Gas-phase studies with FELs

Maria Novella Piancastelli

Sorbonne Université, CNRS,
Laboratoire de Chimie Physique-Matière et Rayonnement, LCPMR,
75005 Paris, France

Department of Physics and Astronomy, Uppsala University,
75120 Uppsala, Sweden

*Extremely high number of photons per pulse (10^{12}-10^{14} ph/shot)

Multiphoton non-linear processes

*Very short pulses (few to hundreds of femtoseconds, 10^{-15} sec)

Time-resolved spectroscopies

Detailed insight on electron and nuclear dynamics on a “real” timescale

Photoexcitation-deexcitation-fragmentation processes

Formation and breaking of chemical bonds

“Molecular movie”

FLASH, Hamburg, Germany

LCLS, Stanford, California, USA

FERMI, Trieste, Italy

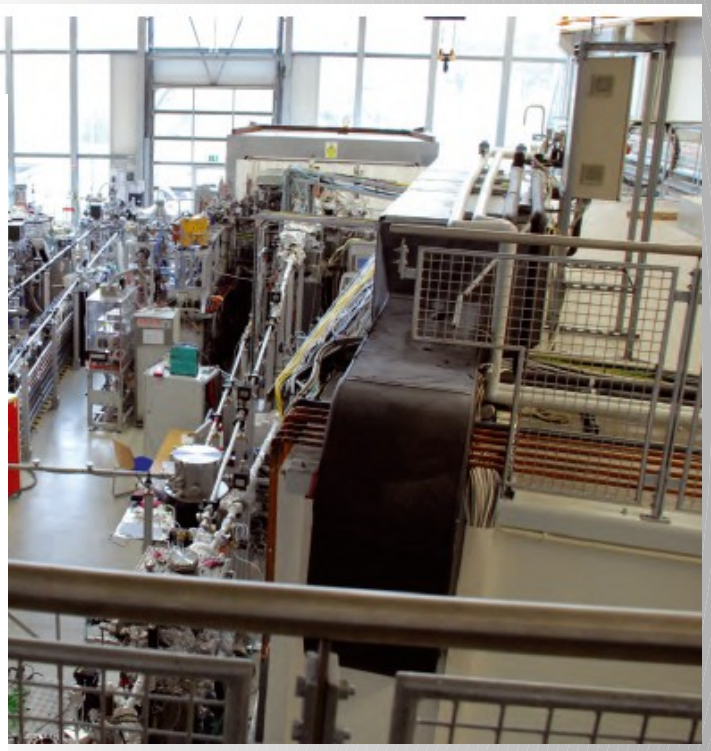
(SACLA, Japan)

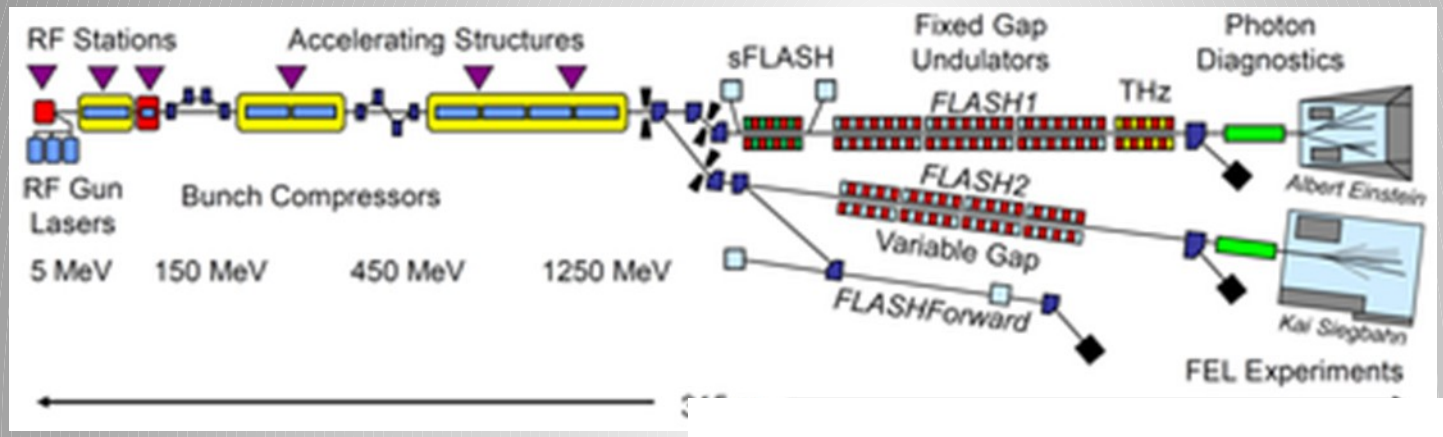
European XFEL (Hamburg, Germany)

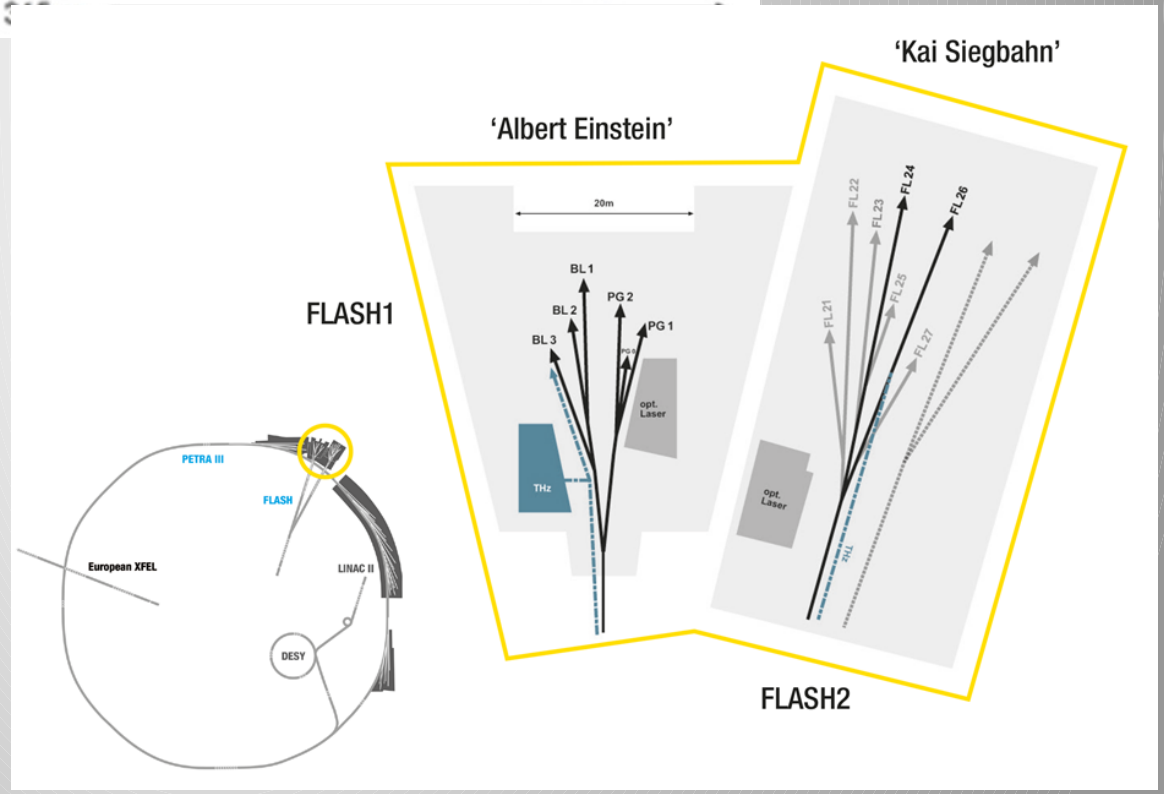
FLASH

DESY, Hamburg, Germany

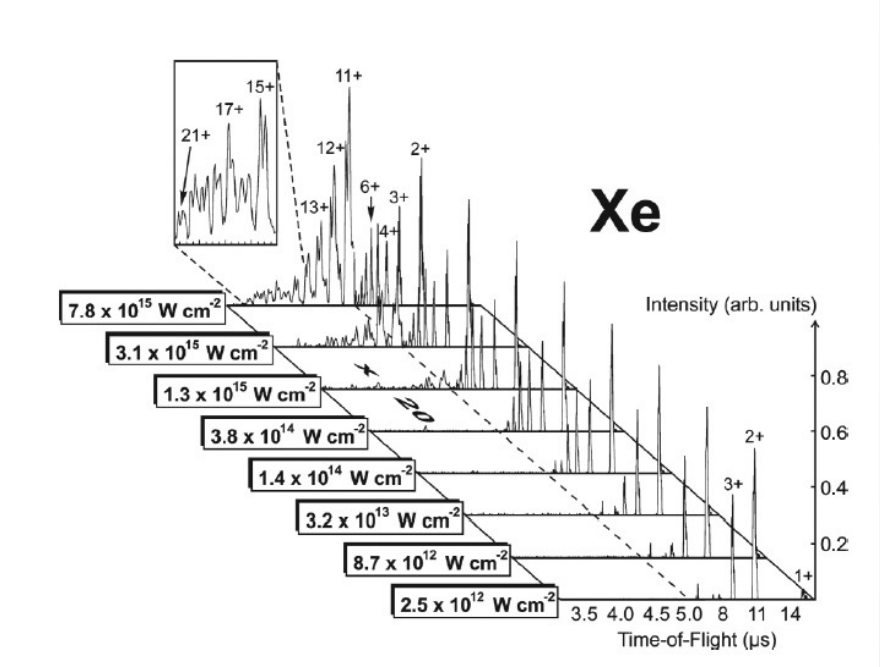
Parameter	FLASH1	FLASH2
Electron beam energy	0.35 - 1.25 GeV	0.4 - 1.25 GeV
Normalised emittance at 1 nC (rms)	1.4 mm mrad	1.4 mm mrad
Energy spread	200 keV	500 keV
Electron bunch charge	0.1 - 1.2 nC	0.02 - 1 nC
Peak current	1 - 2.5 kA	1 - 2.5 kA
Electron bunches per second (typ./max)	300 / 5000	300 / 5000
Photon energy (fundamental)	24 - 295 eV	14 - 310 eV
Photon wavelength (fundamental)	51 - 4.2 nm	90 - 4 nm
Photon pulse duration (FWHM)	<30 - 200 fs	<10 - 200 fs
Peak Power (from av.)	1 - 5 GW	1 - 5 GW
Single photon pulse energy (average)	1 - 500 µJ	1 - 1000 µJ
Spectral Width (FWHM)	0.7 - 2 %	0.5 - 2 %
Photons per Pulse	10^{11} - 10^{14}	10^{11} - 10^{14}
Peak Brilliance	10^{28} - 10^{31} B	10^{28} - 10^{31} B

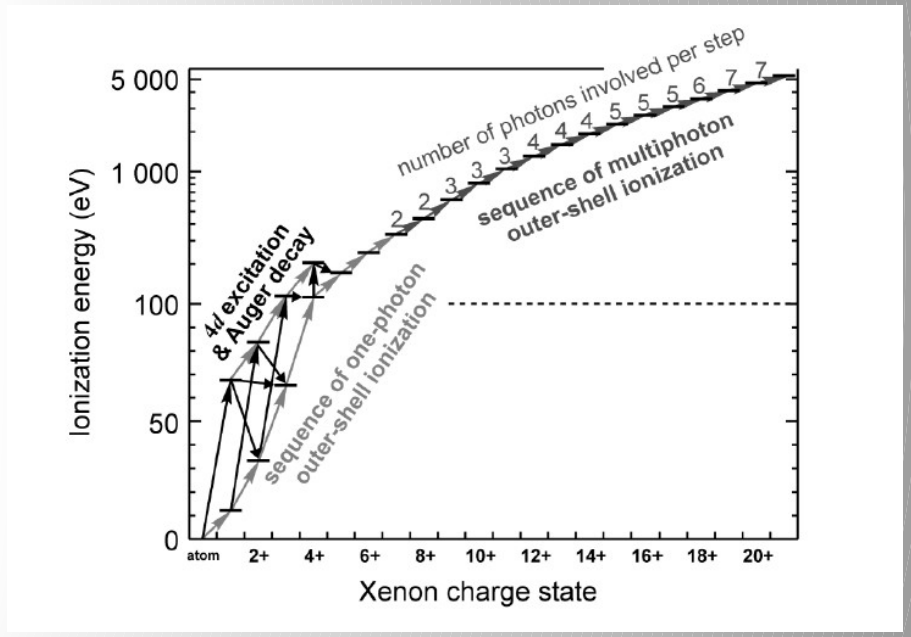



RF Stations
Accelerating Structures
sFLASH
Fixed Gap Undulators
Photon Diagnostics
THz
FLASH1
FLASH2
Variable Gap
FLASHForward
Albert Einstein
Kai Siegbahn
RF Gun Lasers
Bunch Compressors
5 MeV
150 MeV
450 MeV
1250 MeV
FEL Experiments


'Kai Siegbahn'
'Albert Einstein'
FLASH1
FLASH2
20m
BL 1
BL 2
BL 3
PG 2
PG 1
opt. Laser
THz
FL21
FL22
FL23
FL24
FL25
FL26
FL27
PETRA III
FLASH
European XFEL
LINAC II
DESY

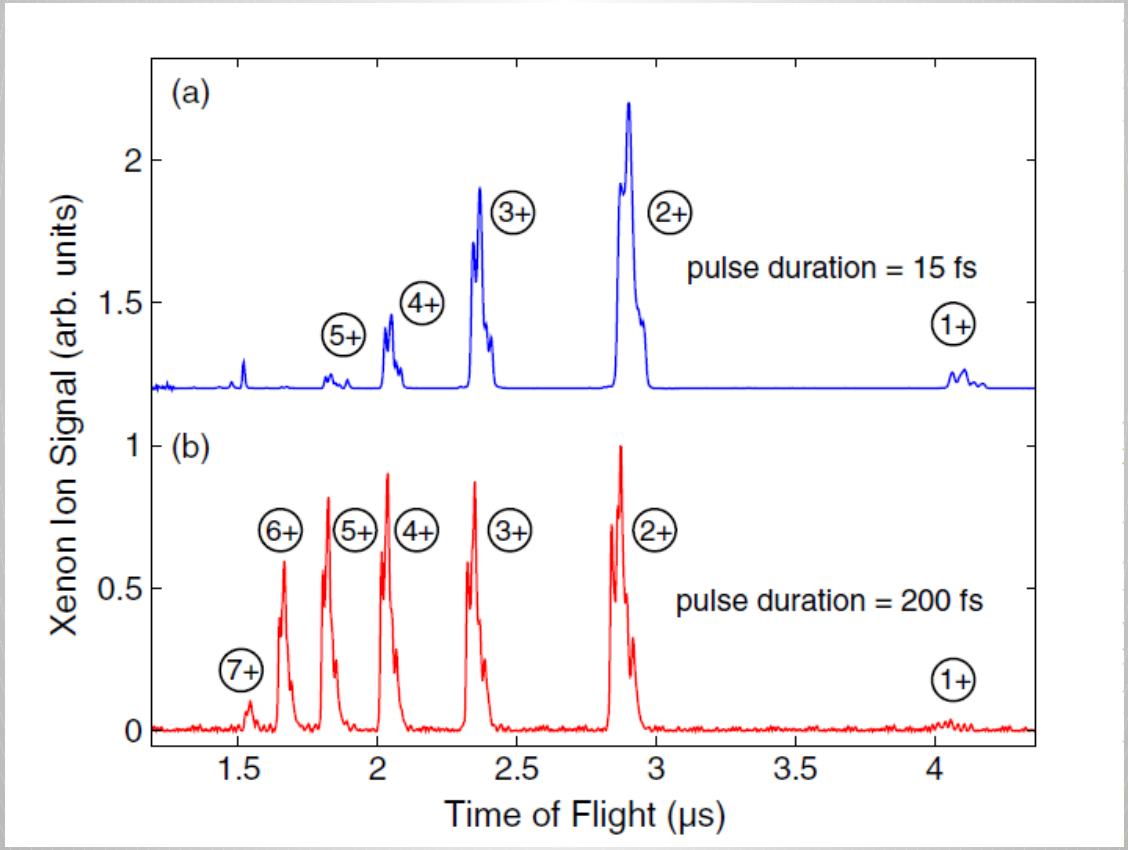
Photoelectric Effect at Ultrahigh Intensities



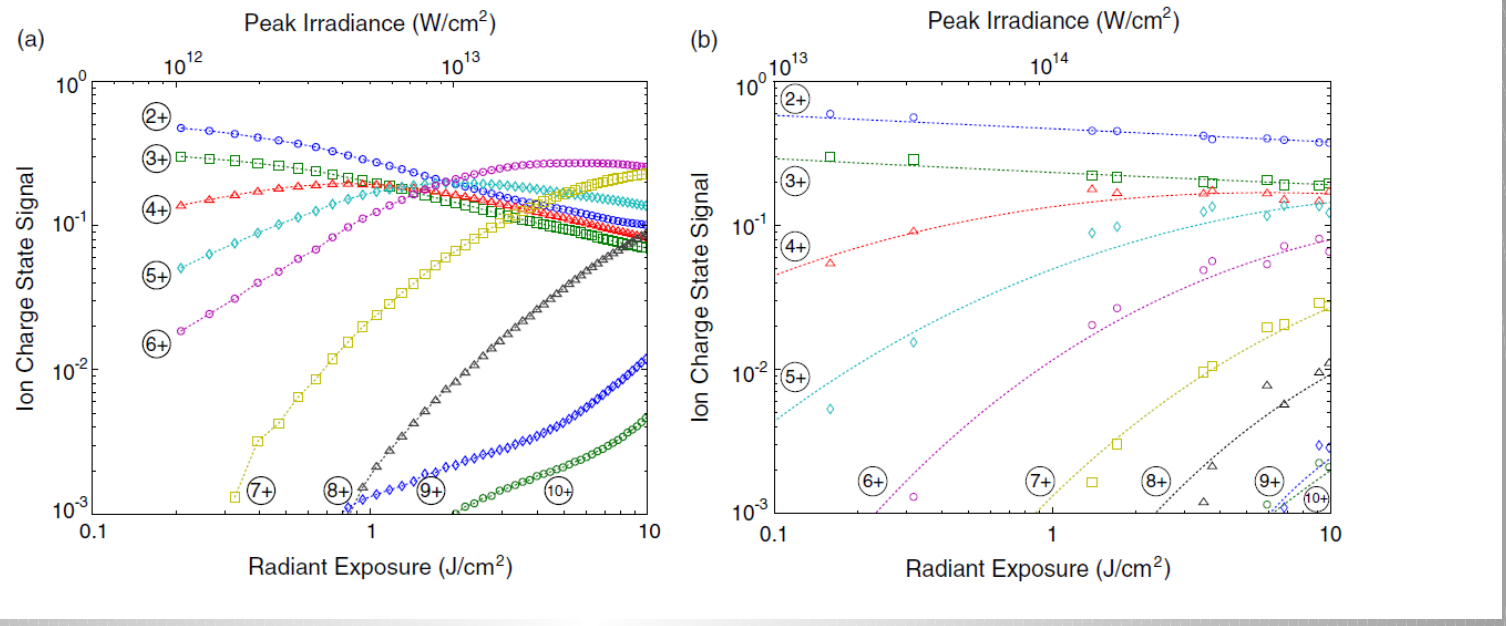


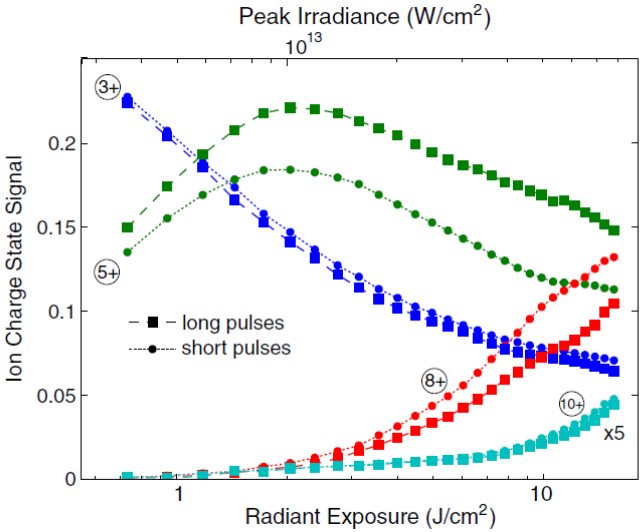
A. Sorokin, S.V. Bobashev, T. Feigl, K. Tiedtke, H. Wabnitz and M. Richter, Phys.Rev.Lett. 99 (2007) 213002

Time-Dependent Multiphoton Ionization of Xenon in the Soft-X-Ray Regime

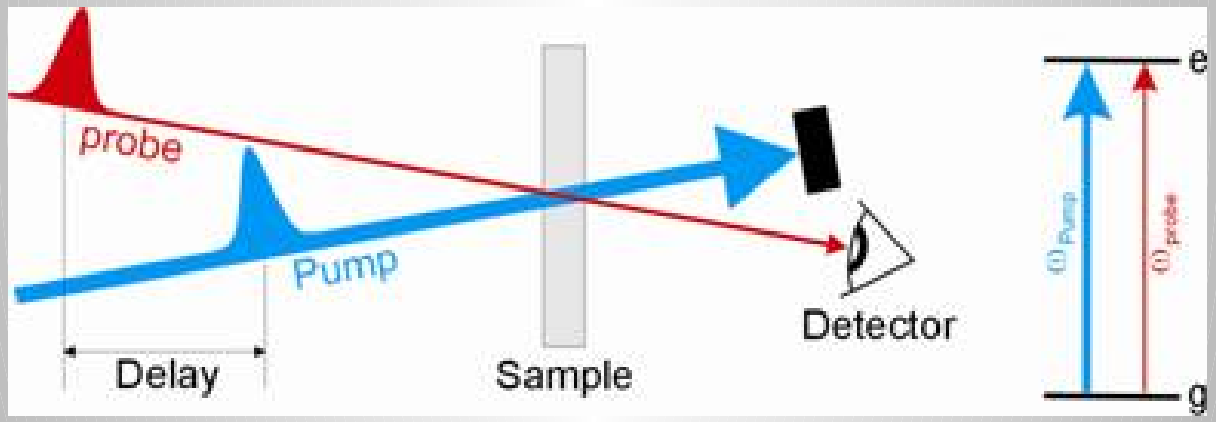


N. Gerken, S. Klumpp, A. A. Sorokin, K. Tiedtke, M. Richter, V. Bürk, K. Mertens, P. Juranić and M. Martins, Phys.Rev.Lett. 112, 213002 (2014)

