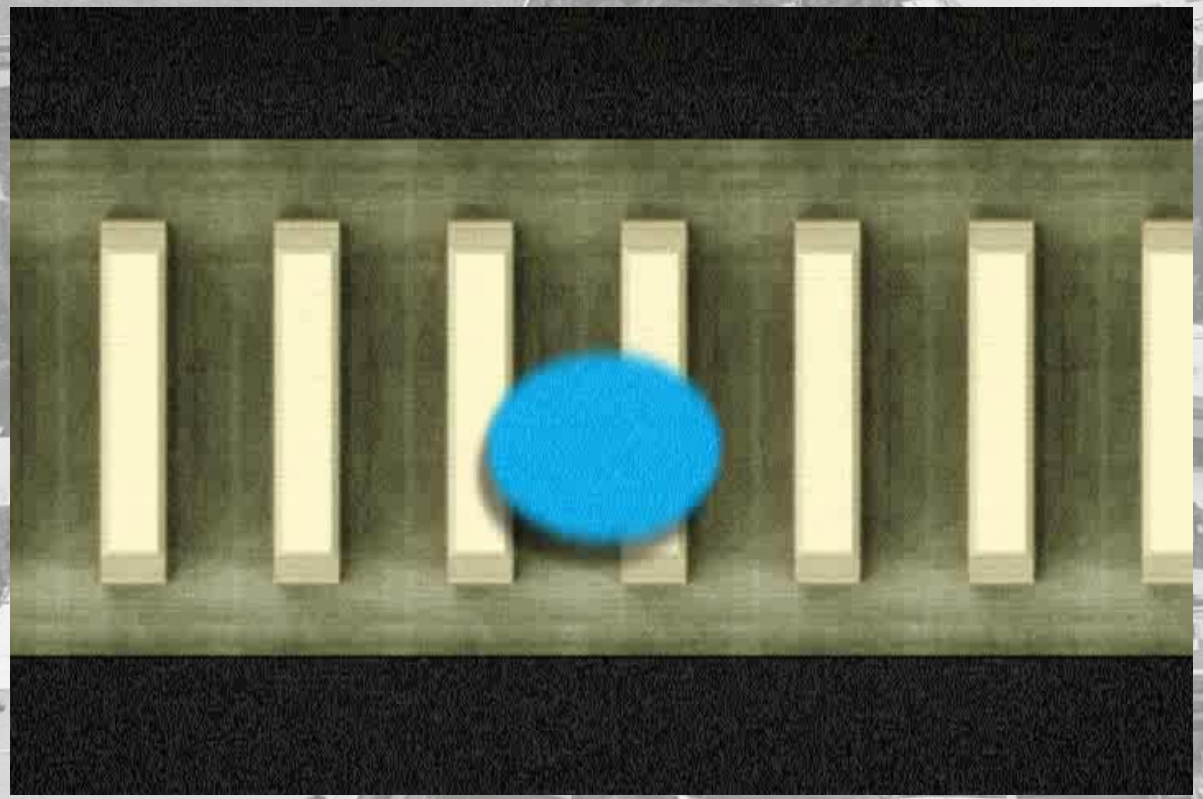
Working principle of a Free Electron Laser