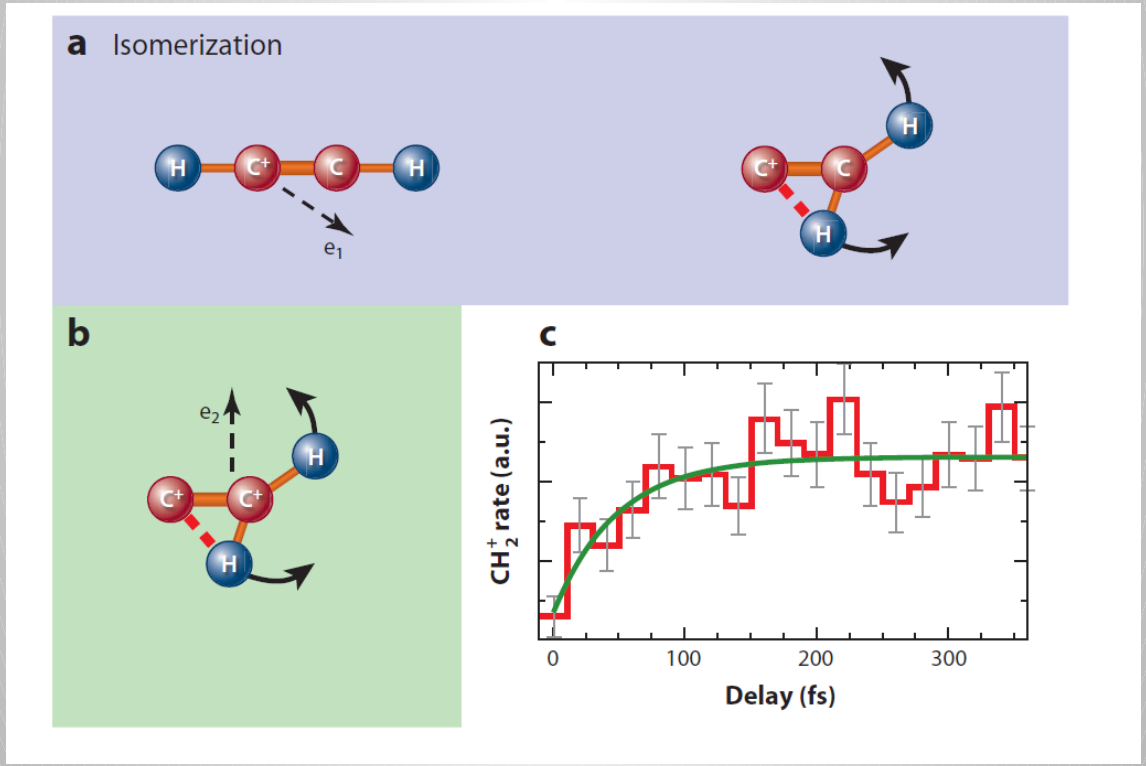

(a)
Peak Irradiance (W/cm^2)
10^{12}
10^{13}
10^0
10^{-1}
10^{-2}
10^{-3}
Ion Charge State Signal
2+
3+
4+
5+
6+
7+
8+
9+
10+
0.1
1
10
Radiant Exposure (J/cm^2)
(b)
Peak Irradiance (W/cm^2)
10^{13}
10^{14}
10^0
10^{-1}
10^{-2}
10^{-3}
Ion Charge State Signal
2+
3+
4+
5+
6+
7+
8+
9+
10+
0.1
1
10
Radiant Exposure (J/cm^2)


Peak Irradiance (W/cm^2)
10^{13}
0.2
0.15
0.1
0.05
0
Ion Charge State Signal
3+
5+
8+
10+
x5
long pulses
short pulses
1
10
Radiant Exposure (J/cm^2)

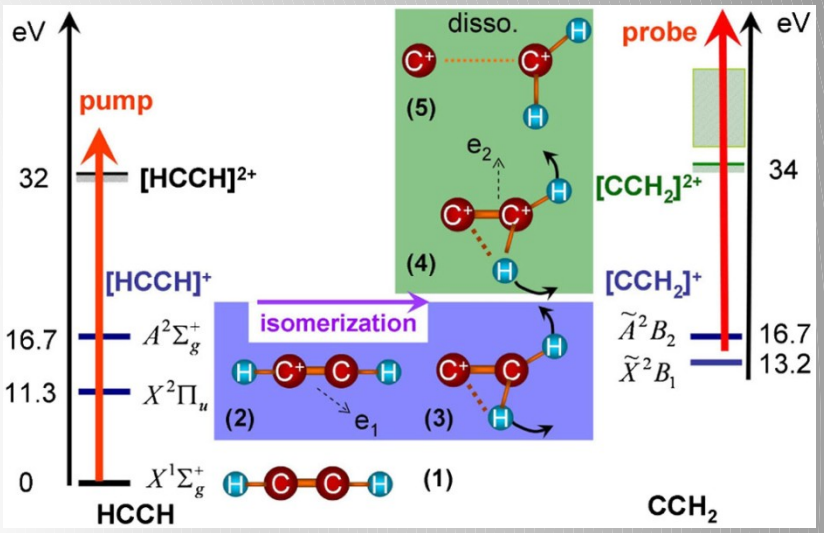
Pump-probe experiments



Ultrafast Extreme Ultraviolet Induced Isomerization of Acetylene Cations



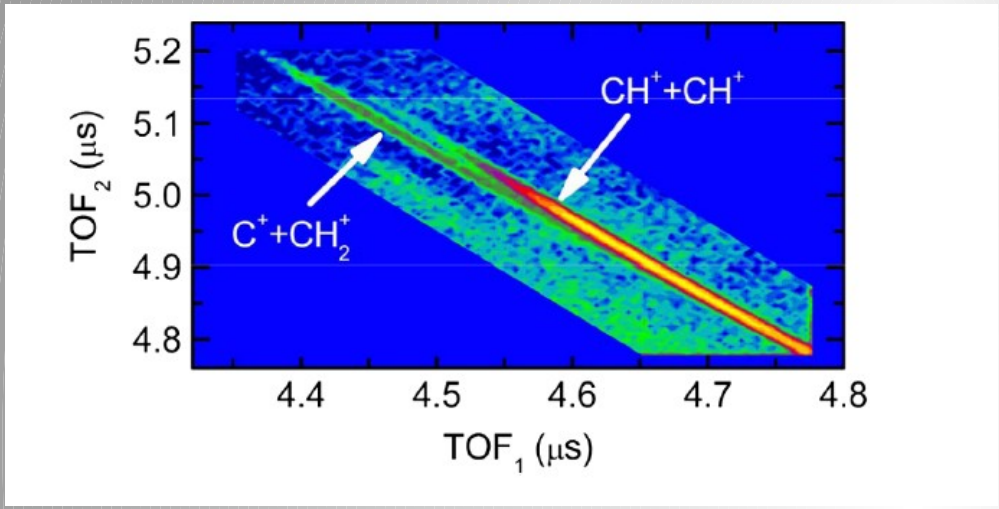
Y. H. Jiang et al., Phys.Rev.Lett. 105, 263002 (2010)

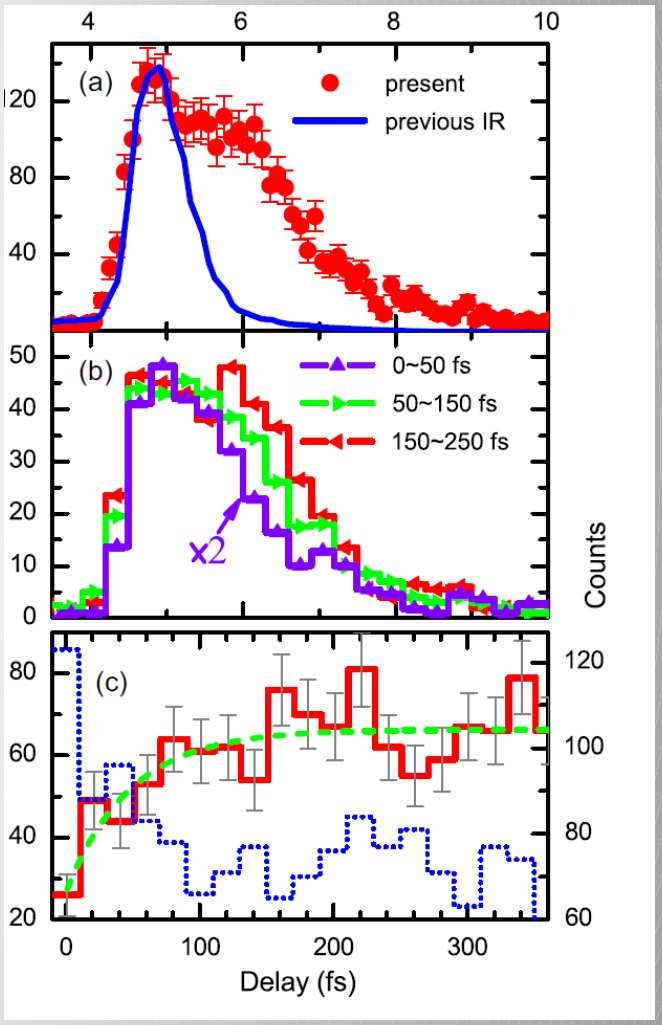


$$\mathrm{HCCH}(X^1\Sigma_g^+) + h\upsilon(\mathrm{pump}) \rightarrow [\mathrm{HCCH}]^+(X^2\Pi_u, A^2\Sigma_g) + e_1 \xrightarrow{\text{migra}} [\mathrm{H_2CC}]^+(\tilde{X}^2B_1, \tilde{A}^2B_2) + e_1, \quad (1)$$

and

$$[\mathrm{H_2CC}]^+(\tilde{X}^2B_1, \tilde{A}^2B_2) + h\upsilon(\mathrm{probe}) \rightarrow [\mathrm{H_2CC}]^{2+} + e_2 \xrightarrow{\text{diss}} \mathrm{CH_2^+} + \mathrm{C^+} + e_2, \quad (2)$$

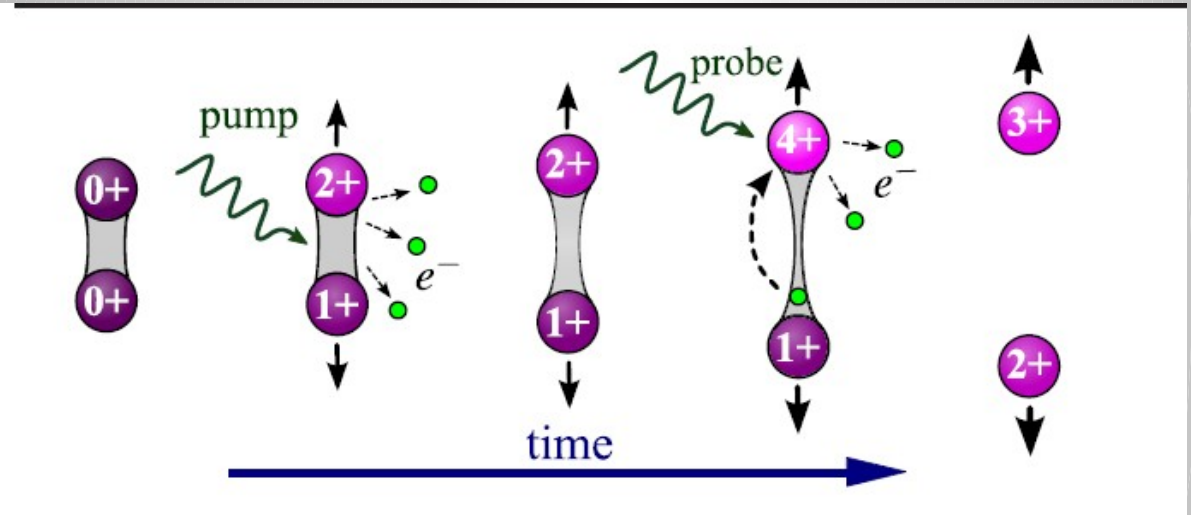




Mean isomerization time:

52 ± 15 fs

Electron Rearrangement Dynamics in Dissociating I_2^{n+} Molecules Accessed by Extreme Ultraviolet Pump-Probe Experiments

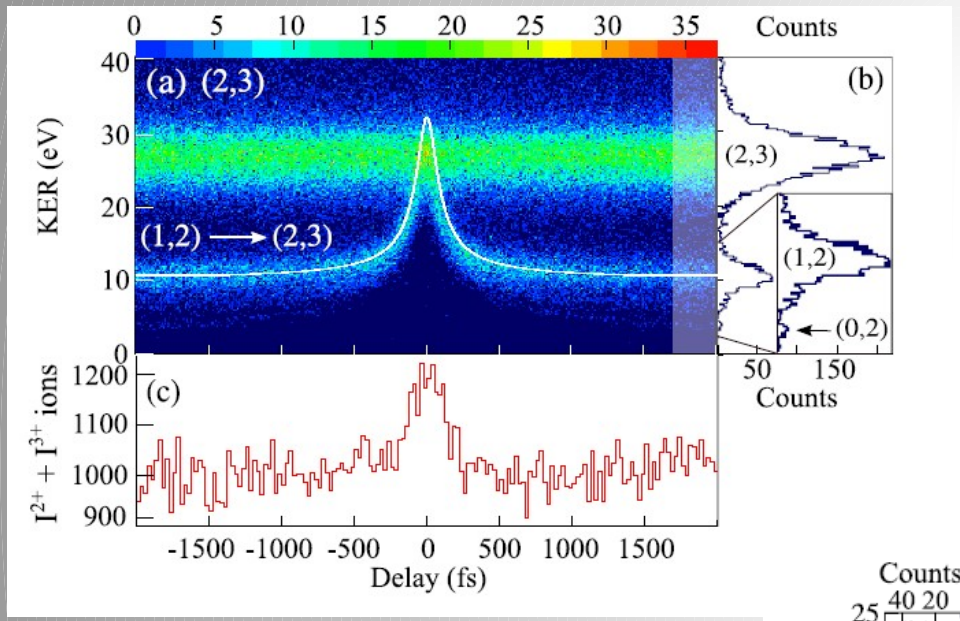


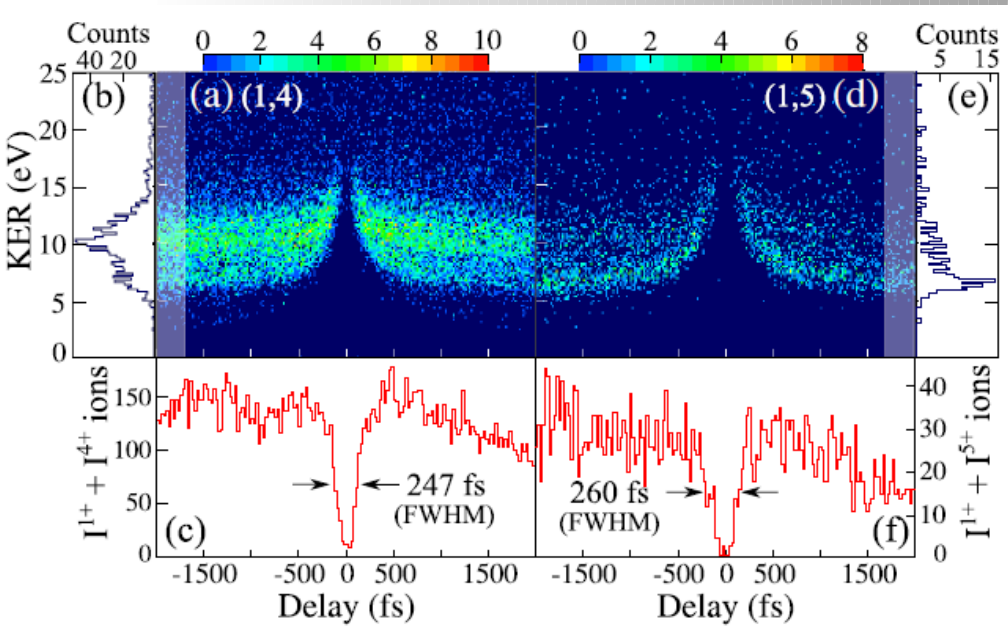
$$I_2 \xrightarrow{h\nu} I_2^{*+} \xrightarrow{A1+A2} I_2^{3+} \longrightarrow I^{1+} + I^{2+} \quad (55\%), \qquad (1)$$

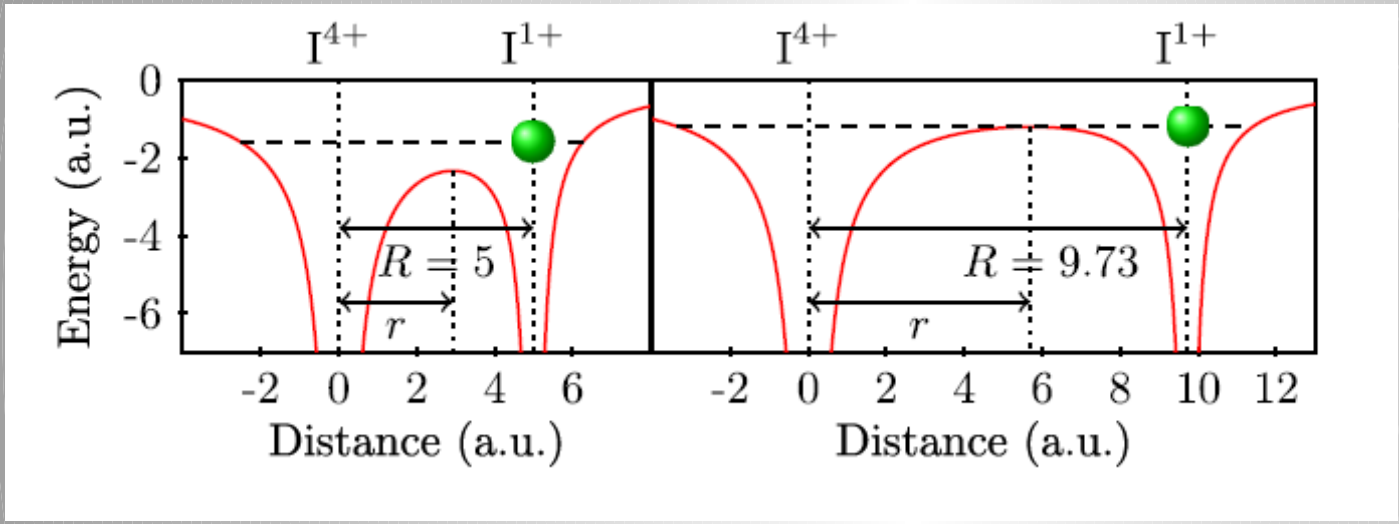
$$I_2 \xrightarrow{h\nu} I_2^{*+} \xrightarrow{A1} I_2^{2+} \longrightarrow I^{1+} + I^{1+} \quad (44\%), \qquad (2)$$

$$I_2 \xrightarrow{h\nu} I_2^{*+} \xrightarrow{A1} I_2^{2+} \longrightarrow I + I^{2+} \quad (< 1\%). \qquad (3)$$

K. Schnorr, A. Senftleben, M. Kurka, A. Rudenko, G. Schmid,T. Pfeifer, K. Meyer, M. Kübel, M. F. Kling,Y. H. Jiang, R. Treusch,S. Düsterer, B. Siemer, M. Wöstmann, H. Zacharias, R. Mitzner, T. J. M. Zouros, J. Ullrich, C. D. Schröter and R. Moshammer, Phys.Rev.Lett. 113, 073001 (2014)

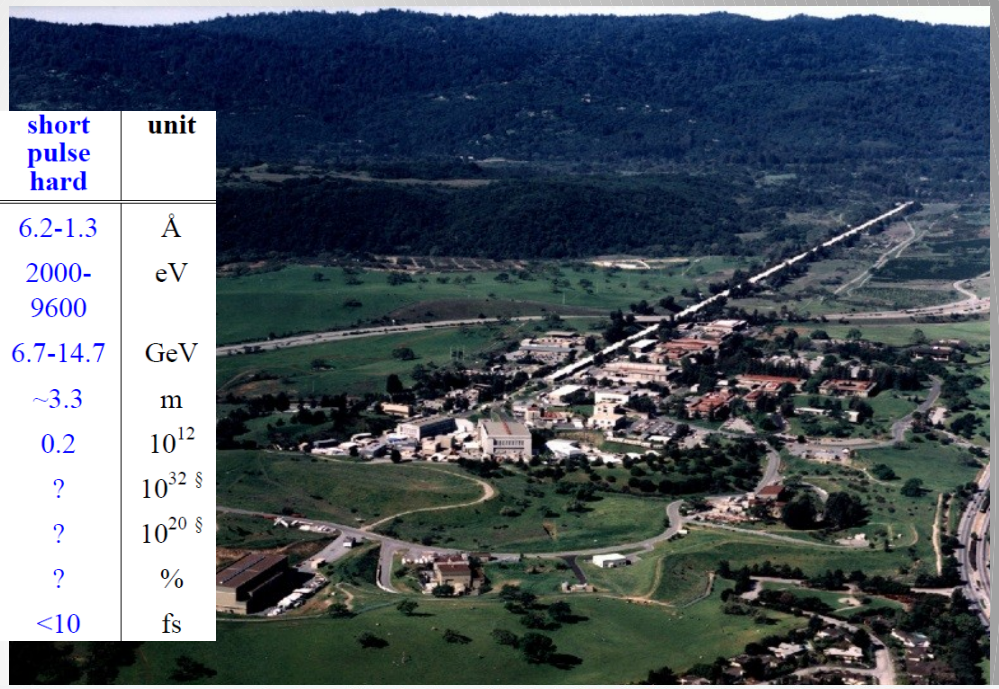

Counts
(a) (2,3)
(1,2) → (2,3)
KER (eV)
(b)
(2,3)
(1,2)
(0,2)
Counts
(c)
$I^{2+} + I^{3+}$ ions
Delay (fs)


Counts
(b)
(a) (1,4)
(1,5) (d)
(e)
KER (eV)
(c)
247 fs
(FWHM)
260 fs
(FWHM)
(f)
$I^{1+} + I^{4+}$ ions
$I^{1+} + I^{5+}$ ions
Delay (fs)
Delay (fs)



$$V_e(r,R) = -\frac{P_f + 1}{R - r} - \frac{Q_f}{r}.$$

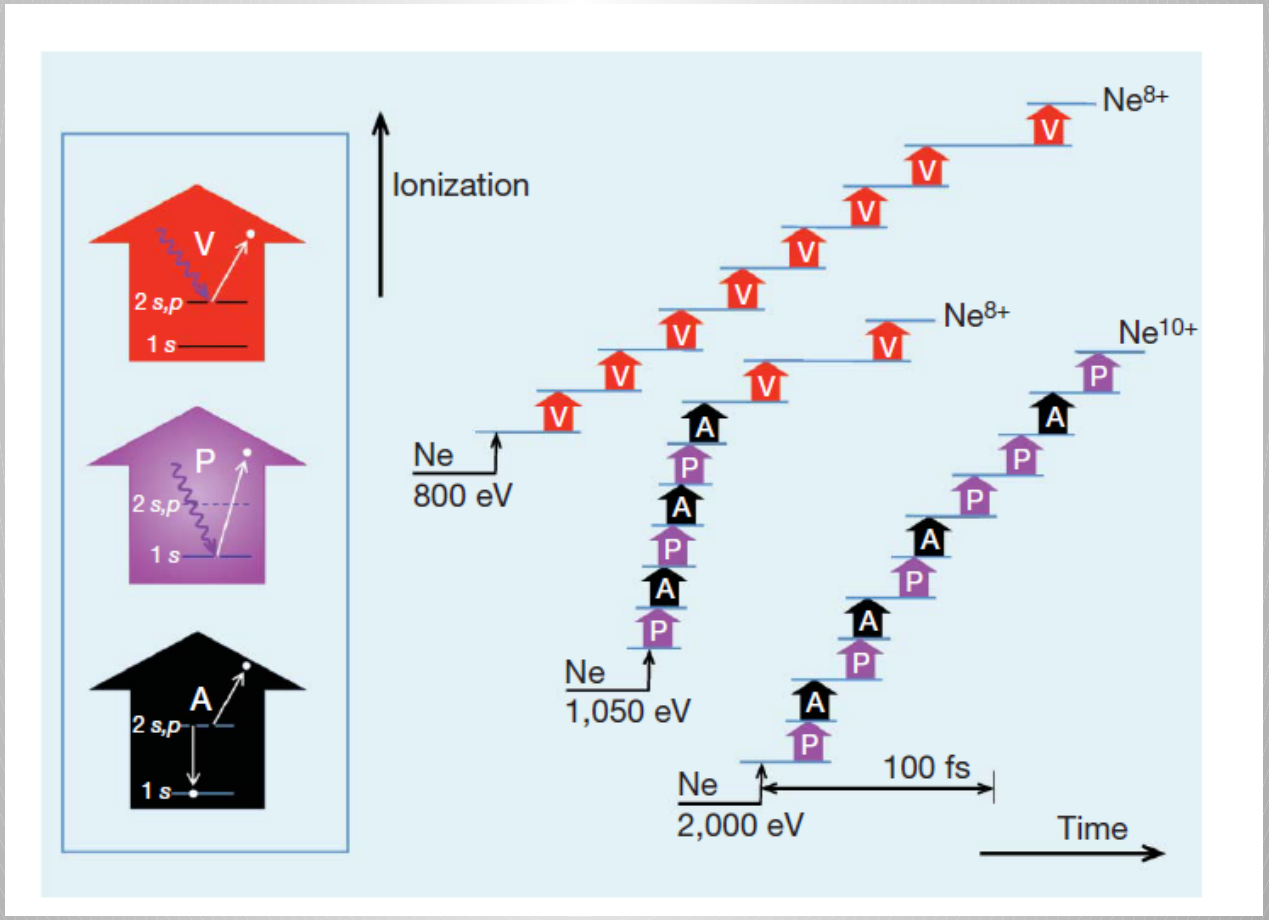
Photon Beam Parameters	Symbol	hard x-rays	soft x-rays	short pulse soft	short pulse hard	unit
Fundamental wavelength	λ_r	6.2-1.3	43.7-6.2	43.7-6.2	6.2-1.3	Å
Photon energy	$\hbar\omega$	2000-9600	285-2000	285-2000	2000-9600	eV
Final linac e^- energy	γmc^2	6.7-14.7	2.5-6.7	2.5-6.7	6.7-14.7	GeV
FEL 3-D gain length	L_G	3.3	1.5	~1.5	~3.3	m
Photons per pulse	N_γ	2	20	0.5	0.2	10^{12}
Peak brightness	B_{pk}	20	0.3	?	?	10^{32} §
Average brightness (120 Hz)	$\langle B \rangle$	160	8	?	?	10^{20} §
SASE bandwidth (fwhm)	$\Delta\omega/\omega$	~0.2-0.5	~0.2-1.0	?	?	%
Final pulse duration (fwhm)	$\Delta\tau_f$	50-250	70-400	<10	<10	fs



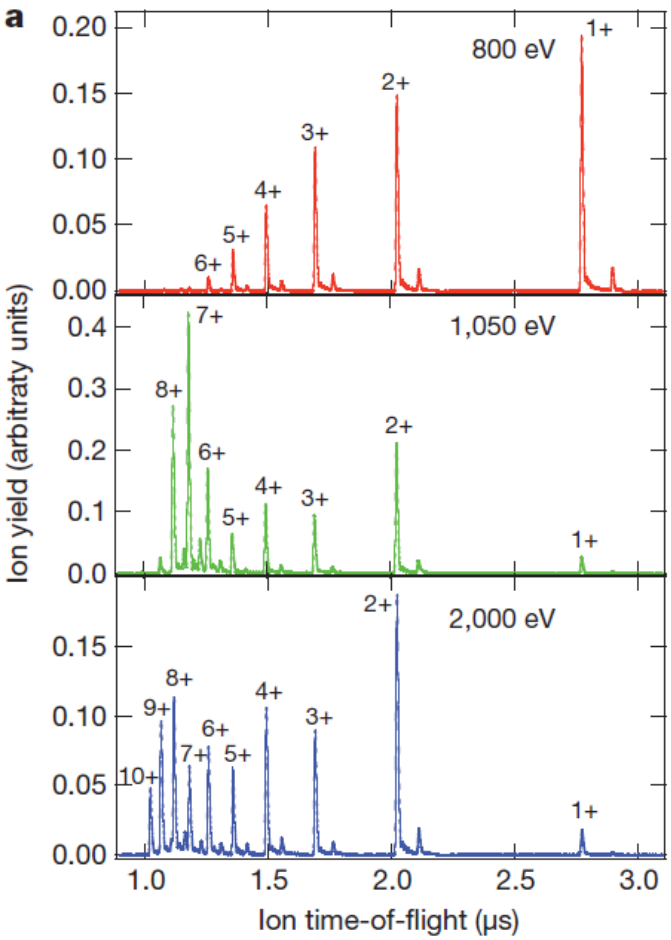
LCLS

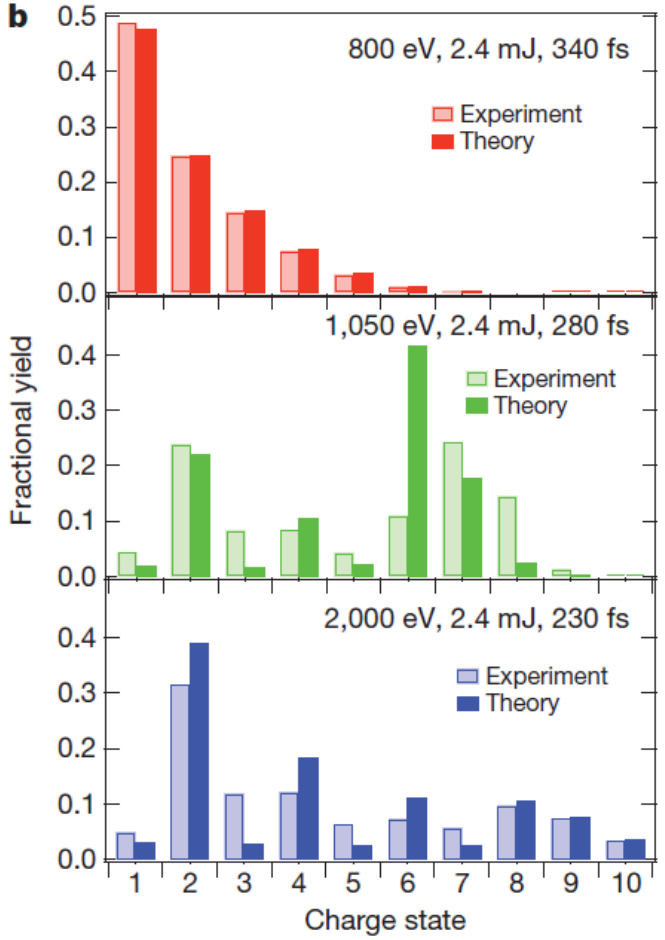
SLAC, Stanford, CA, USA

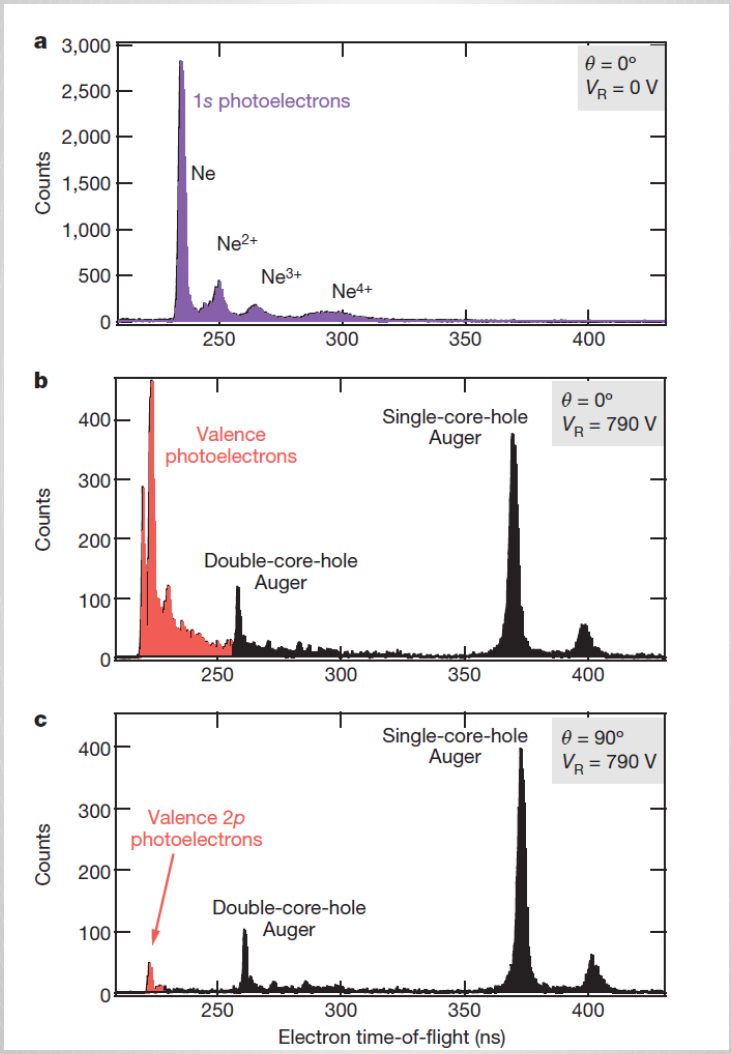
Femtosecond electronic response of atoms to ultra-intense X-rays

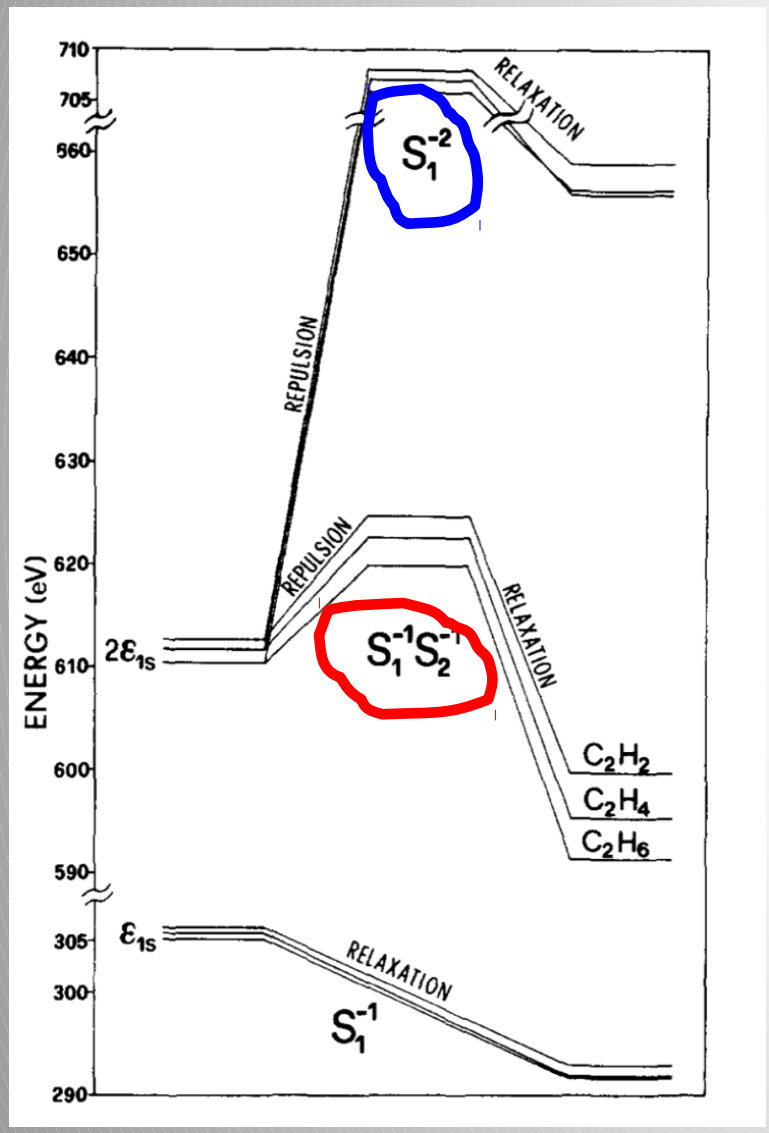


L.Young et al., Nature 466, 56 (2010)


a
800 eV
1,050 eV
2,000 eV
1+
2+
3+
4+
5+
6+
7+
8+
9+
10+
Ion yield (arbitraty units)
Ion time-of-flight (μs)


b
800 eV, 2.4 mJ, 340 fs
1,050 eV, 2.4 mJ, 280 fs
2,000 eV, 2.4 mJ, 230 fs
Experiment
Theory
Fractional yield
Charge state


a
3,000
2,500
2,000
1,500
1,000
500
0
Counts
1s photoelectrons
Ne
Ne2+
Ne3+
Ne4+
θ = 0°
VR = 0 V
250
300
350
400
b
400
300
200
100
0
Counts
Valence photoelectrons
Double-core-hole Auger
Single-core-hole Auger
θ = 0°
VR = 790 V
250
300
350
400
c
400
300
200
100
0
Counts
Valence 2p photoelectrons
Double-core-hole Auger
Single-core-hole Auger
θ = 90°
VR = 790 V
250
300
350
400
Electron time-of-flight (ns)



DCH Single-Site (SS)

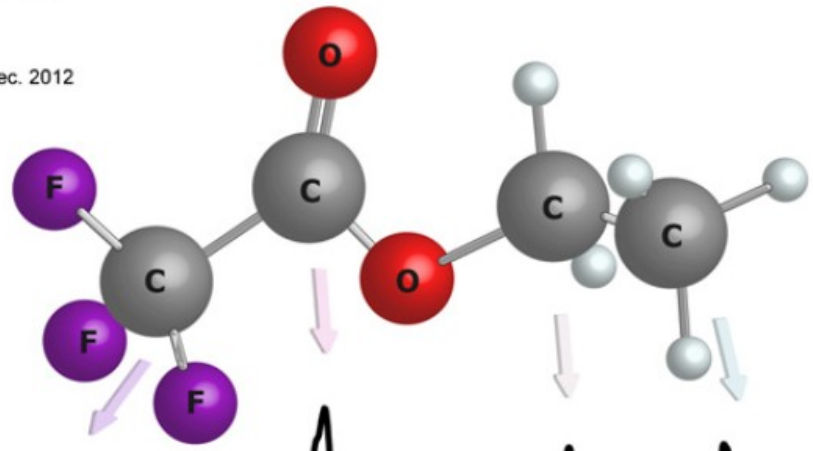
DCH Two-Site (TS)

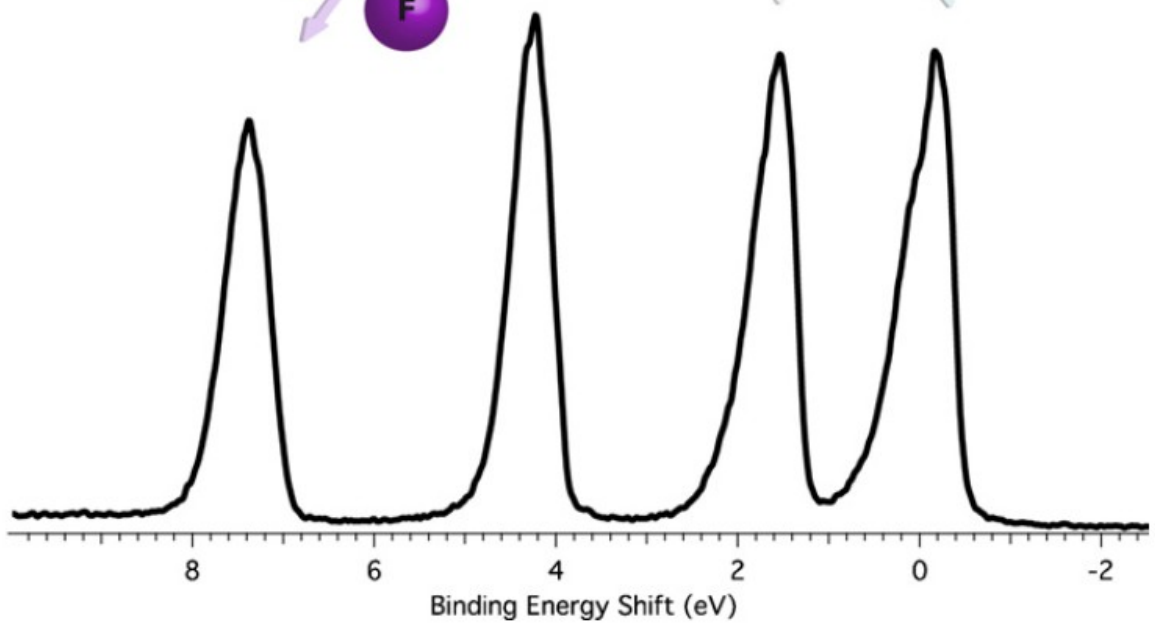
Substantially enhanced chemical sensitivity