https://science.hzbblog.de/what-is-an-undulator

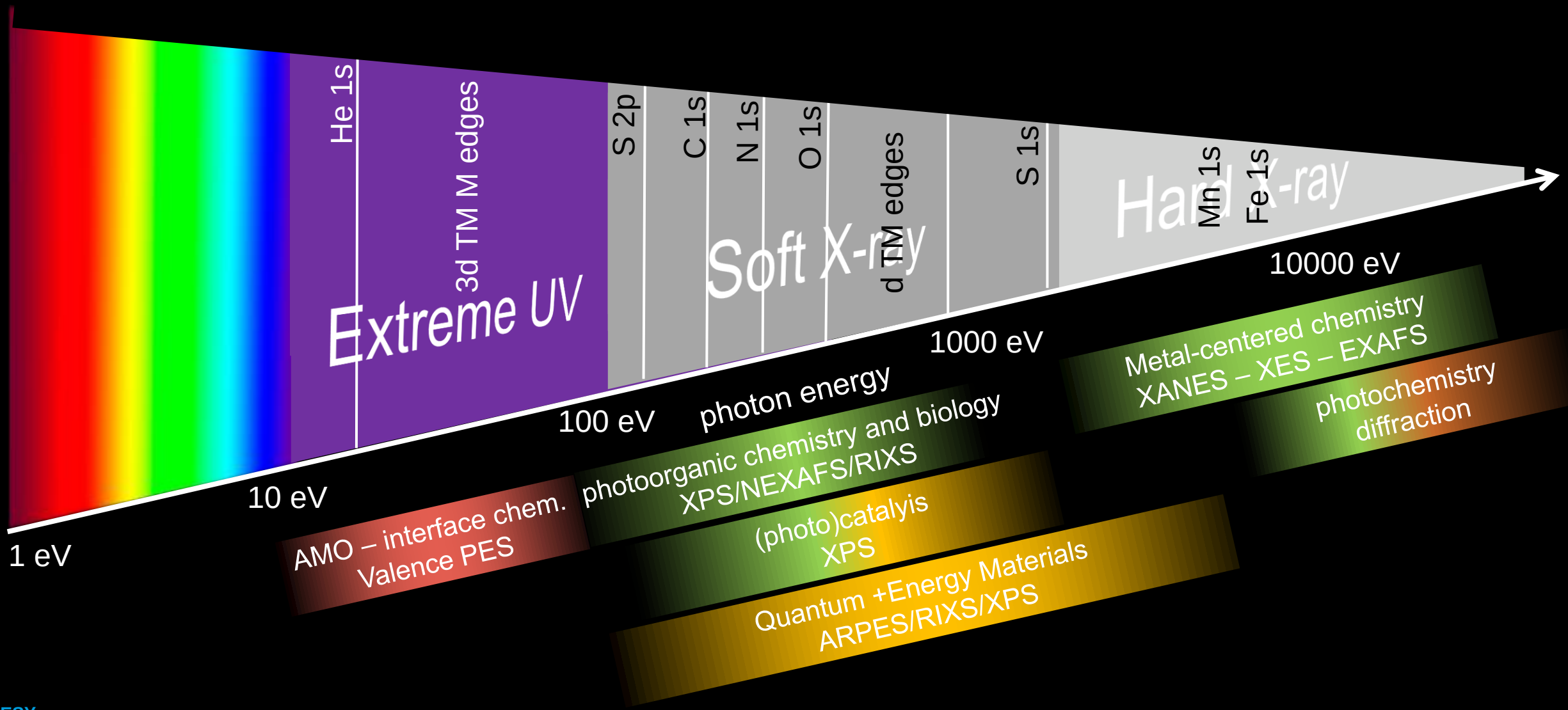
Undulator

Working principle of a Free Electron Laser



Undulator

https://www.youtube.com/watch?v=RG-PYmeq2XE


He 1s
3d TM M edges
Extreme UV
S 2p
C 1s
N 1s
O 1s
d TM edges
Soft X-ray
S 1s
Mn 1s
Fe 1s
Hard X-ray
1 eV
10 eV
100 eV
photon energy
1000 eV
10000 eV
AMO – interface chem.
Valence PES
photoorganic chemistry and biology
XPS/NEXAFS/RIXS
(photo)catalysis
XPS
Quantum +Energy Materials
ARPES/RIXS/XPS
Metal-centered chemistry
XANES – XES – EXAFS
photochemistry
diffraction