L.S.Cederbaum et al, J.Chem.Phys. 85, (1986) 6513

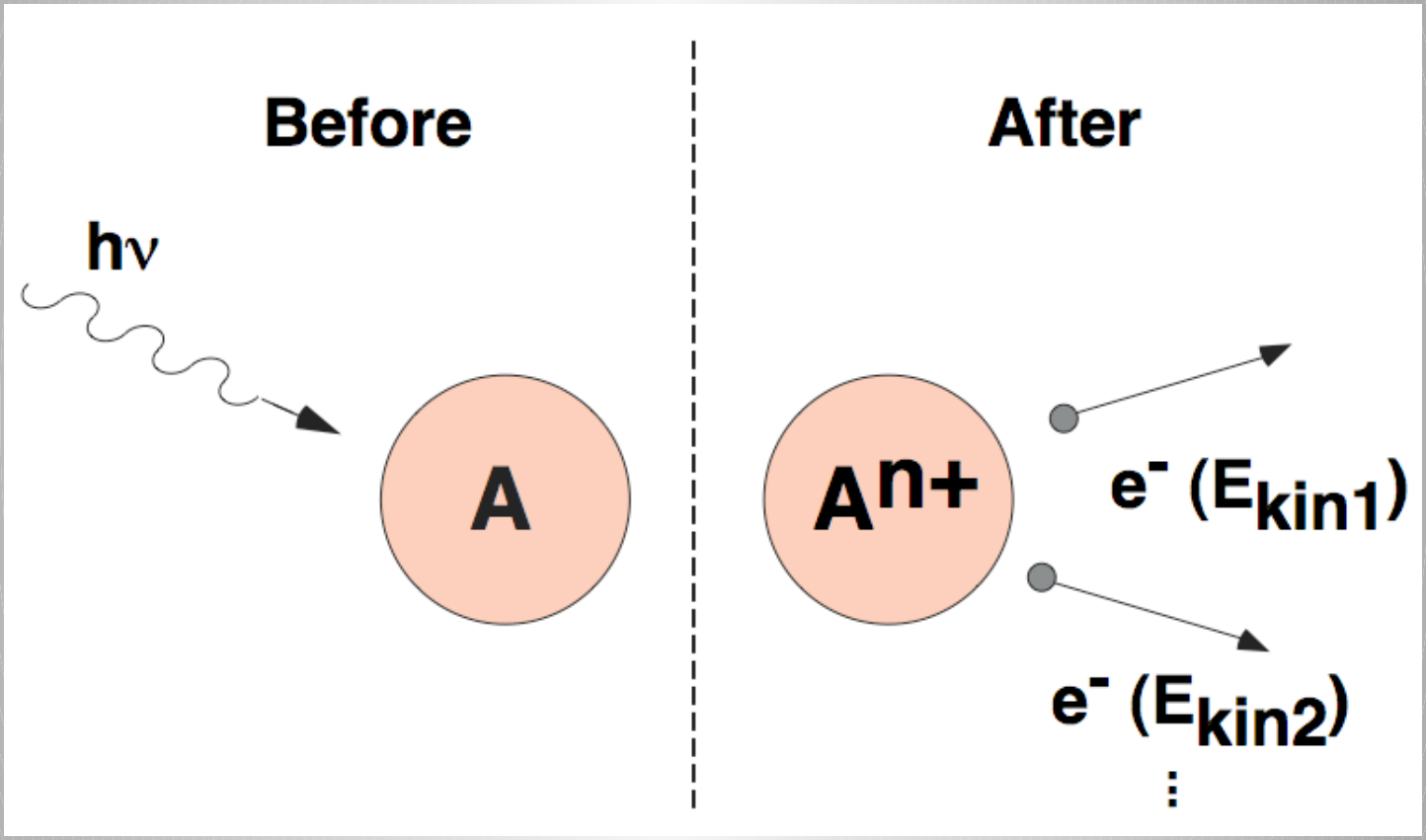
Ethyl trifluoroacetate
C1s XPS

Travnikova *et al.* J.El.Spec. 2012





Single Photon – Multiple Ionisation

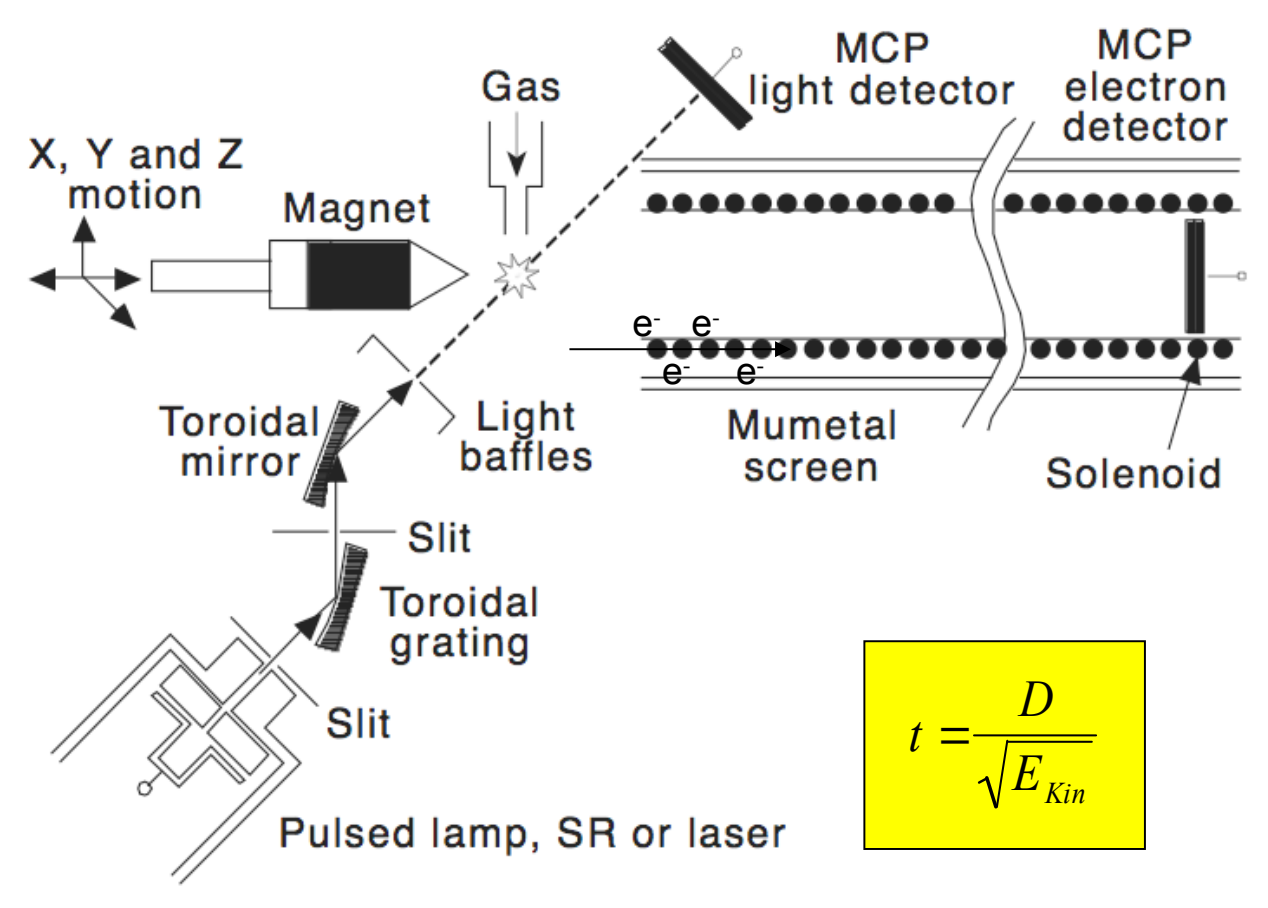


$$E_{B1} + E_{B2} (+ \ldots) = h\nu - E_{kin1} - E_{kin2} (- \ldots)$$

Double (multiple) ionisation energy (DIP, …)

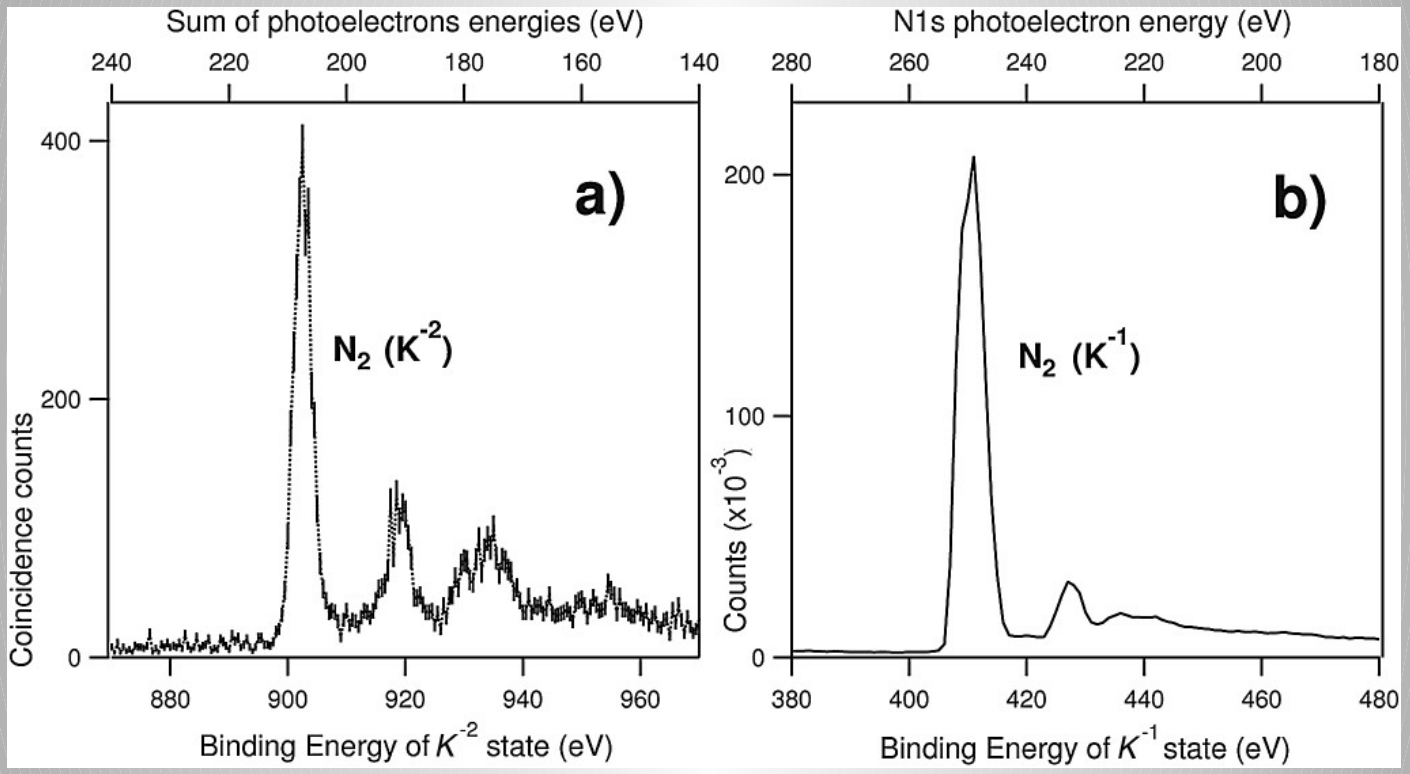
Time-Of-Flight Magnetic Bottle Multi-Electron Spectrometer

"4π" correlation device

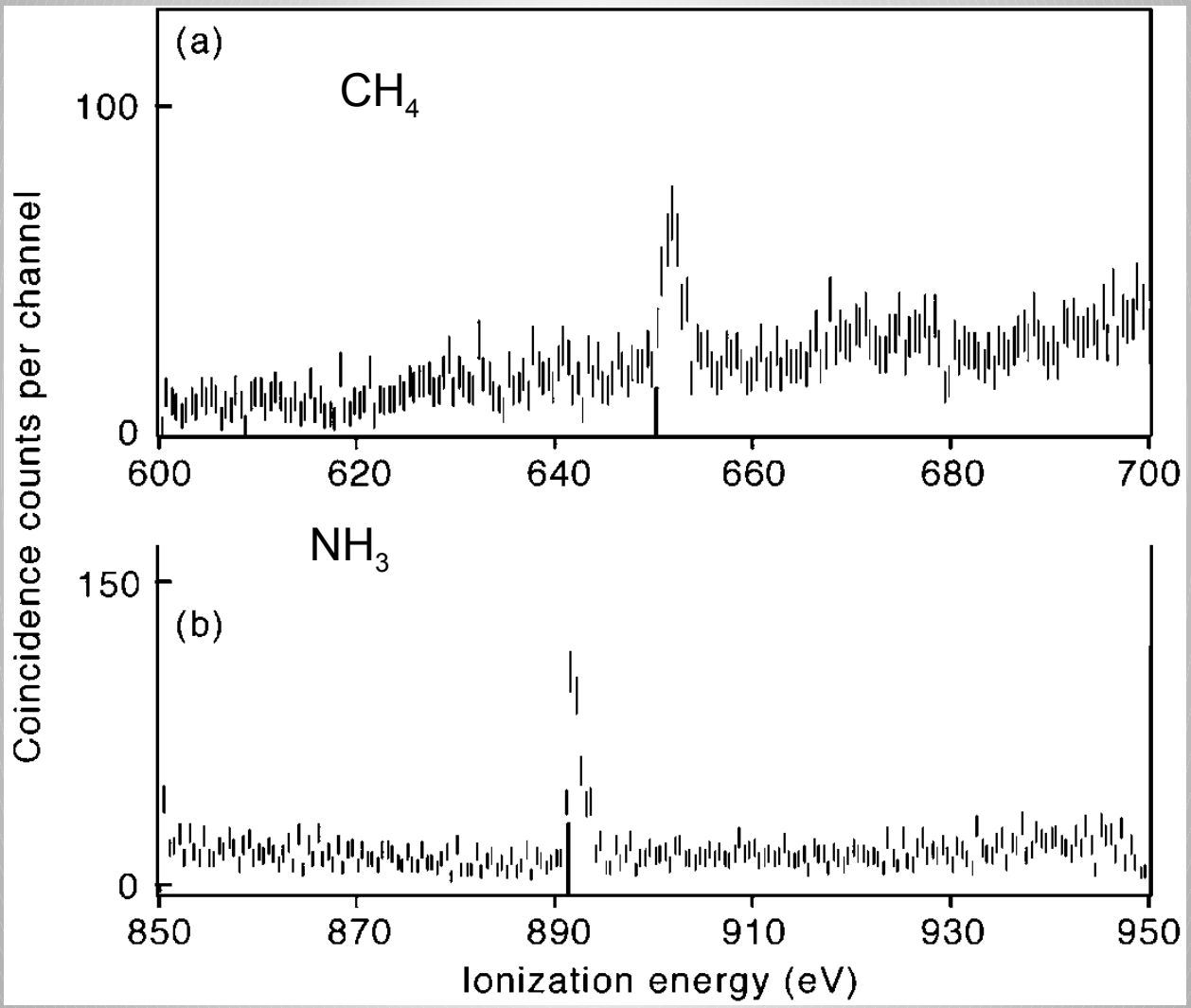


Pulsed light source: He-lamp, SR, fs-laser system, FEL

J.H.D. Eland *et al*., Phys. Rev. Lett. **90**, 053003 (2003)

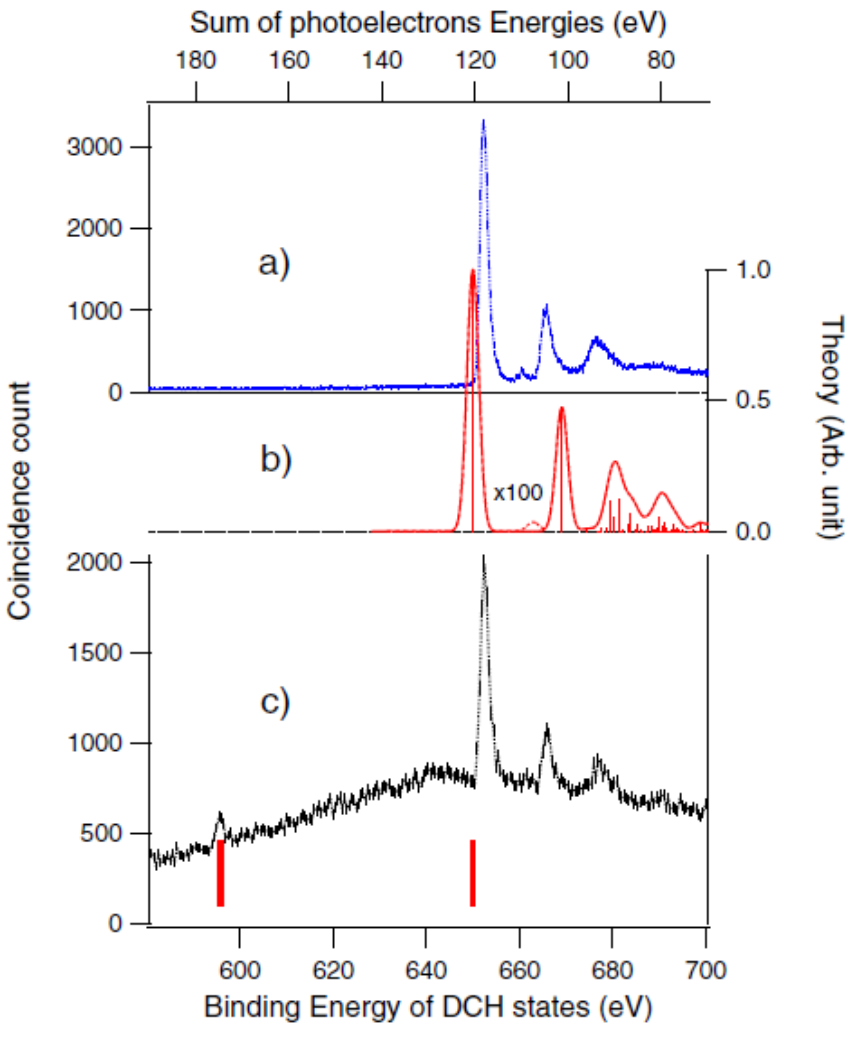


P.Lablanquie, F.Penent,J.Palaudoux, L.Andric, P.Selles, S.Carniato, K.Bučar, M.Žitnik, M. Huttula, J.H.D.Eland, E.Shigemasa, K.Soejima, Y.Hikosaka, I.H.Suzuki, M.Nakano and K.Ito, PRL 106, 063003 (2011)



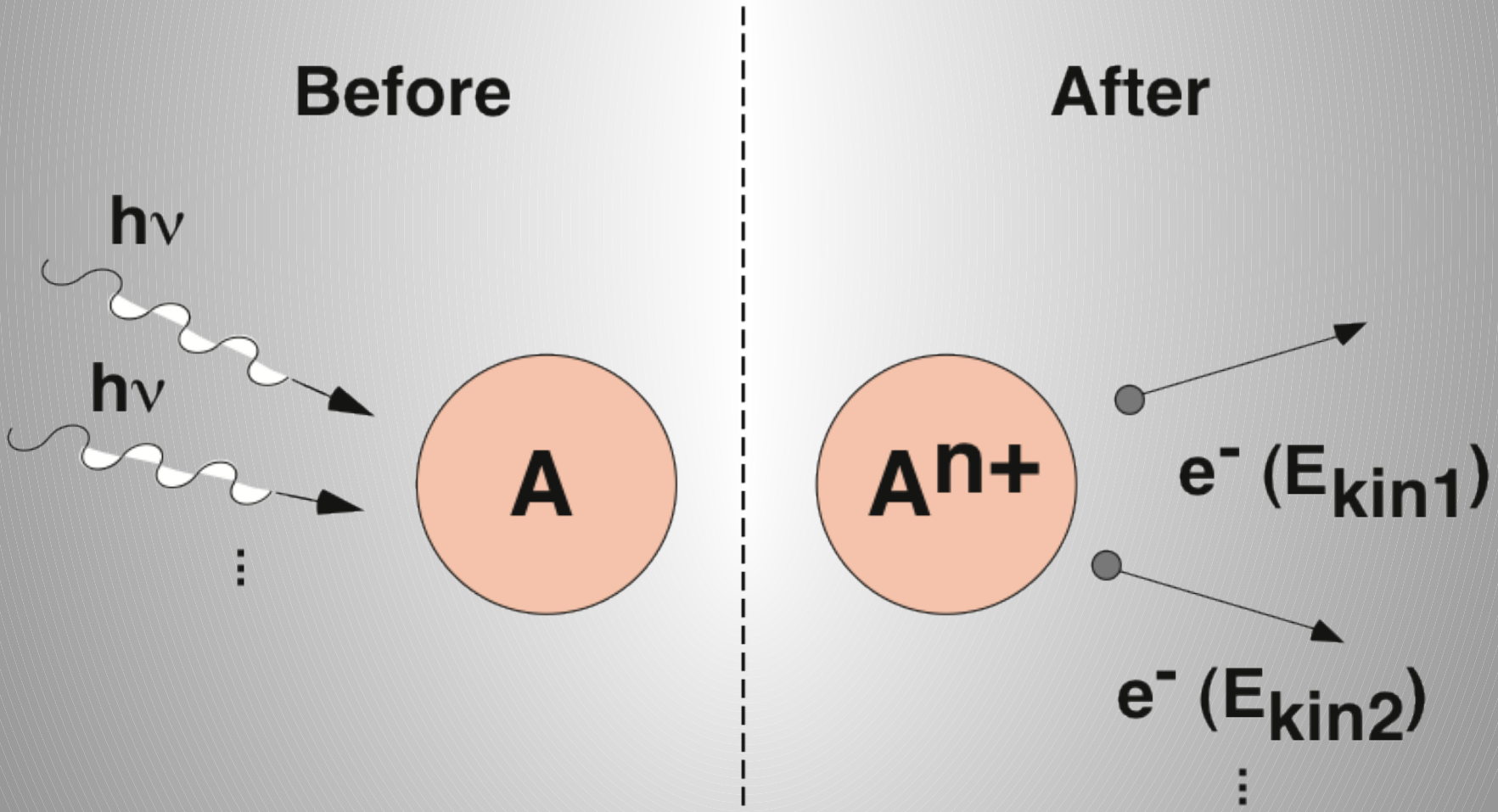
J.H.D.Eland, M.Tashiro, P.Linusson, M.Ehara, K.Ueda and R. Feifel, PRL 105, 213005 (2010)