Extreme UV

Soft X-ray

S 2p
C 1s
N 1s
O 1s
d TM edges
S 1s
Mn
Fe

100 eV photon energy 1000 eV

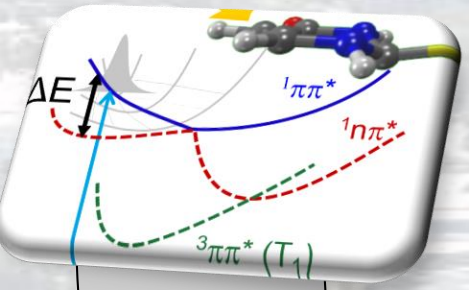
– interface chem.
PES

photoorganic chemistry and biology
XPS/NEXAFS/RIXS

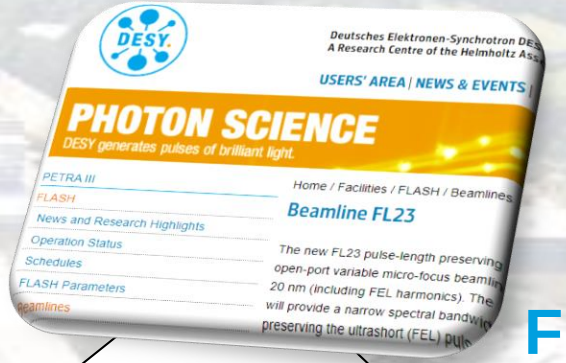
(photo)catalysis
XPS

Metal-centered ch
XANES – XES –

Outline

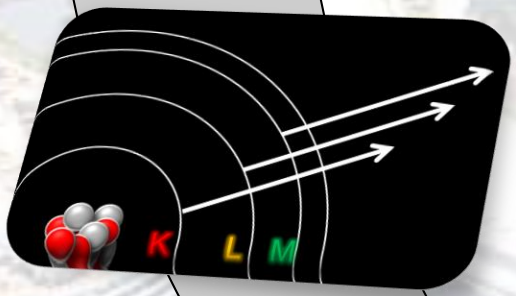


Molecular Photoenergy Conversion

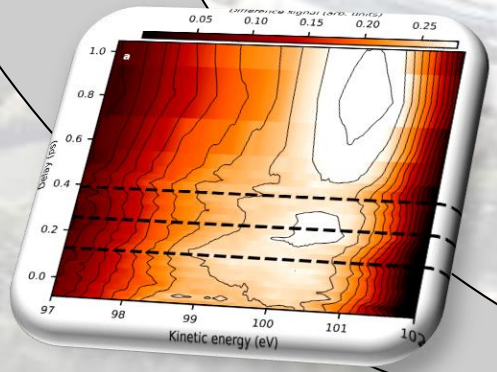


FLASH Beamtime

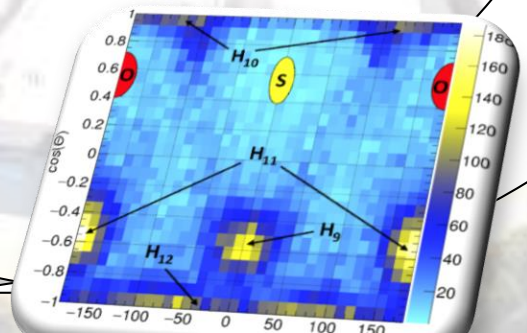
X-ray Probing

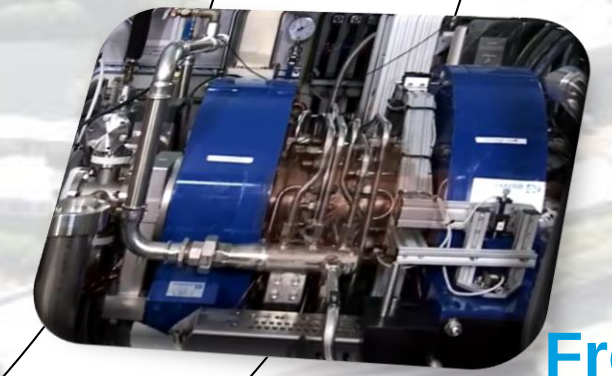


Electronic Movie



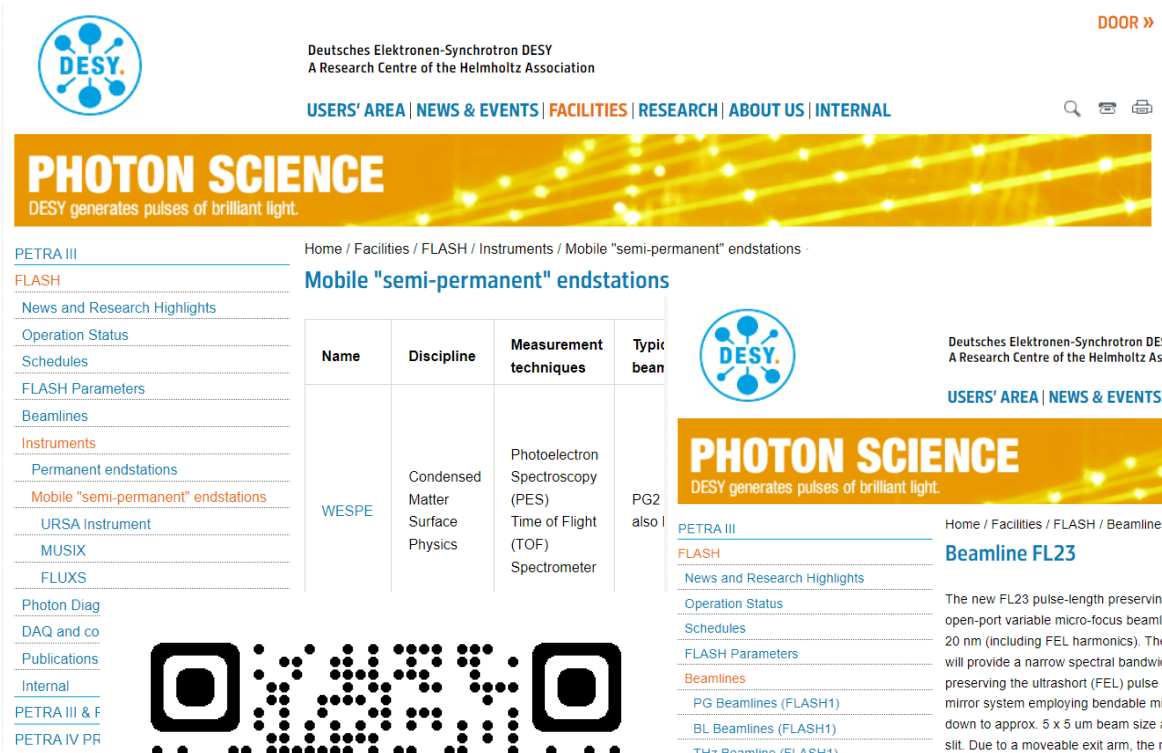
Geometry Movie

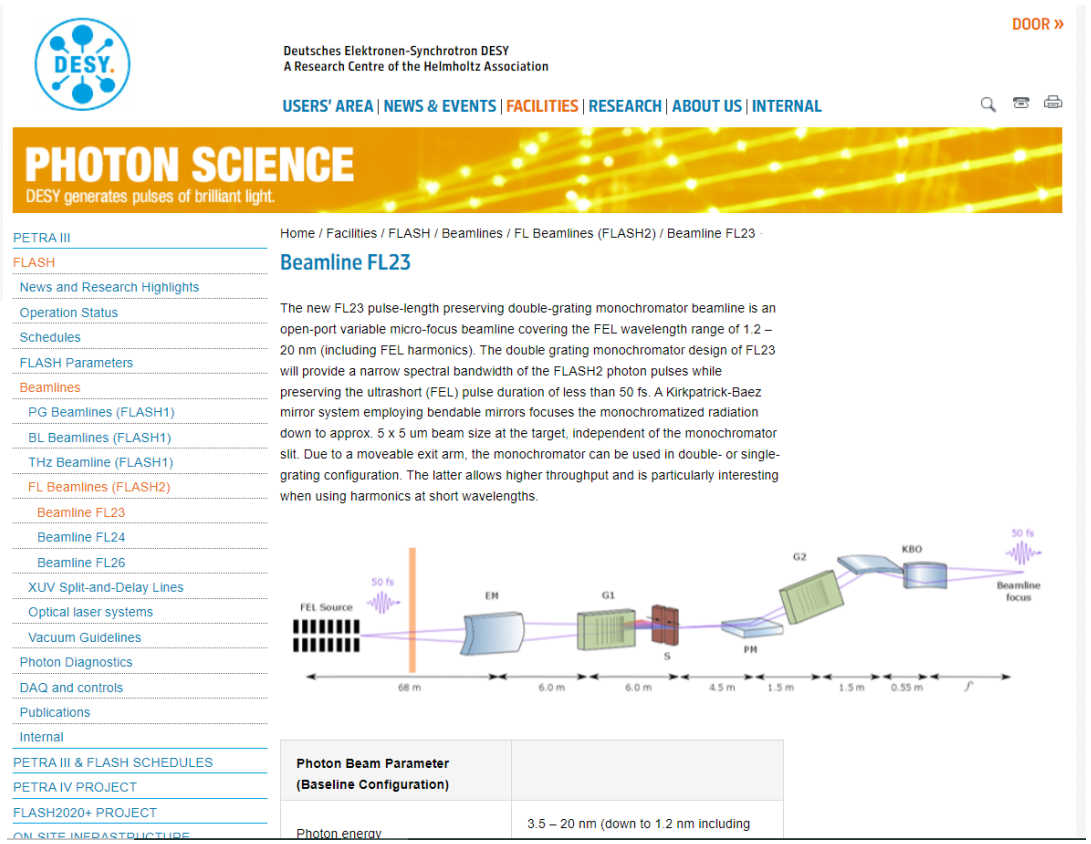




Free-electron laser physics