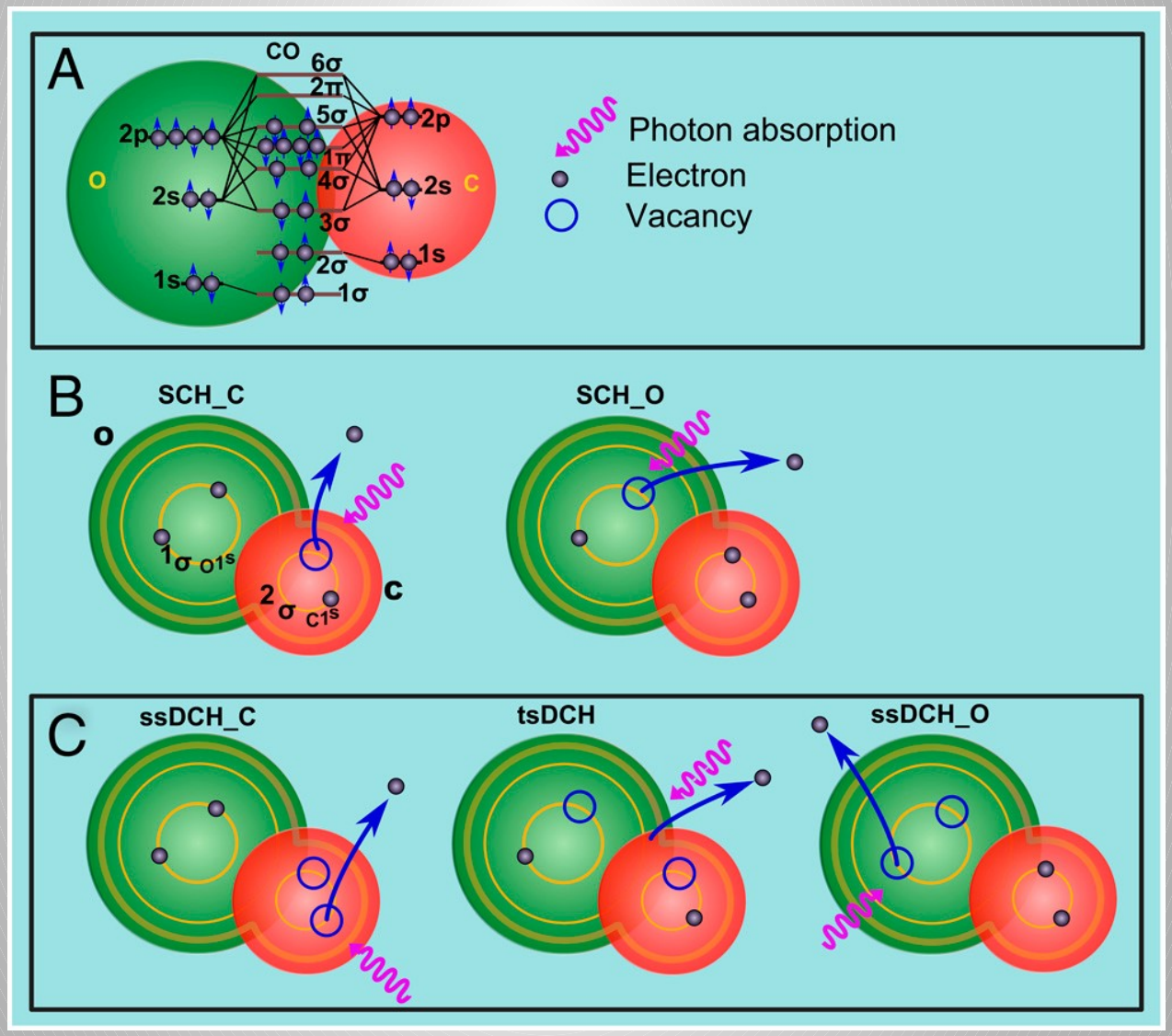
C_2H_2



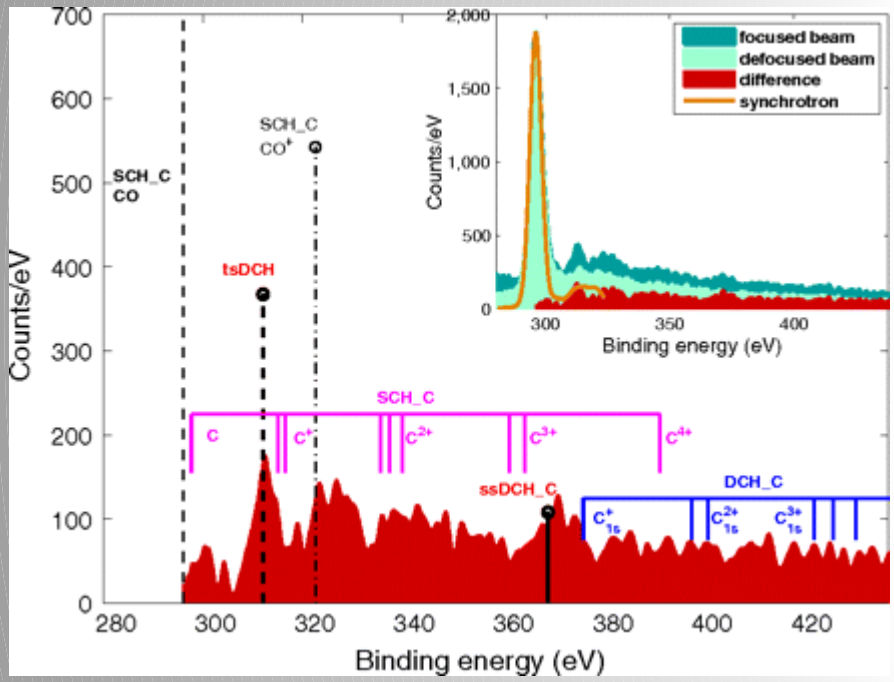
P. Lablanquie,T. P. Grozdanov, M. Žitnik, S. Carniato, P. Selles, L. Andric, J. Palaudoux, F. Penent, H. Iwayama, E. Shigemasa, Y. Hikosaka, K. Soejima, M. Nakano, I. H. Suzuki and K. Ito, PRL 107, 193004 (2011)

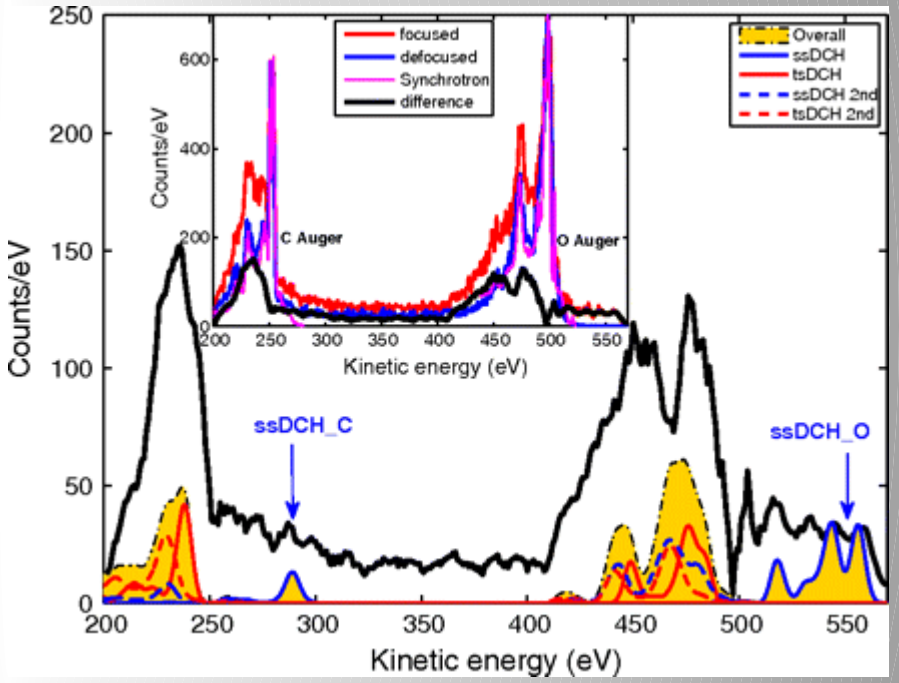
Few Photon – Multiple Ionisation




A
CO
6σ
2π
5σ
1π
4σ
3σ
2σ
1σ
2p
2s
1s
O
C
Photon absorption
Electron
Vacancy
B
SCH_C
SCH_O
O
C
1σ O1s
2σ C1s
C
ssDCH_C
tsDCH
ssDCH_O

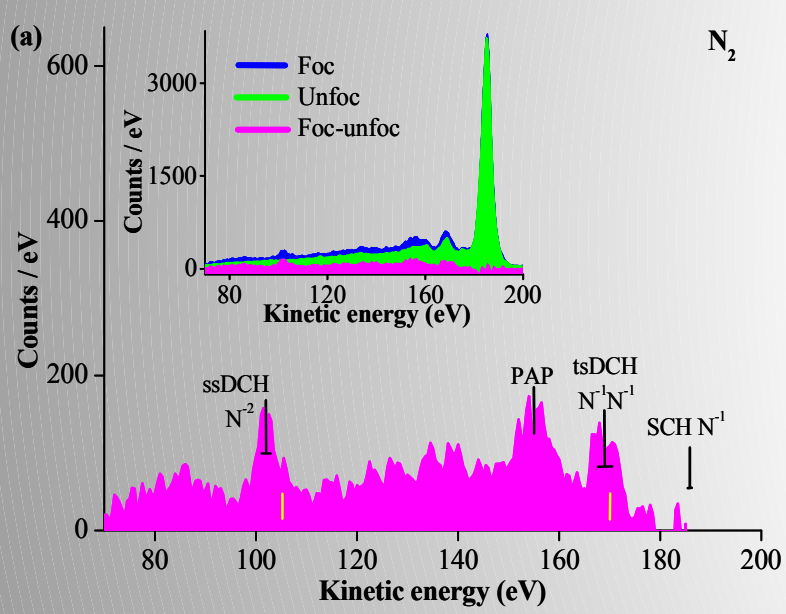
DCH measurements: CO

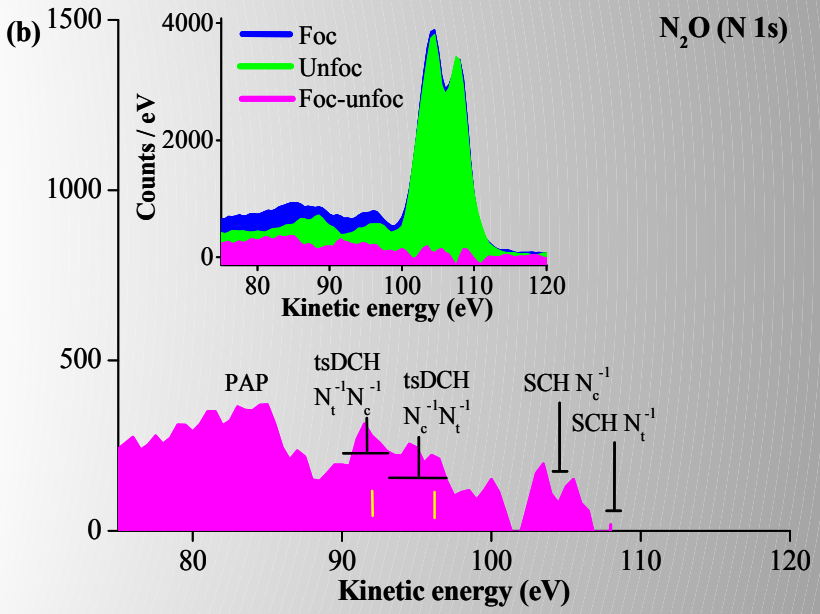




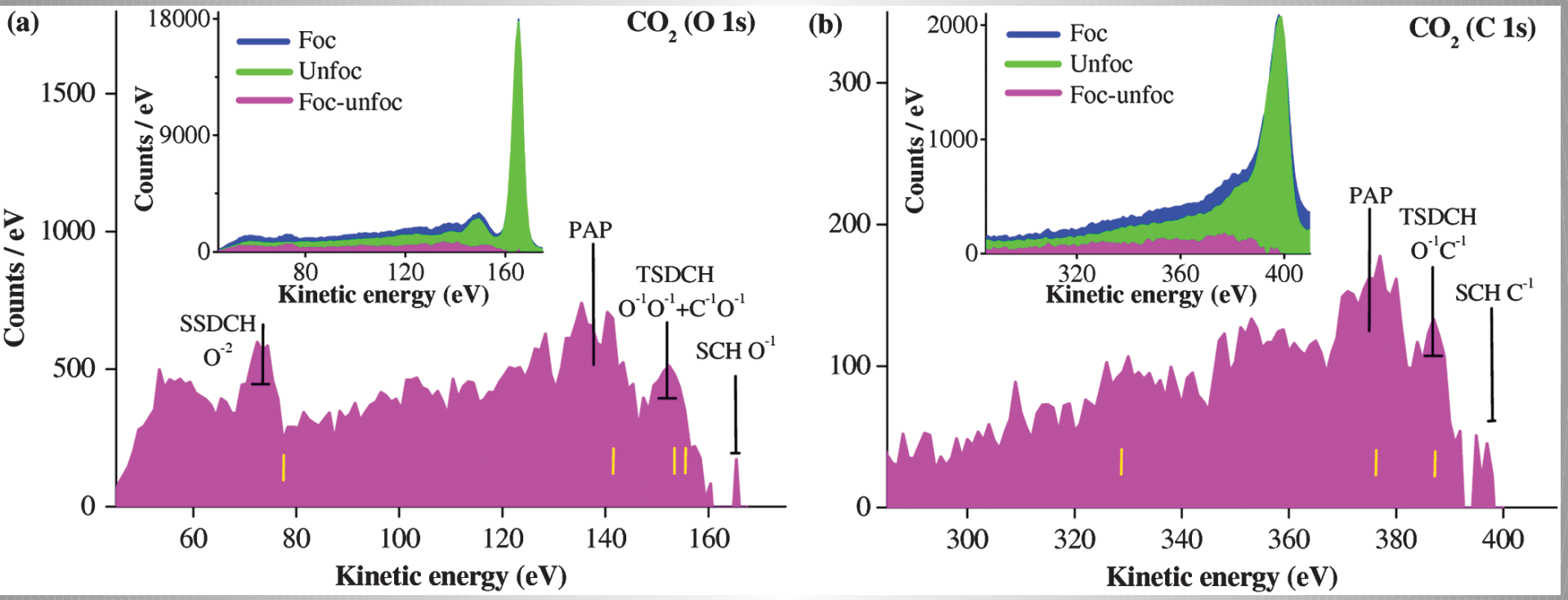
N. Berrah, ……M.N.Piancastelli *et al.*,
PNAS 108, 16912 (2011)

Challenge remains:
TS-DCH → CVV/VVVV Auger
and Auger from other channels overlap





P. Salén, P. van der Meulen, H.T. Schmidt, R.D. Thomas, M. Larsson, R. Feifel, M.N. Piancastelli, L.Fang, B. Murphy, T. Osipov, N. Berrah, E. Kukk, K. Ueda, J.D. Bozek, C. Bostedt, S. Wada, R. Richter, V. Feyer and K.C. Prince, PRL 108, 153003 (2012)

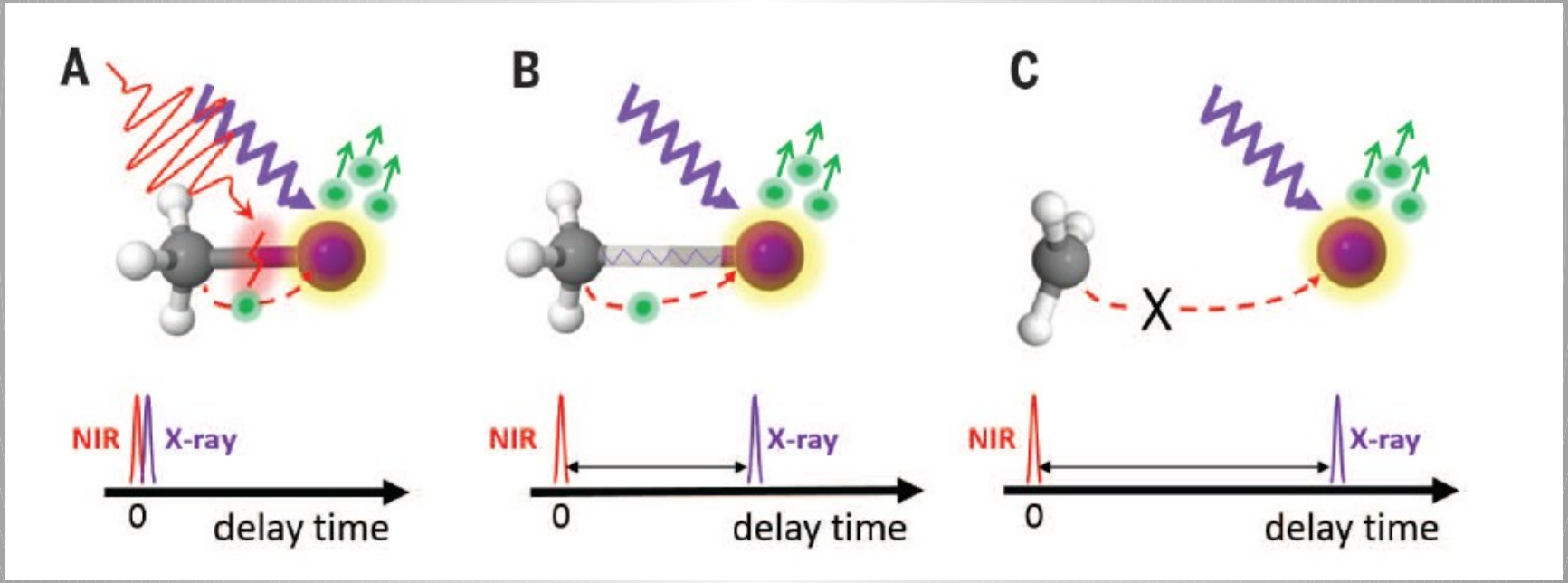


P. Salén, P. van der Meulen, H.T. Schmidt, R.D. Thomas, M. Larsson, R. Feifel, M.N. Piancastelli, L.Fang, B. Murphy, T. Osipov, N. Berrah, E. Kukk, K. Ueda, J.D. Bozek, C. Bostedt, S. Wada, R. Richter, V. Feyer and K.C. Prince, PRL 108, 153003 (2012)

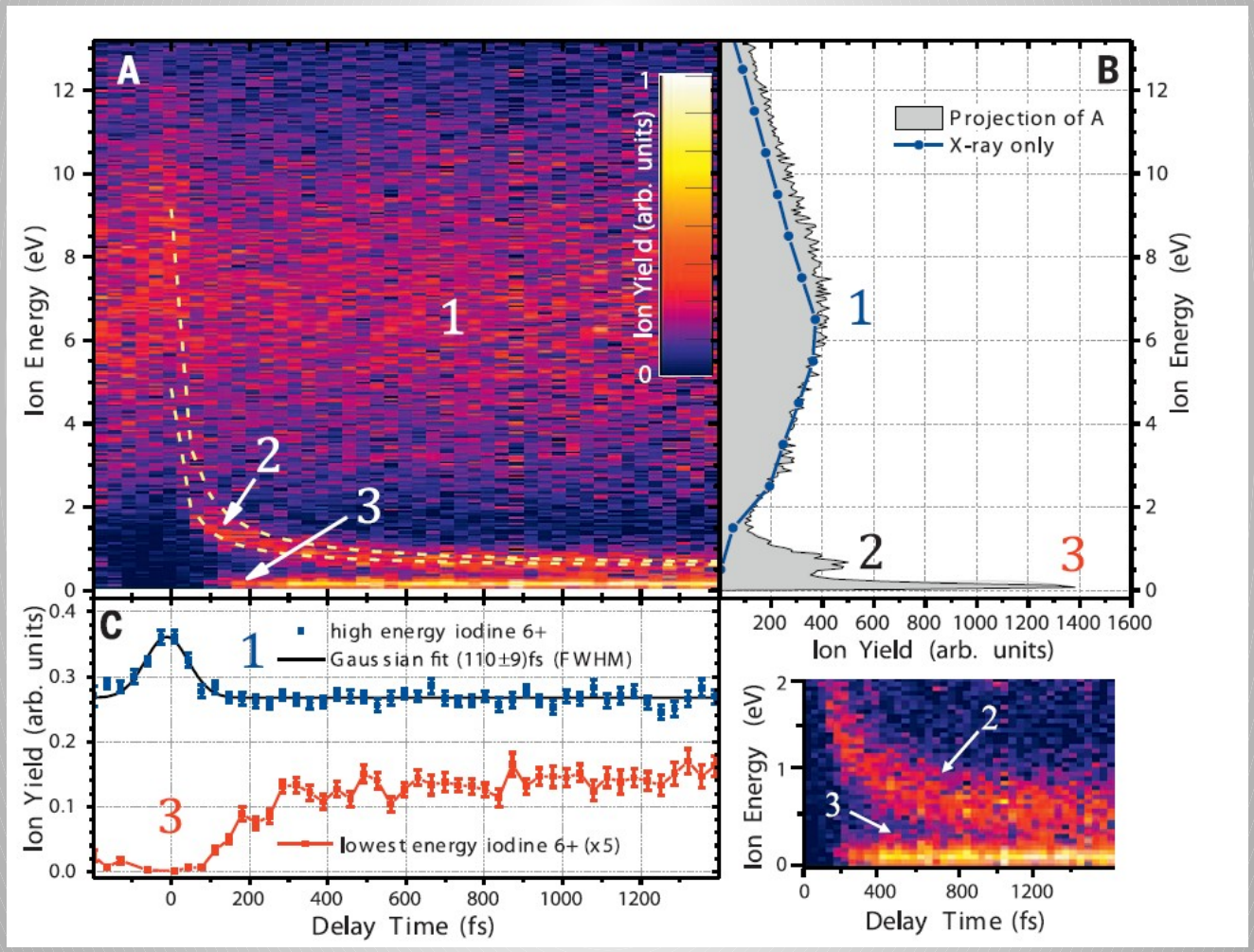
Molecule	IP(S^{-1}) (eV)	DIP(S^{-2}) (eV)	DIP(S_i^{-1}, S_j^{-1}) (eV)	ΔE_1(S^{-2}) (eV)	ΔE_2(S_i^{-1}, S_j^{-1}) (eV)	IRC (eV)
N_2	(N^{-1})	(N^{-2})	($N^{-1}N^{-1}$)	(N^{-2})	($N^{-1}N^{-1}$)	($N^{-1}N^{-1}$)
Exp.	409.9 ± 0.3 [29]	903.2 ± 1.1	836.2 ± 1.6	83.4 ± 1.1	16.4 ± 1.6	−3.29 ± 1.6
Theory [6]	411.0	901.2	836.4	79.2	14.3	−0.65
N_2O (N_t)	(N_t^{-1})	(N_t^{-2})	($N_c^{-1}N_t^{-1}$)	(N_t^{-2})	($N_c^{-1}N_t^{-1}$)	($N_c^{-1}N_t^{-1}$)
Exp.	409.0 ± 0.5		834.2 ± 2.1		12.7 ± 2.1	0.09 ± 2.1
Theory [6]	408.6	893.9	833.2	76.7	12.1	1.11
N_2O (N_c)	(N_c^{-1})	(N_c^{-2})	($N_t^{-1}N_c^{-1}$)	(N_c^{-2})	($N_t^{-1}N_c^{-1}$)	($N_t^{-1}N_c^{-1}$)
Exp.	412.5 ± 0.5 [29]		834.2 ± 1.6		12.7 ± 1.6	0.09 ± 1.6
Theory [6]	412.5	902.3	833.2	77.3	12.1	1.11
CO_2 (O 1s)	(O^{-1})	(O^{-2})		(O^{-2})	($O^{-1}O^{-1}$ + $C^{-1}O^{-1}$)	
Exp.	540.6 ± 0.5 [30]	1173.2 ± 1.6		92.0 ± 1.5	12.8 ± 1.6	
Theory [6]	542.9	1171.9		86.2	9.1	
CO_2 (C 1s)	(C^{-1})	(C^{-2})	($O^{-1}C^{-1}$)	(C^{-2})	($O^{-1}C^{-1}$)	($O^{-1}C^{-1}$)
Exp.	296.8 ± 0.5 [30]		848.6 ± 1.6		11.2 ± 1.6	1.21 ± 1.6
Theory [6]	297.6	664.6	851.2	69.3	10.6	1.79
CO (C 1s)	(C^{-1})	(C^{-2})	($O^{-1}C^{-1}$)	(C^{-2})	($O^{-1}C^{-1}$)	($O^{-1}C^{-1}$)
Exp. [8]	296.5 ± 0.5	667.9 ± 3.6	855.3 ± 1.2	74.9 ± 4.0	16.3 ± 1.2	−3.53 ± 1.2
Theory [6]	296.4	664.4	855.2	71.7	15.9	−2.8