FLASH - support in beamline, instrument, and data





We don‘t only offer x-ray light, but:

- Beamline and optical lasers
- Instrumentation which can be tailored to your samples
- A rich data analysis library for user during and after beamtime

All you need to do is getting in contact with us

AND THEN

Write a proposal

Why would you want to use FLASH?

Femtosecond duration soft x-ray pulses

1-400 eV photon energy in fundamental

Up to ~1000 eV in third harmonic

5000 bunches/second, up to 1mJ per bunch

THz undulator

Optical lasers

X-ray split and delay

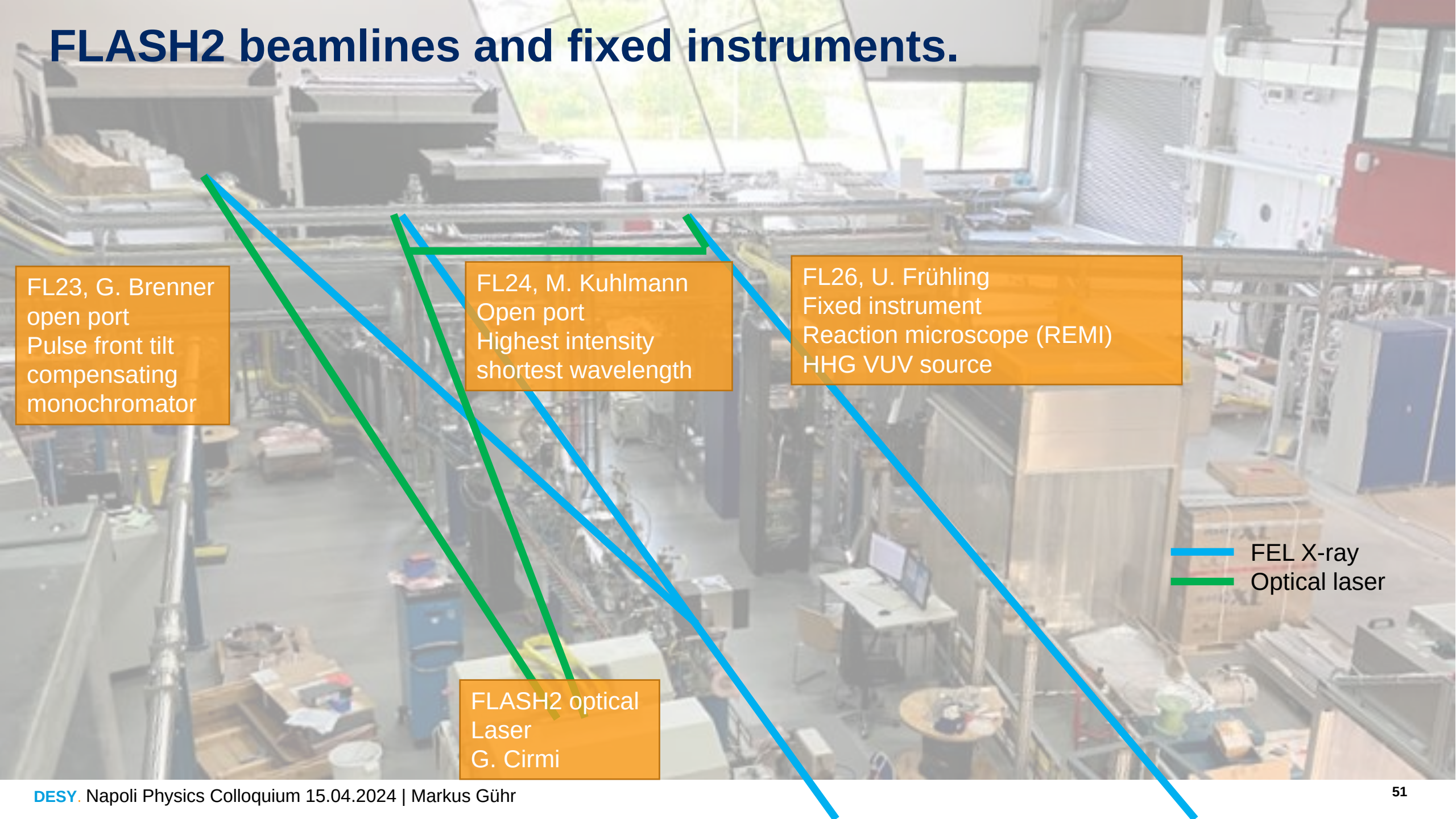
FLASH2 FLASH1

Ultrafast dynamics

Nonlinear probe

Probe before destroy

FLASH2 beamlines and fixed instruments.