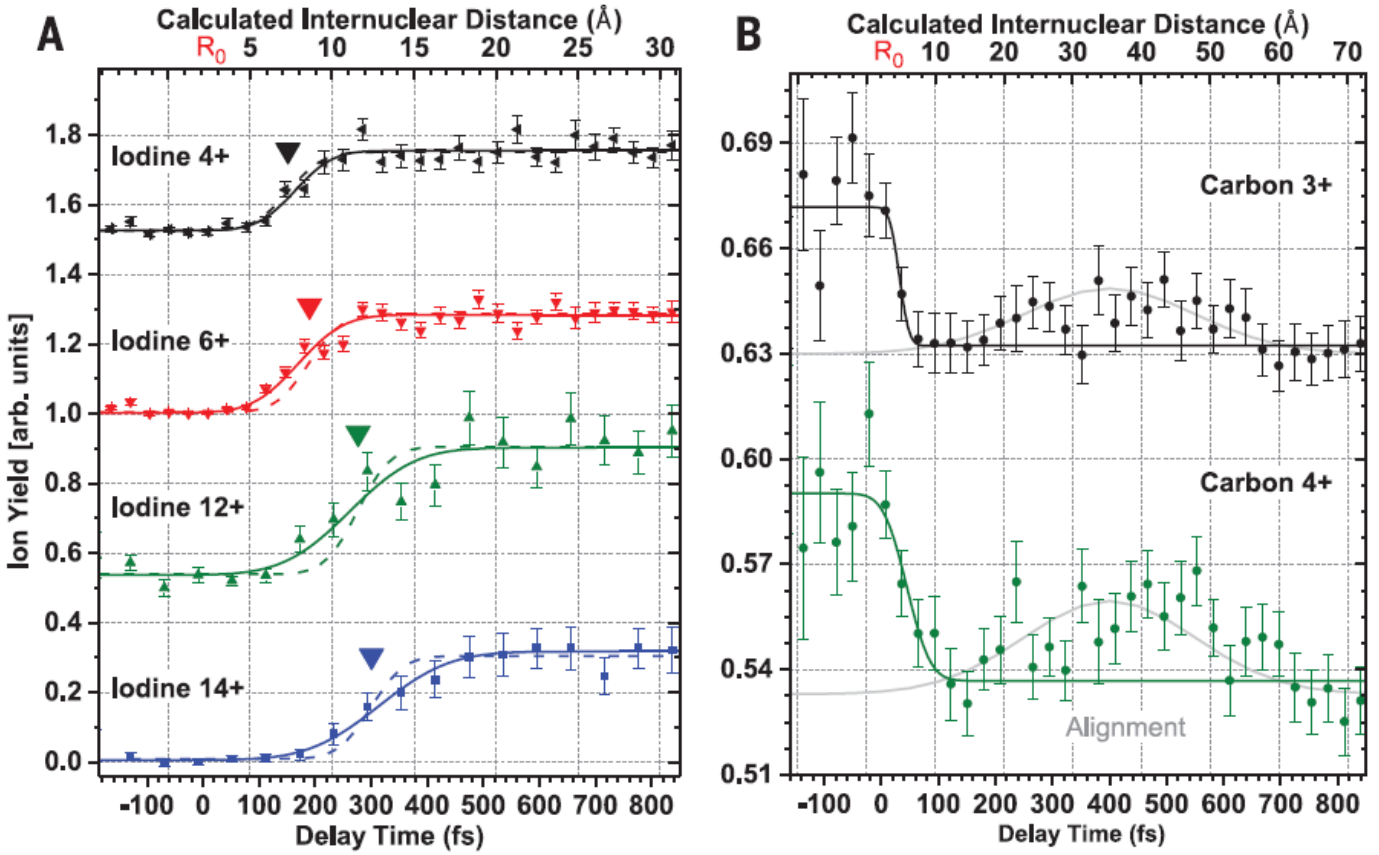
P. Salén, P. van der Meulen, H.T. Schmidt, R.D. Thomas, M. Larsson, R. Feifel, M.N. Piancastelli, L.Fang, B. Murphy, T. Osipov, N. Berrah, E. Kukk, K. Ueda, J.D. Bozek, C. Bostedt, S. Wada, R. Richter, V. Feyer and K.C. Prince, PRL 108, 153003 (2012)

Imaging charge transfer in iodomethane upon x-ray photoabsorption

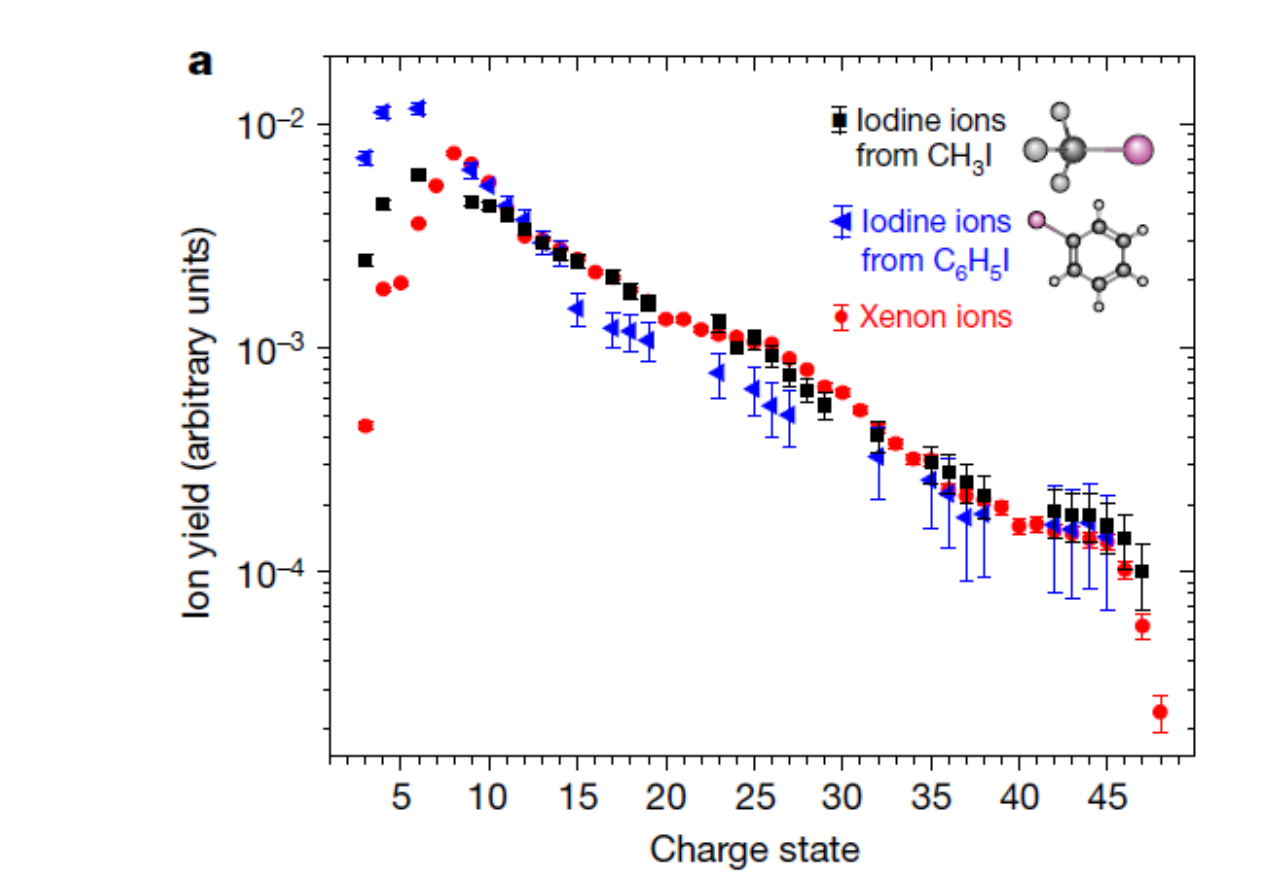


B.Erk et al., Science 345, 288 (2014)

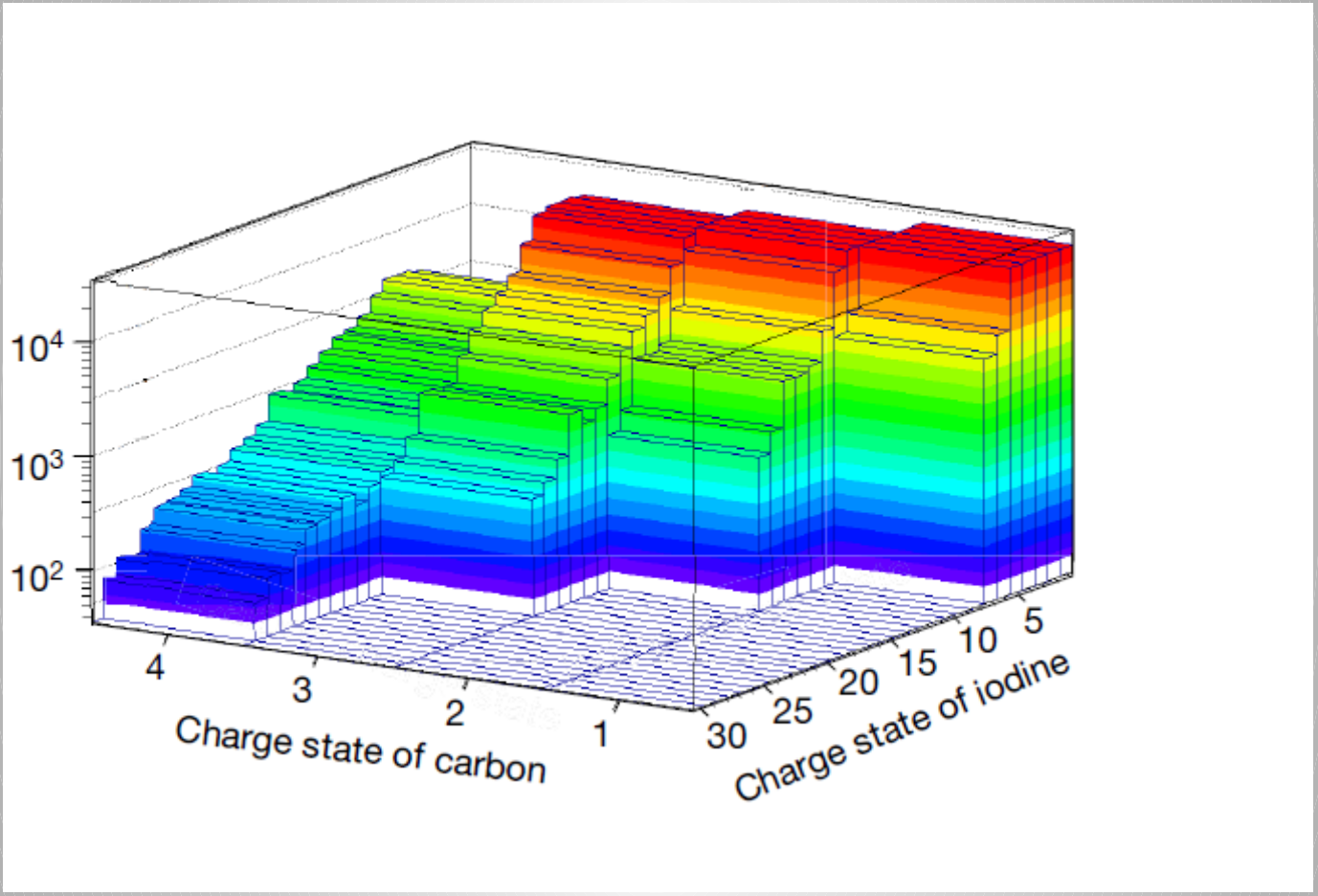

A
B
C
Ion Energy (eV)
Ion Yield (arb. units)
Delay Time (fs)
Projection of A
X-ray only
high energy iodine 6+
Gaussian fit (110±9)fs (FWHM)
lowest energy iodine 6+ (x5)
1
2
3

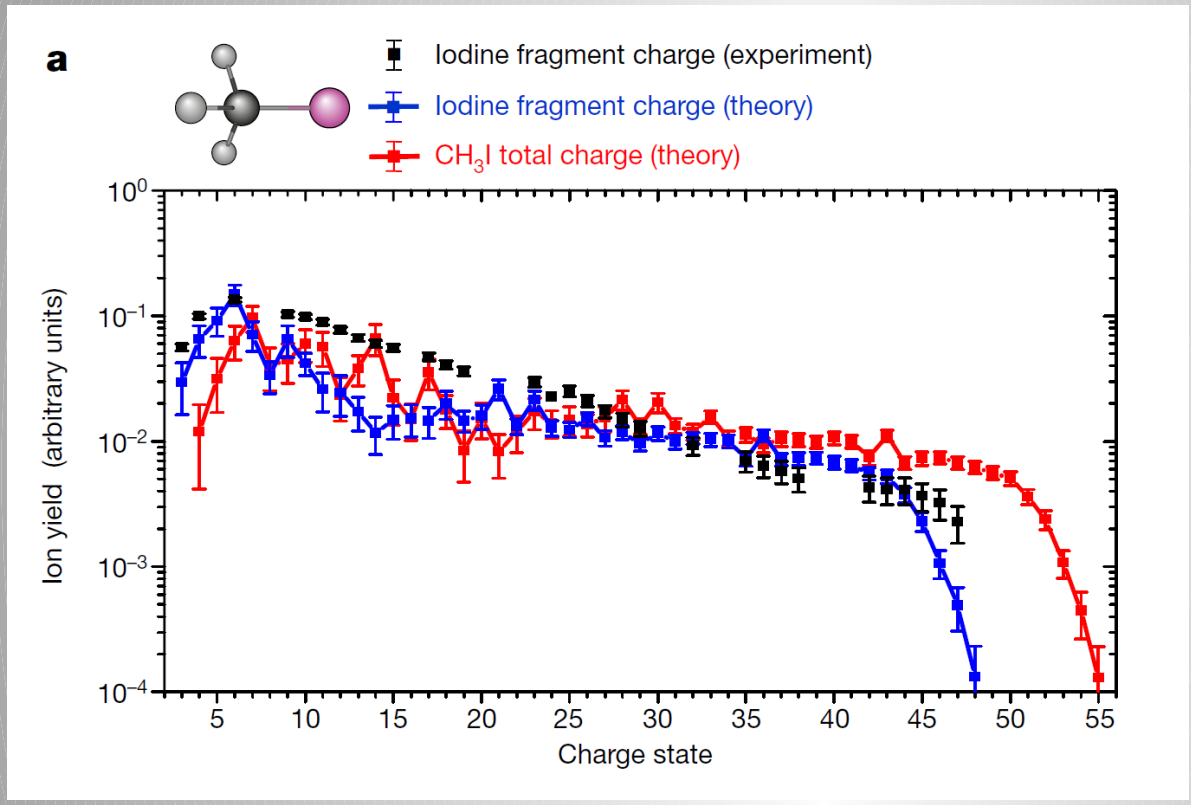

A
Calculated Internuclear Distance (Å)
R0 5 10 15 20 25 30
Iodine 4+
Iodine 6+
Iodine 12+
Iodine 14+
Ion Yield [arb. units]
Delay Time (fs)
B
Calculated Internuclear Distance (Å)
R0 10 20 30 40 50 60 70
Carbon 3+
Carbon 4+
Alignment
Delay Time (fs)

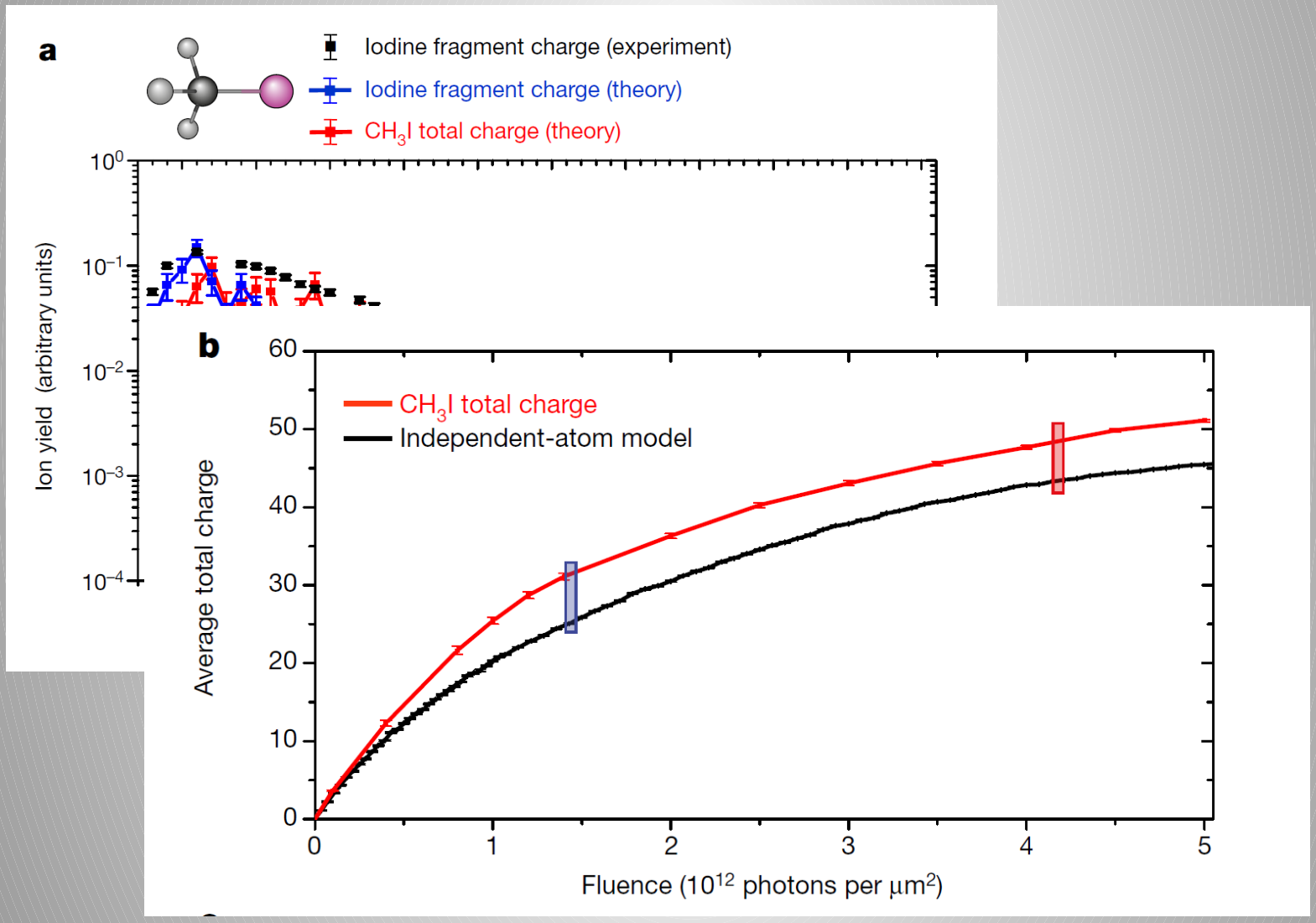
Femtosecond response of polyatomic molecules to ultra-intense hard X-rays