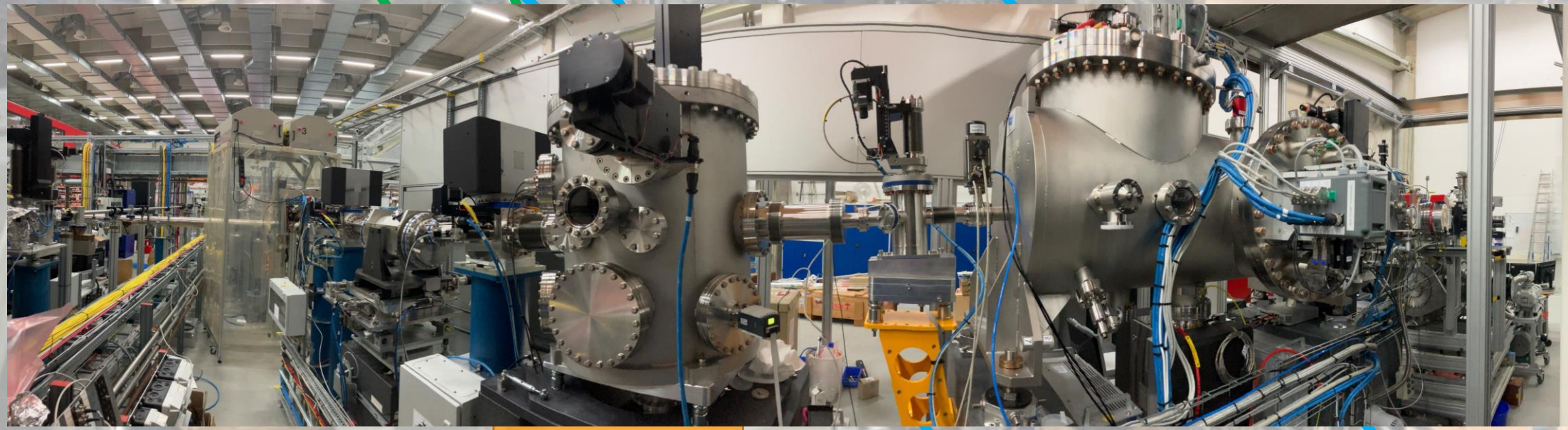


FLASH2 beamlines and fixed instruments.

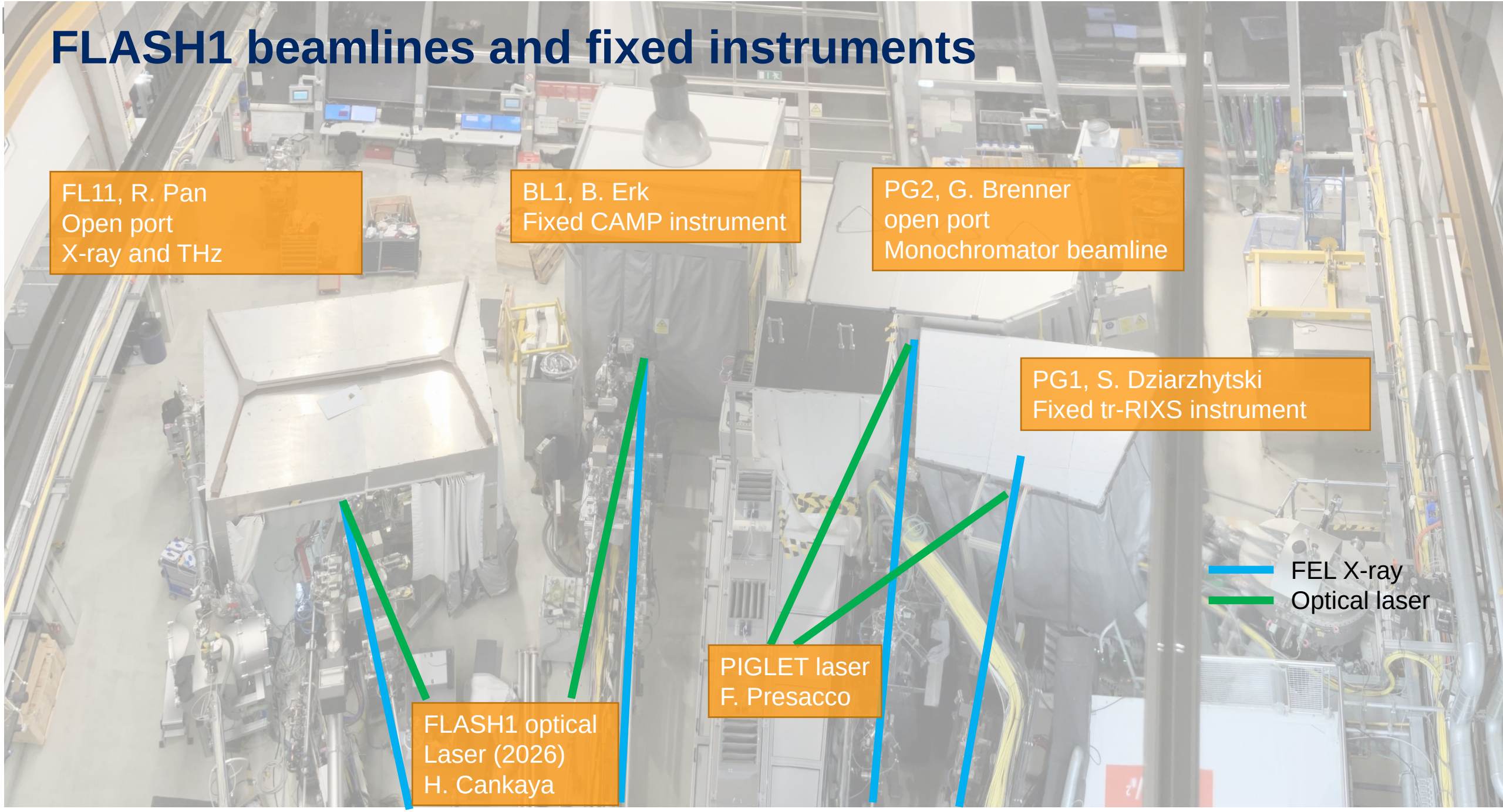
FL23, G. Brenner
open port
Pulse front tilt compensating monochromator