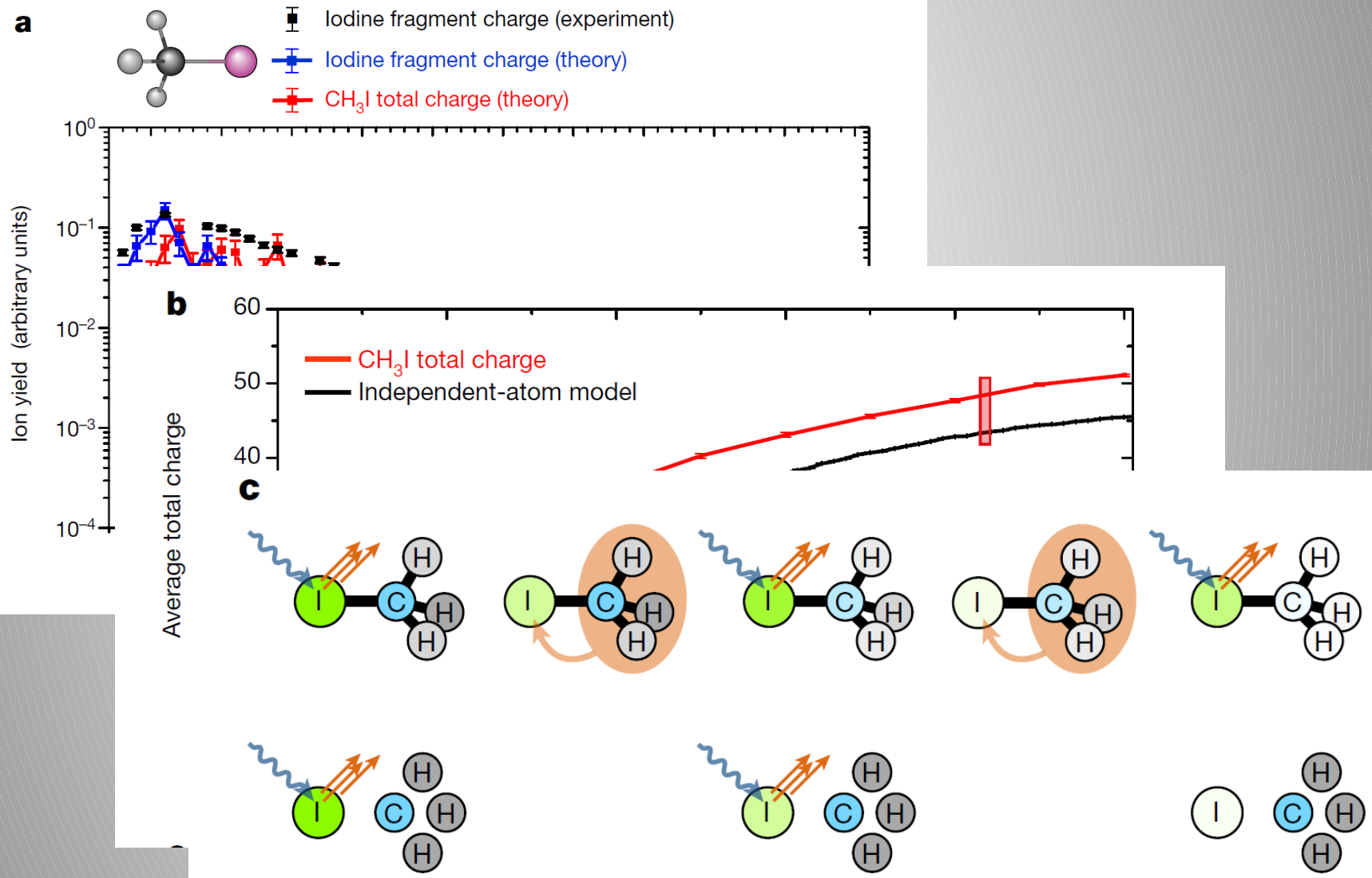


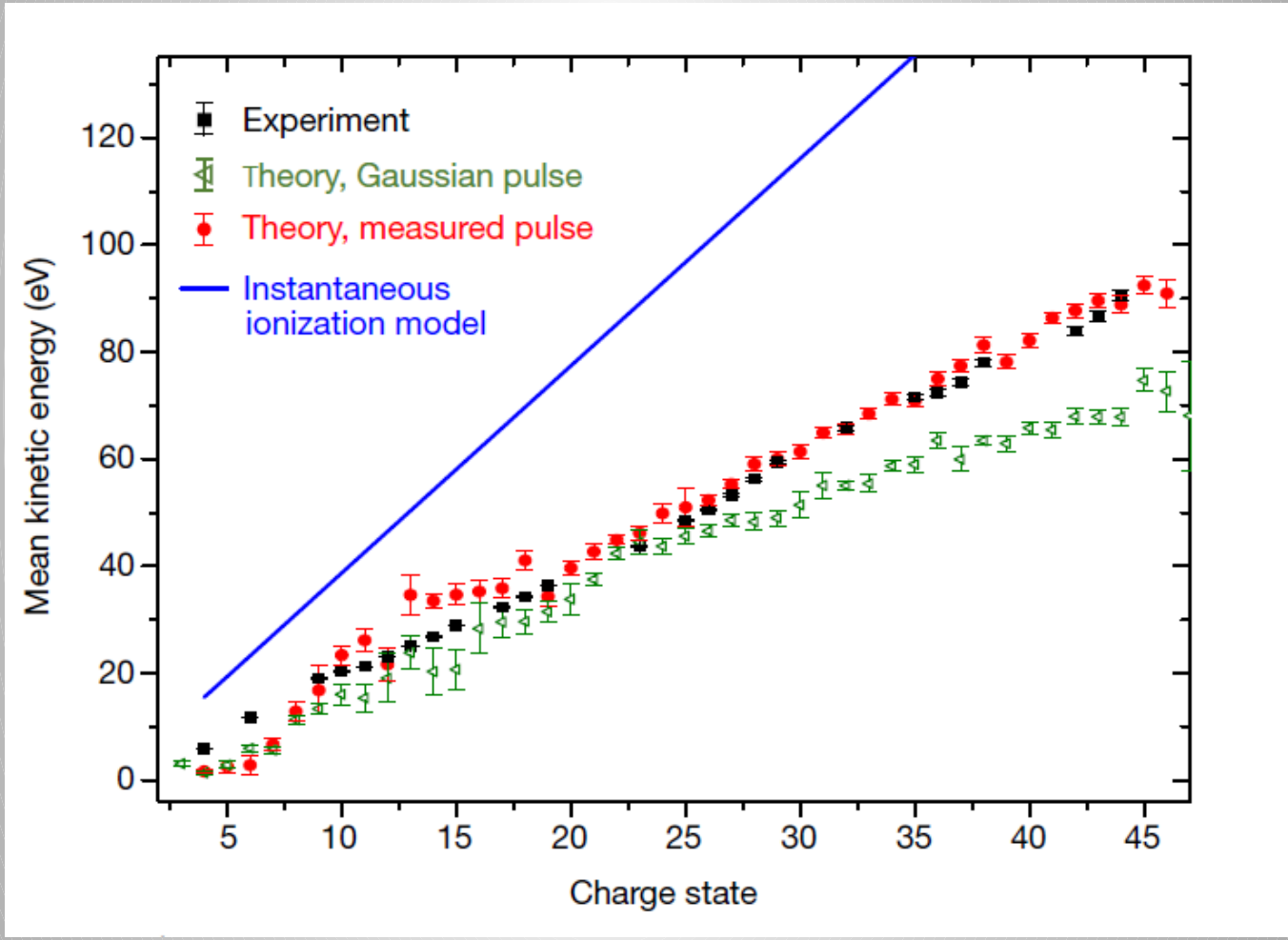
A. Rudenko et al, Nature Comm. 546, (2017) 129


10^4
10^3
10^2
4
3
2
1
Charge state of carbon
30
25
20
15
10
5
Charge state of iodine


a
Iodine fragment charge (experiment)
Iodine fragment charge (theory)
CH3I total charge (theory)
Ion yield (arbitrary units)
10^0
10^-1
10^-2
10^-3
10^-4
5
10
15
20
25
30
35
40
45
50
55
Charge state


a
Iodine fragment charge (experiment)
Iodine fragment charge (theory)
CH3I total charge (theory)
Ion yield (arbitrary units)
10^0
10^-1
10^-2
10^-3
10^-4
b
CH3I total charge
Independent-atom model
Average total charge
0
10
20
30
40
50
60
0
1
2
3
4
5
Fluence (10^12 photons per μm^2)

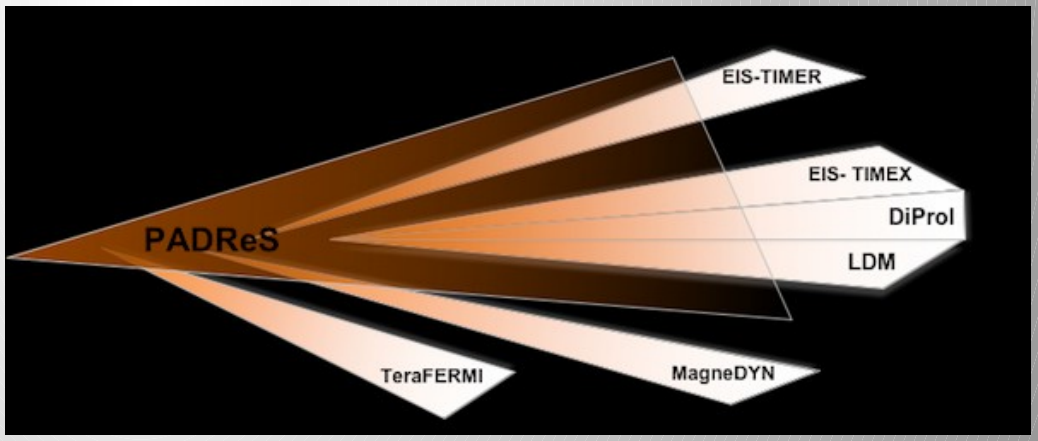

a
Iodine fragment charge (experiment)
Iodine fragment charge (theory)
CH3I total charge (theory)
Ion yield (arbitrary units)
10^0
10^−1
10^−2
10^−3
10^−4
b
60
50
40
CH3I total charge
Independent-atom model
Average total charge
c
H
C
I


Experiment
Theory, Gaussian pulse
Theory, measured pulse
Instantaneous ionization model
Mean kinetic energy (eV)
Charge state
0
20
40
60
80
100
120
5
10
15
20
25
30
35
40
45

FERMI

Elettra, Trieste, Italy

Aerial view



Beam transport and beamlines

FERMI

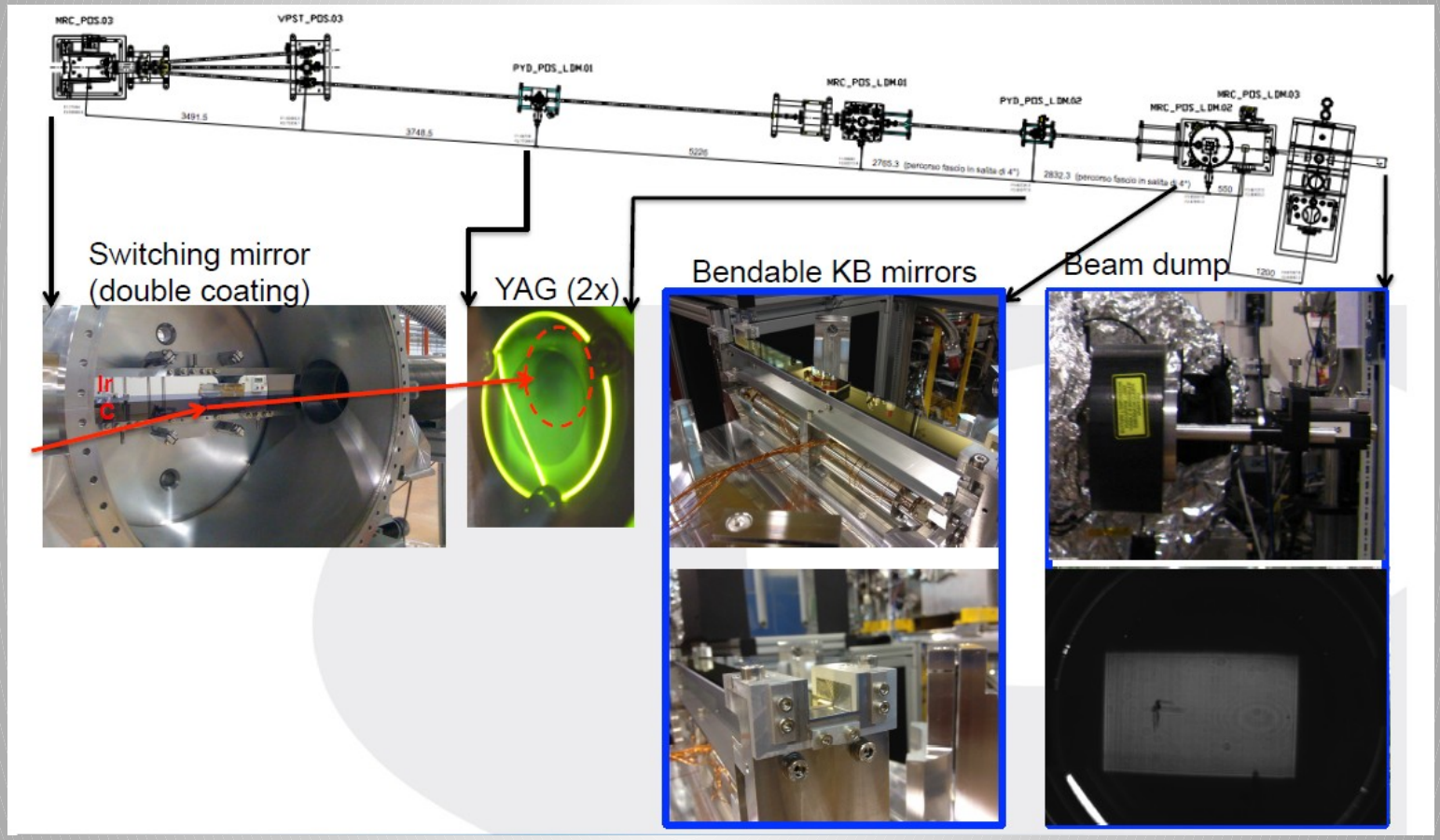
	λ seed	261.60	(±0.5) nm		4.7394	eV
harmonic stage1↓	1st stage wl (nm)	2nd stage wl (nm)				
4	65.40	21.80	16.35	13.08	10.90	9.34
5	52.32	17.44	13.08	10.46	8.72	7.47
6	43.60	14.53	10.90	8.72	7.27	6.23
7	37.37	12.46	9.34	7.47	6.23	5.34
8	32.70	10.90	8.18	6.54	5.45	4.67
9	29.07	9.69	7.27	5.81	4.84	4.15
10	26.16	8.72	6.54	5.23	4.36	
11	23.78	7.93	5.95	4.76		
12	21.80	7.27	5.45	4.36		
13	20.12	6.71	5.03	4.02		
harmonic stage 2→		3	4	5	6	7
harmonic stage1↓	1st stage En. (eV)	2nd stage Energy (eV)				
4	18.96	56.87	75.83	94.79	113.75	132.70
5	23.70	71.09	94.79	118.49	142.18	165.88
6	28.44	85.31	113.75	142.18	170.62	199.06
7	33.18	99.53	132.70	165.88	199.06	232.23
8	37.92	113.75	151.66	189.58	227.49	265.41
9	42.66	127.97	170.62	213.28	255.93	298.59
10	47.39	142.18	189.58	236.97	284.37	
11	52.13	156.40	208.54	260.67		
12	56.87	170.62	227.49	284.37		
13	61.61	184.84	246.45	308.06		

First seeded FEL

Variable polarization

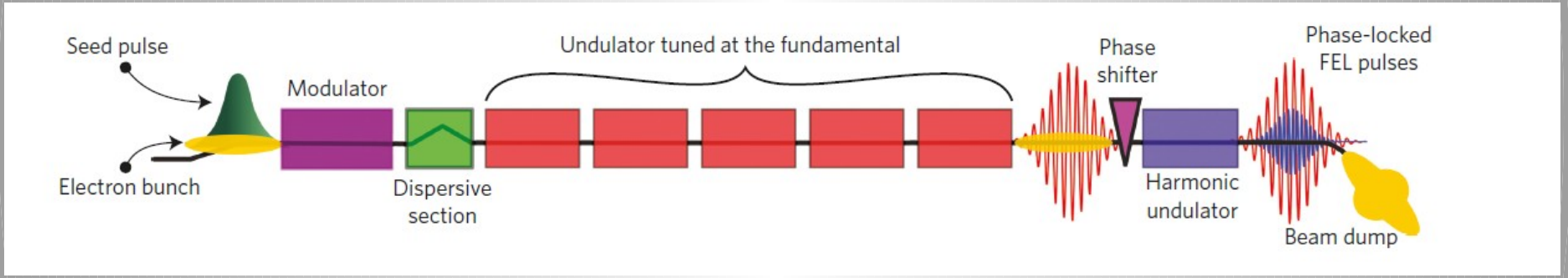
Negligible photon energy jitter

Negligible time jitter

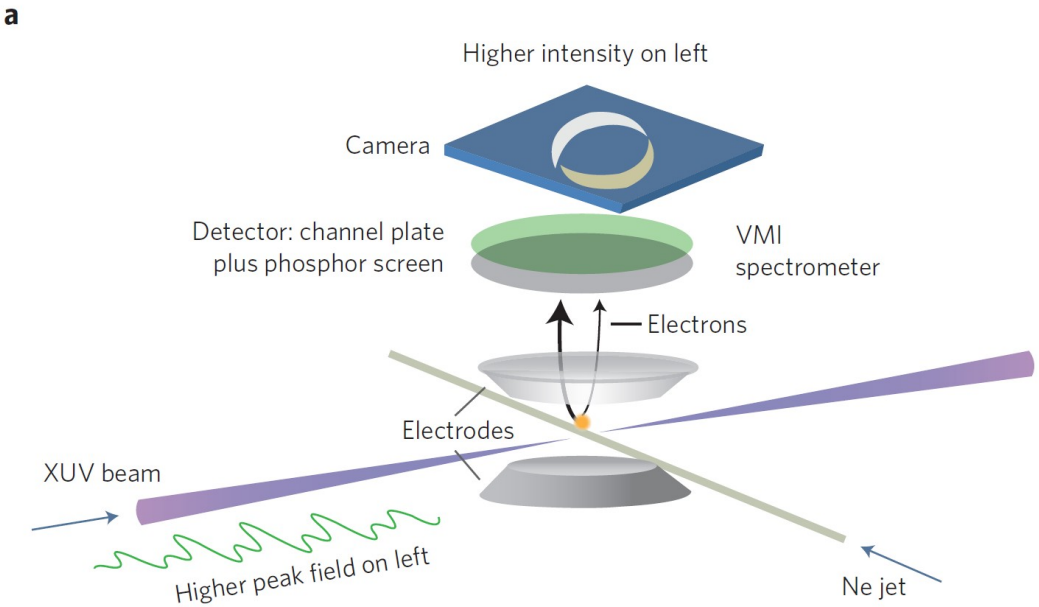


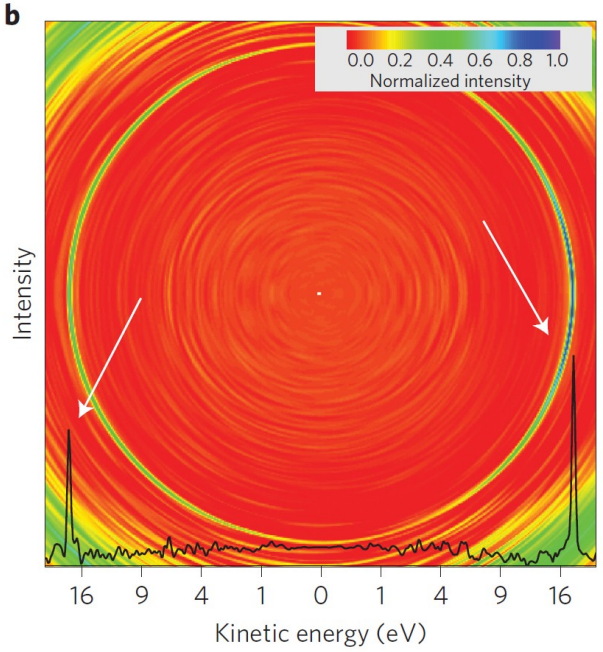
Low Density Matter (LDM)

Coherent control with a short-wavelength free-electron laser



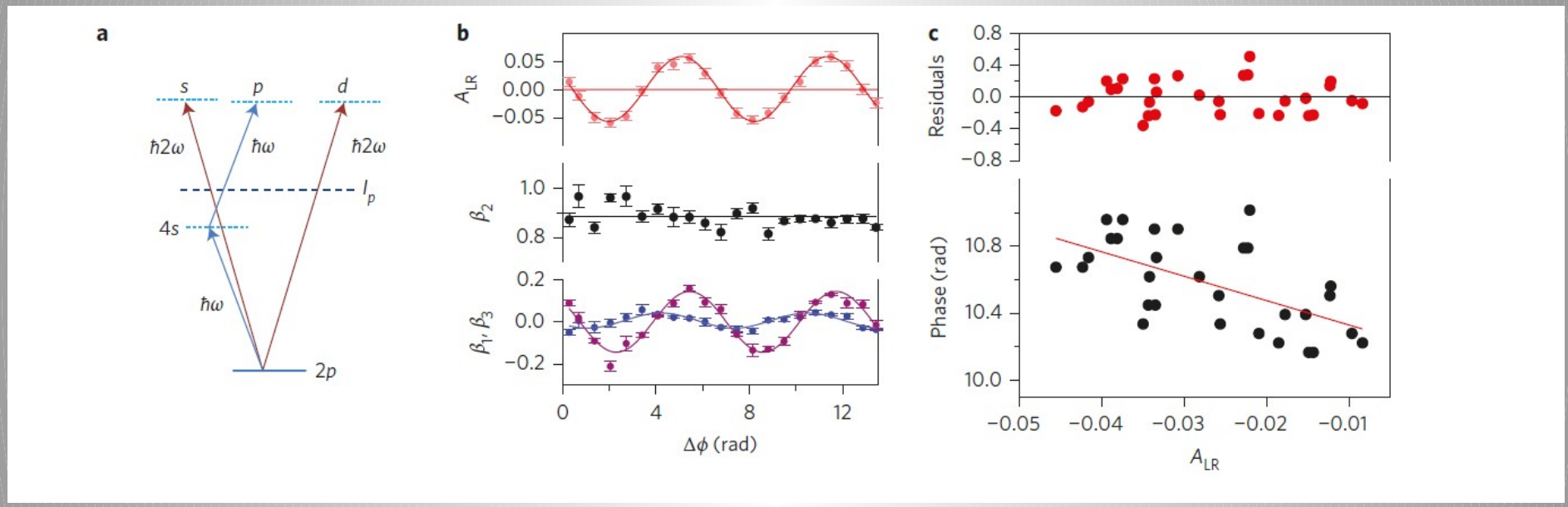
K.C.Prince et al, Nature Photon. 10, (2016) 176