FL24, M. Kuhlmann
Open port
Highest intensity
shortest wavelength

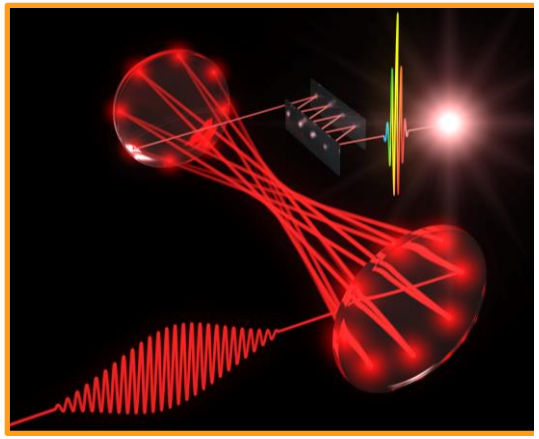
FL26, U. Frühling
Fixed instrument
Reaction microscope (REMI)
HHG VUV source

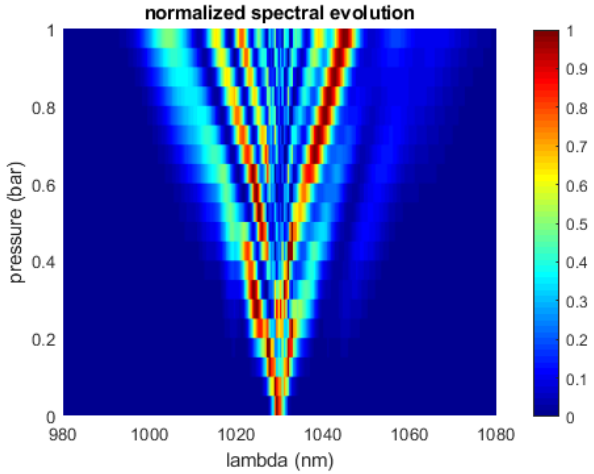


FLASH1 beamlines and fixed instruments

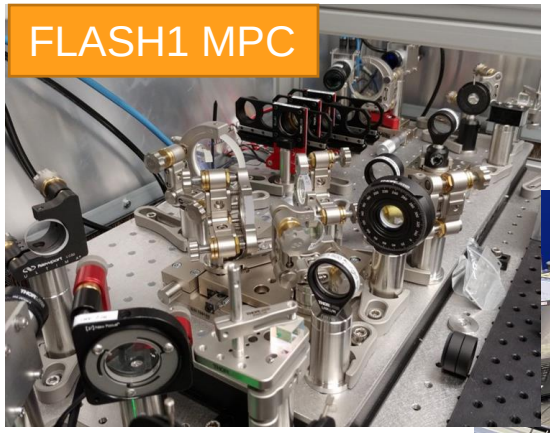


DESY pioneered the use of multi-pass cells.





- FS-LA pioneered MPC for Yb lasers
- Future FLASH1 pp laser also based on MPC and harmonics thereof



MPC in operation:

FLASH1 PIGLET
- MPC based on glass
- low power at high @1MHz, 1030nm, harmonics available

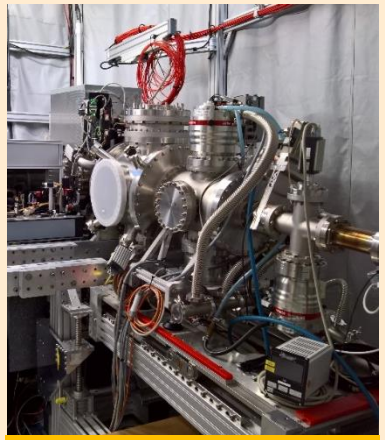
FLASH2 MPC for FL23
- MPC based on gas
- Up to 1mJ@100kHz, 1030nm, harmonics available

M. Seidel et al., Ultrafast Science 754919 (2022).
M. Seidel et al. Laser & Photonics Review 16 (2022).

We provide very flexible instrumentation.

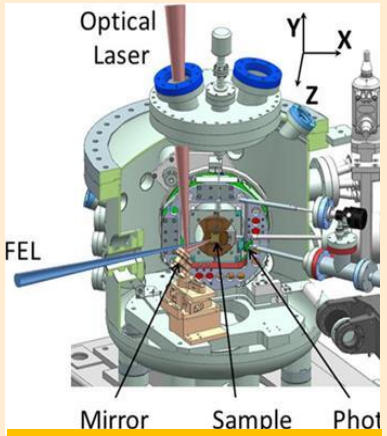
FLASH.

fixed to beamline



CAMP
B. Erk

Diffractive imaging of nanoparticles and clusters

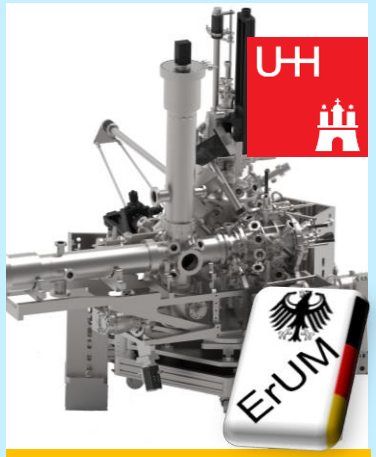


TRIXS
S. Dziarzhytski

Resonant inelastic X-ray scattering

FLASH moved from open port facilty with user delivered instruments to facility owned instruments over the years.

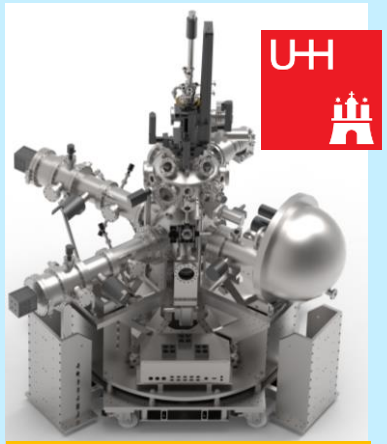
mobile



HEXTOF
D. Kutnyakhov

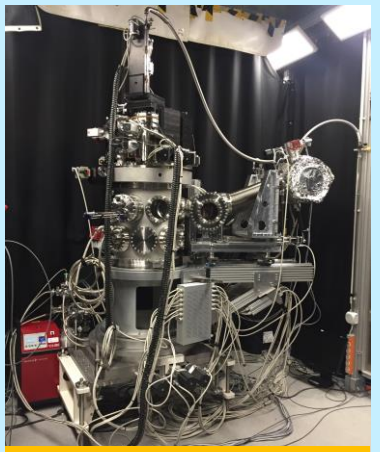
X-ray photoemission spectroscopy and k-microscopy

Instrument pioneered at FLASH spreads in the FEL world (going to EuXFEL and LCLSII)
MML – Rossnagel talk



WESPE
L. Wenthaus

X-ray photoemission Spectroscopy from surfaces



MUSIX
R.-P. Wang

X-ray absorption/emission

Resonant inelastic X-ray scattering

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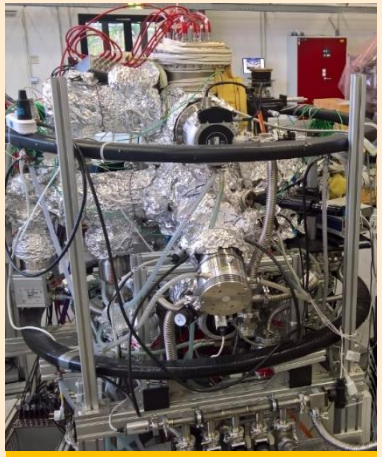
FLASH. DESY.

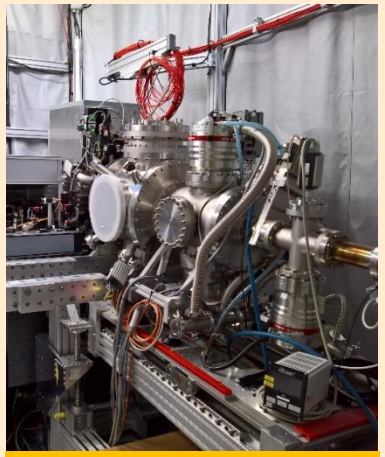
fixed to beamline



REMI
U. Frühling

Reaction microscope

Coincidence spectroscopy of electrons and ions



CAMP
B. Erk

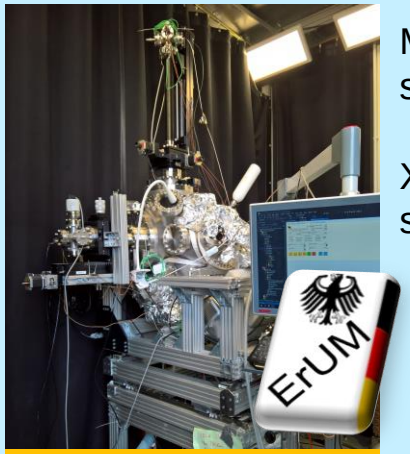
Velocity map imaging of electrons and ions

HHG abs
Ch. Papadopoulou

EUV absorption spectroscopy

HHG continuum and FEL pulse overlap

mobile



URSA
D. Mayer

Magnetic bottle spectrometer

X-ray photoelectron spectroscopy

MULTIP
Sven Toleikis

X-ray transmission

Universal chamber for gas and solid samples

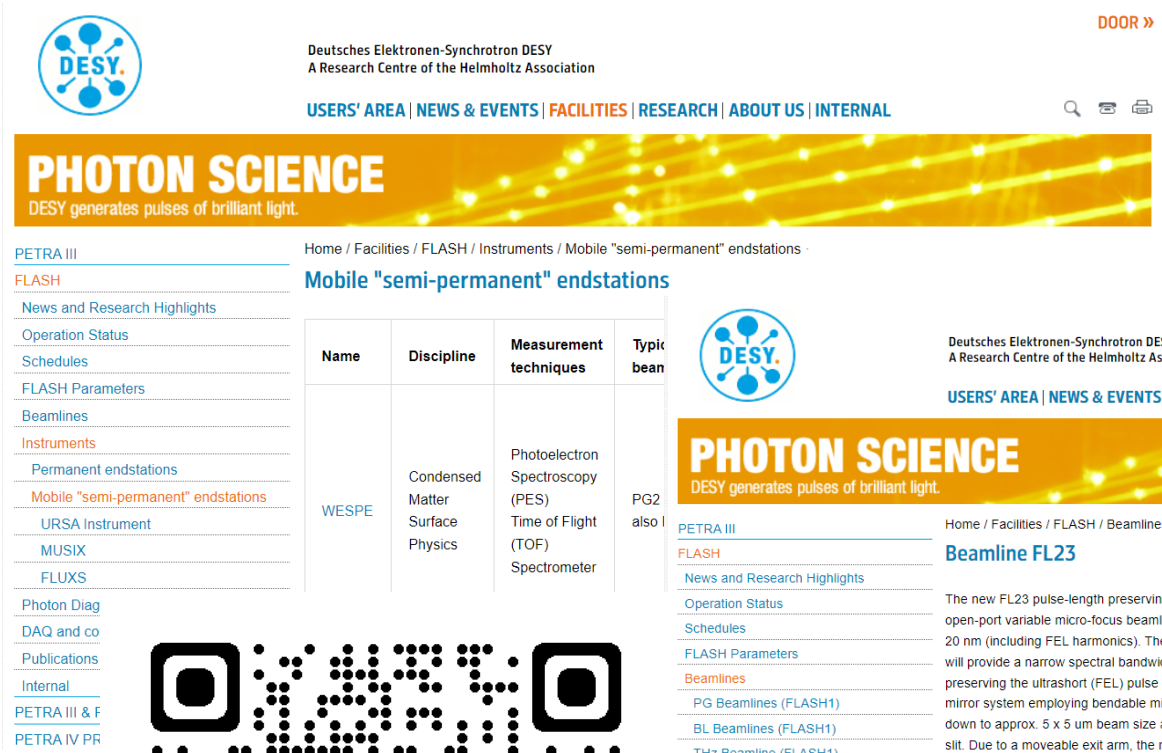
FLUXS
R.P.Wang

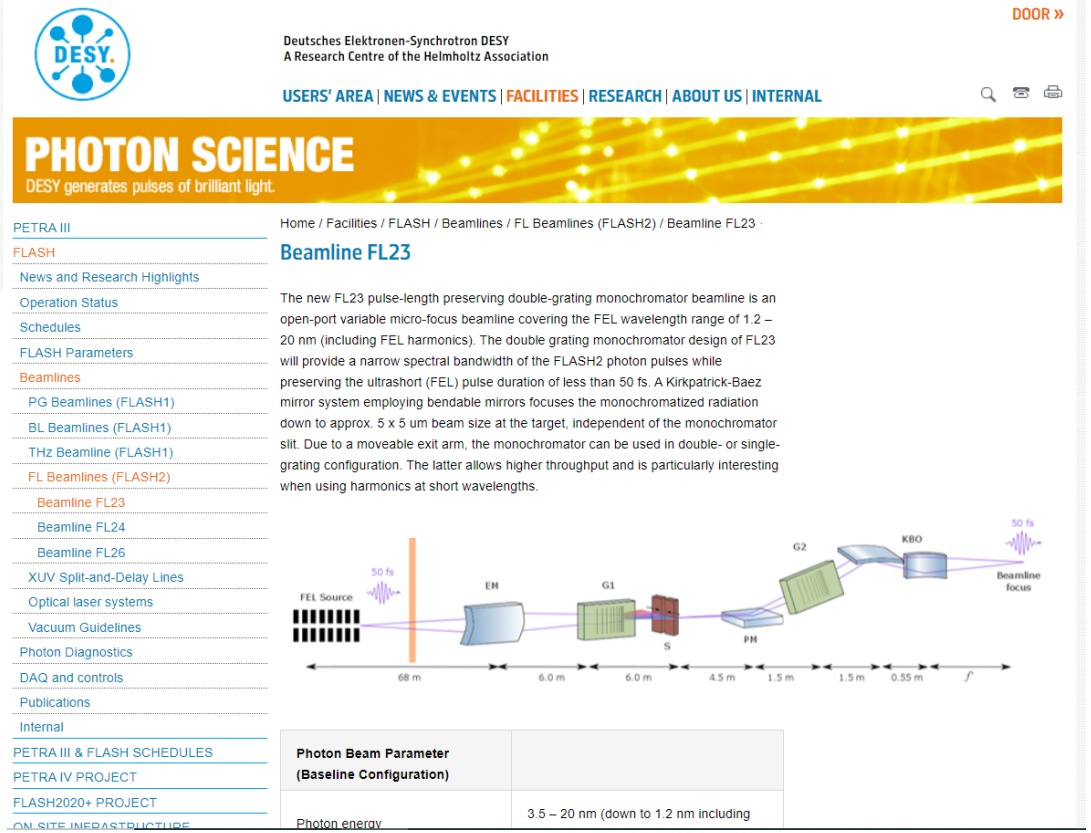
Liquid jet instrument

X-ray absorption and emission

RIXS

FLASH - support in beamline, instrument, and data





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Thanks to the team at FLASH

Thanks for your attention!