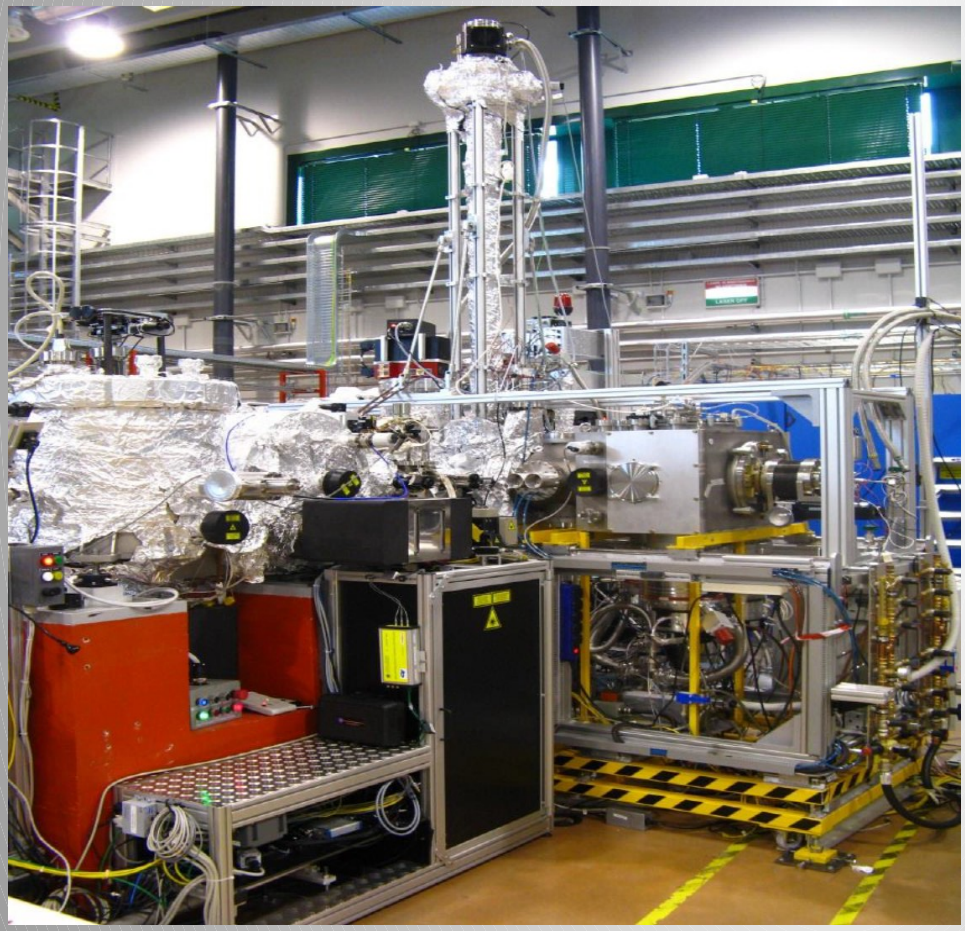


62.97 nm

31.5 nm



$$A_{LR} = \frac{I_L - I_R}{I_L + I_R}$$



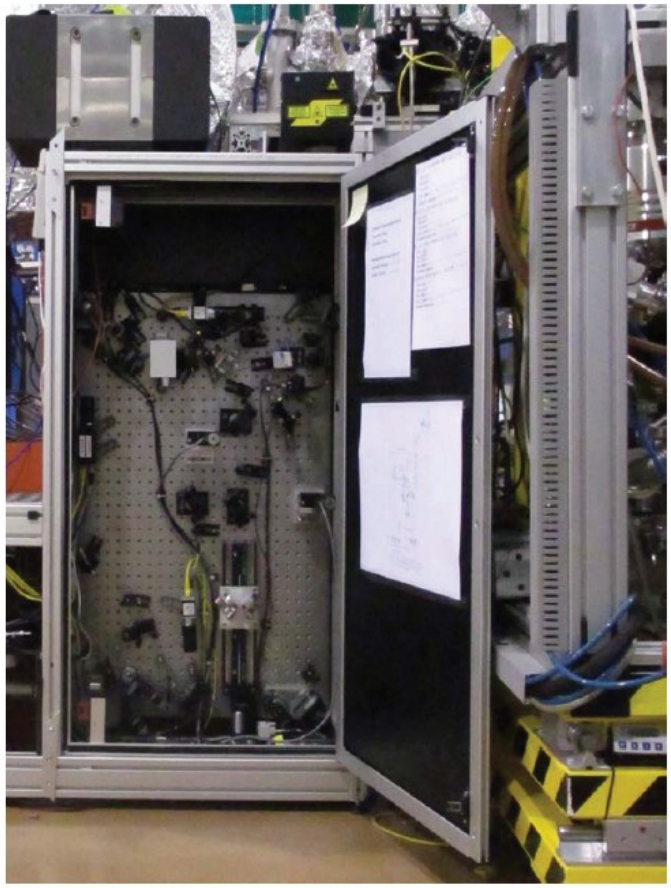
- Magnetic bottle , J.H.D. Eland *et al.*, PRL **90,** 053003 (2003)
- Fast-timing MCP detector combined with signal digitizer
- High collection+detection efficiency
- $E/\Delta E$ = 50-100
- Successfully used for several runs at LCLS

Pump-probe experiments

Two-color experiments are available to users at LDM

The seeded FEL provides high-power,
coherent pulses with 100 femtosecond or less duration,
with a high level of shot-to-shot stability

FEL-1 provides EUV photons in
the range from 65 to 20 nm,
while the 780 nm optical pulses are provided from the same
Ti:sapphire laser used to form the FEL seed pulse



Ti:sapphire (same used to form the FEL pulse)

λ=780 nm

Energy/pulse: 1 mJ

Pulse width 140 fs

(autocorrelation)

USL-LDM Controls	
Attenuation (energy meter avaialble)	0 – 100 %
Polarization	Full control
Delay resolution	2.6 fs
Beam Position resolution	10 µrad (upgrade: piezo tip-tilt)

Acetylacetone femtodynamics

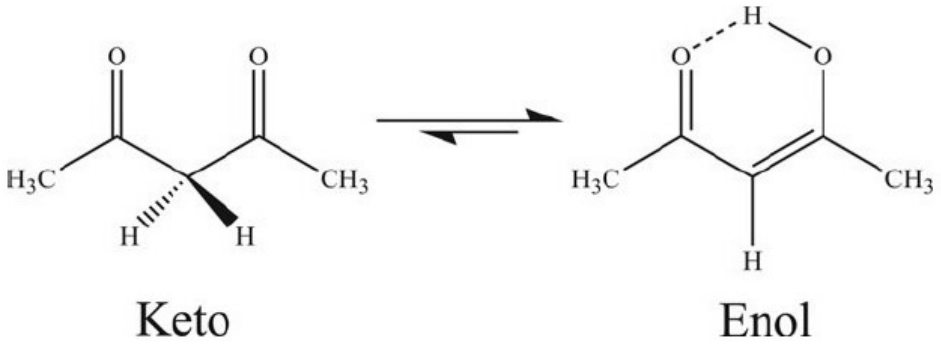
by pump-probe experiments at

FERMI-LDM

R. Squibb,…. and M.N.Piancastelli, Nature Comm. 9, 63 (2018)

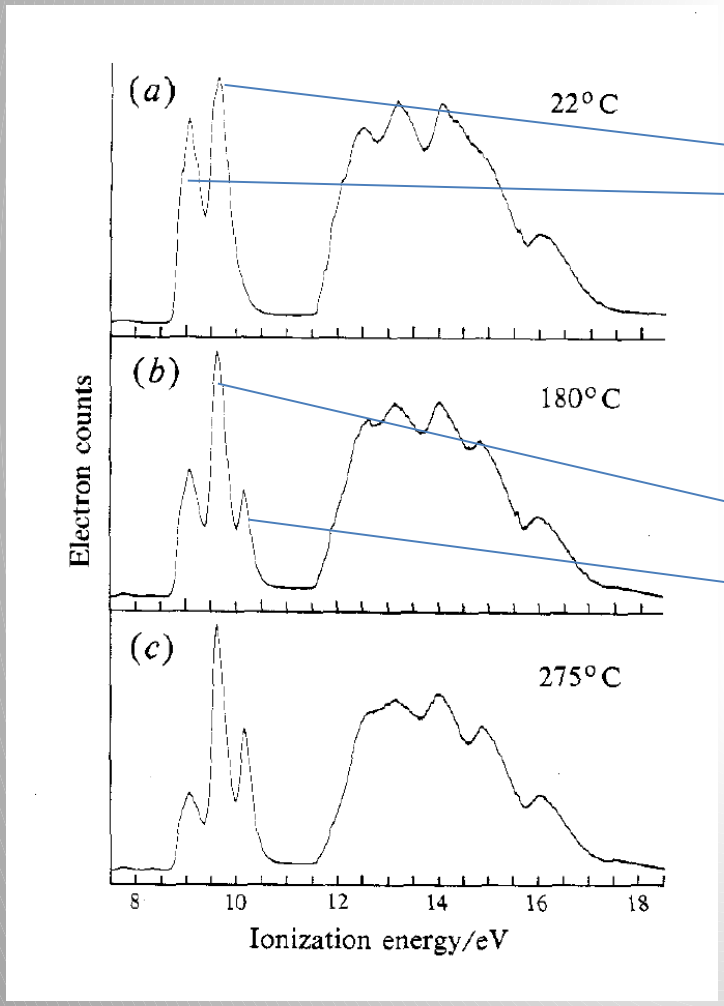
Probing keto-enol tautomerism

in acetylacetone



Keto Enol

Valence Photoelectron spectra are characteristic of the forms (Hush *et al.* Aust. J.Chem. **40,** (1987) 559)



Enol form

Keto form

LDM beam time

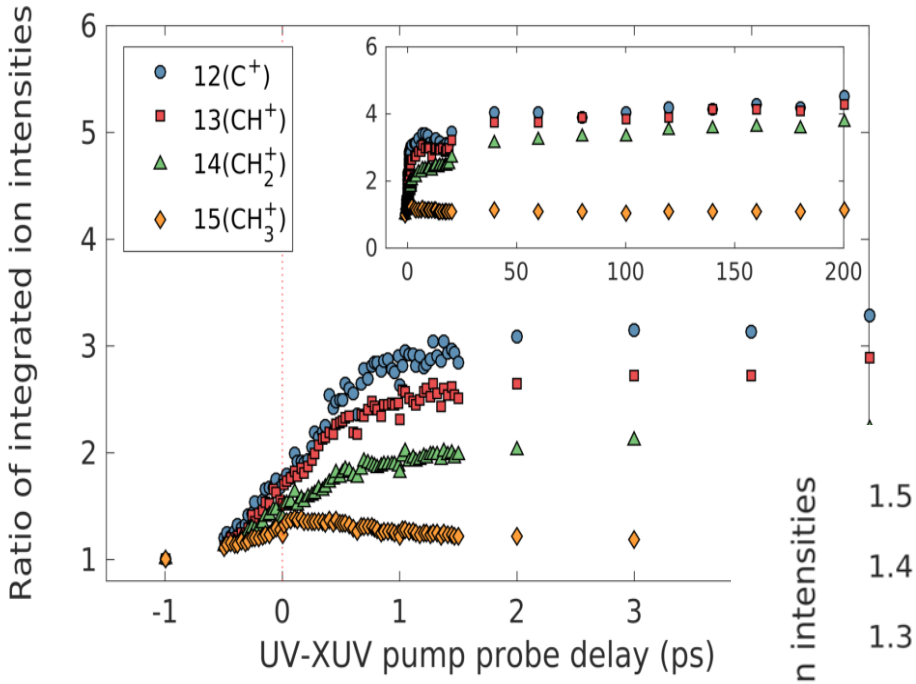
Photon energy pump: 261 nm

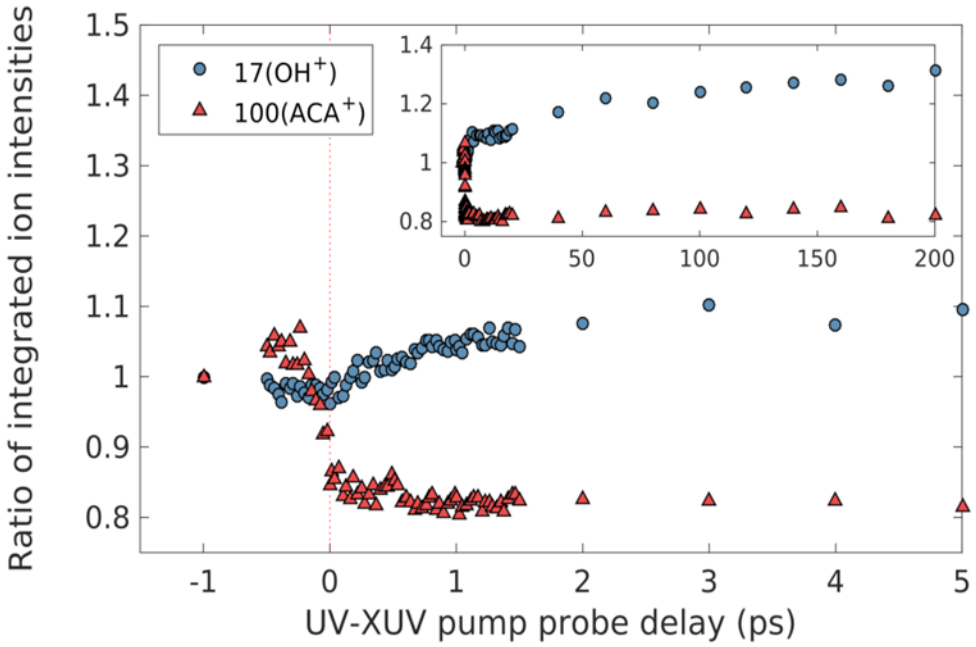
Photon energy probe: 19.24 eV

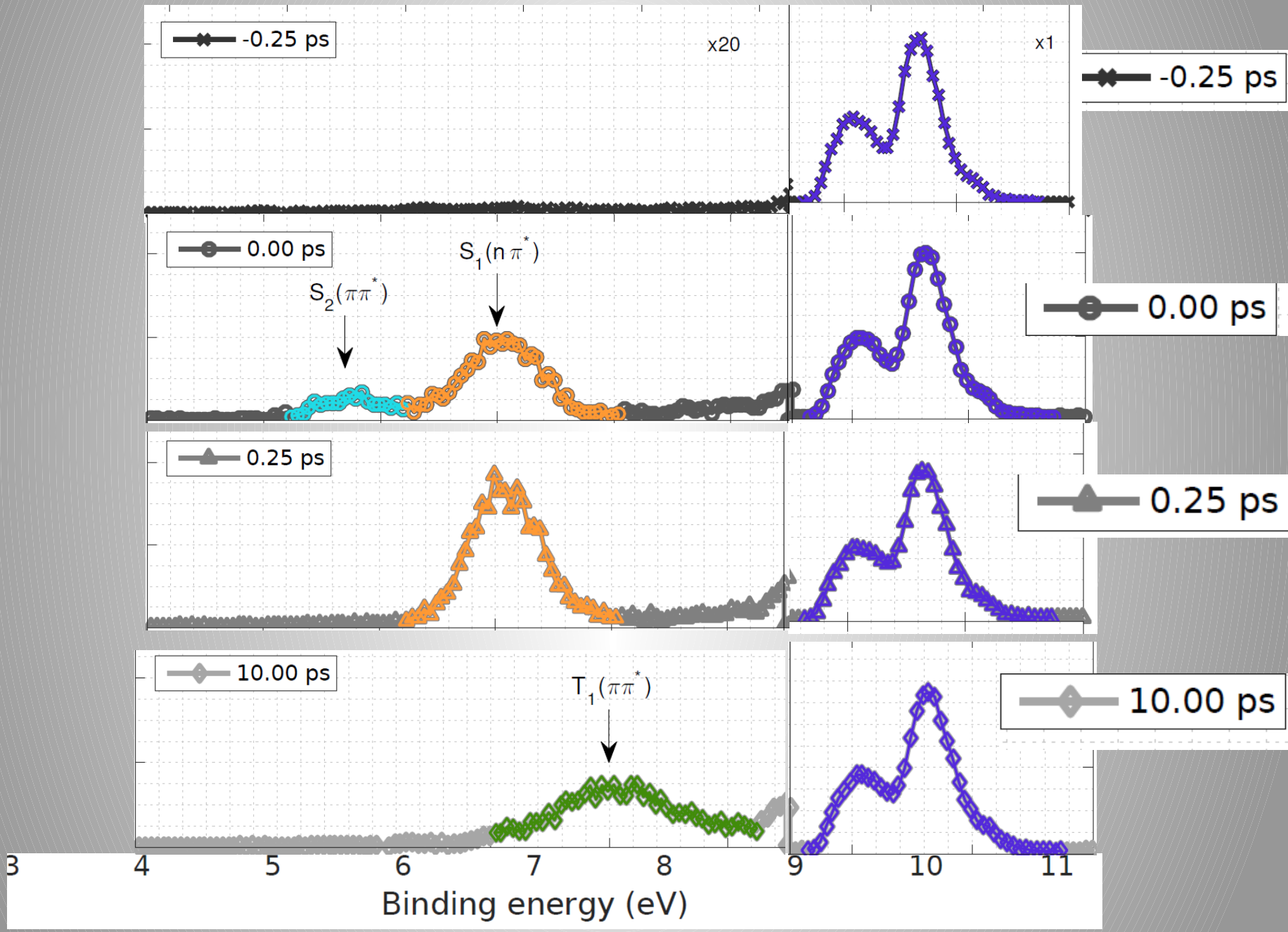
Delay range 0-200 ps

Detection of valence electrons as a function of delay

Detection of ions as a function of delay


Ratio of integrated ion intensities
UV-XUV pump probe delay (ps)
12(C+)
13(CH+)
14(CH2+)
15(CH3+)


Ratio of integrated ion intensities
UV-XUV pump probe delay (ps)
17(OH+)
100(ACA+)

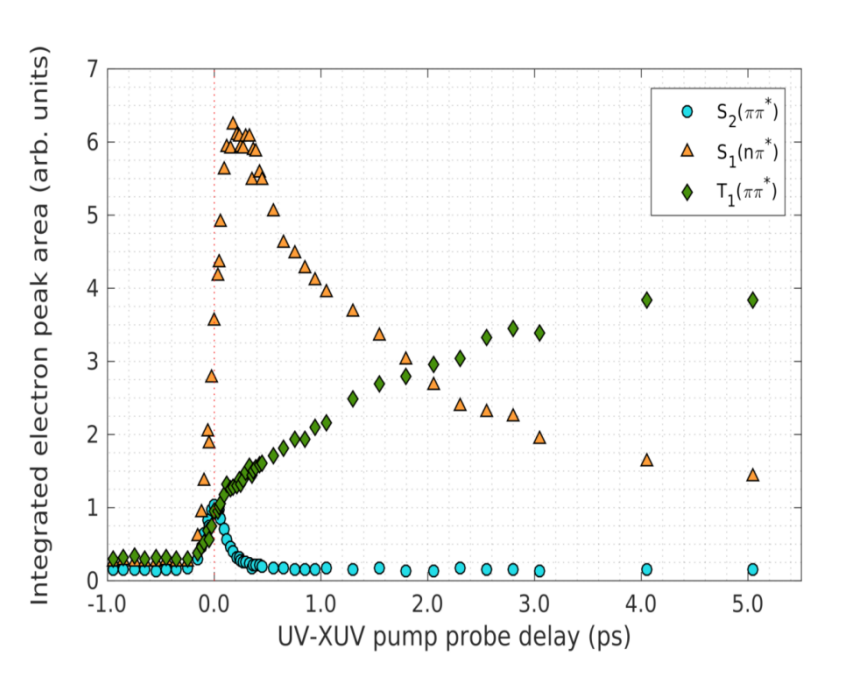

-0.25 ps
x20
x1
0.00 ps
$S_1(n\pi^*)$
$S_2(\pi\pi^*)$
0.25 ps
10.00 ps
$T_1(\pi\pi^*)$
3
4
5
6
7
8
9
10
11
Binding energy (eV)

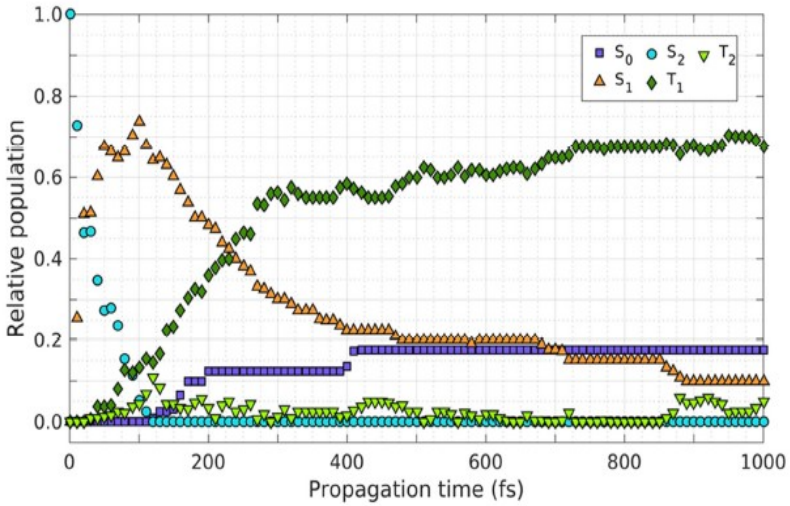
UPPSALA UNIVERSITET

ab initio static (CASPT2) and surface-hopping dynamics (CASSCF) calculations

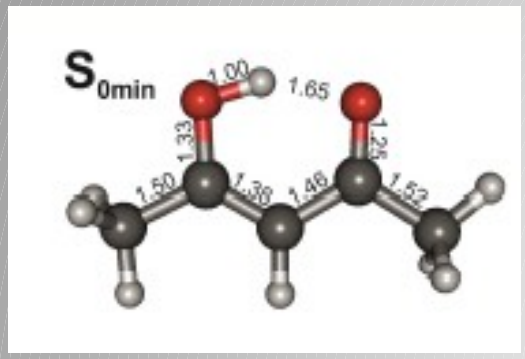
ionization energies at the MS-CASPT2-[10,10] level

CASPT2 ionization energies and fragmentation pathways

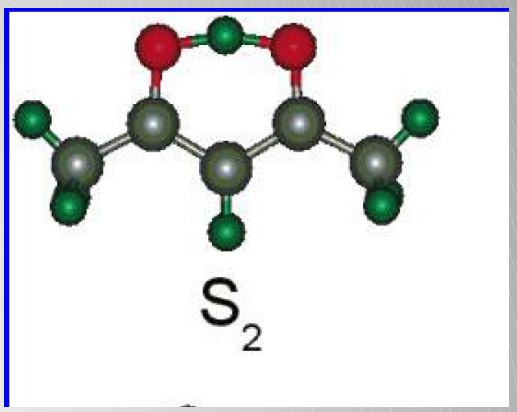




	S_{0min}	S_{1min}	
	$IE(D_0\text{-}S_2)$ (eV)	$IE(D_1\text{-}S_1)$(eV)	$IE(D_0\text{-}T_1)$ (eV)
Experiment	4.64	6.04	7.14
CASPT2[10,10]	4.43	5.71	6.81
Dynamics	4.45 ± 0.39	5.81 ± 0.42	6.89±0.66



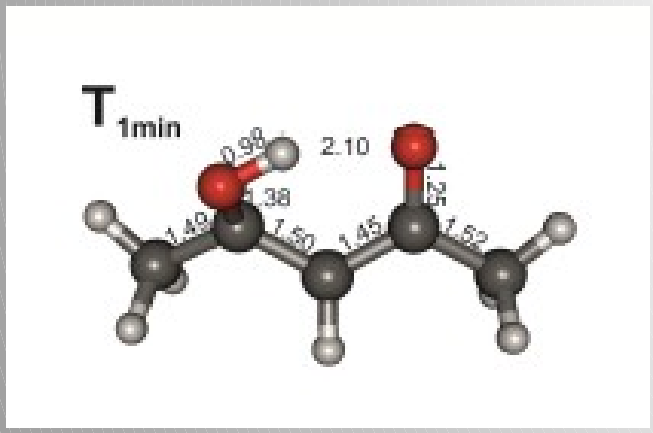
261 nm



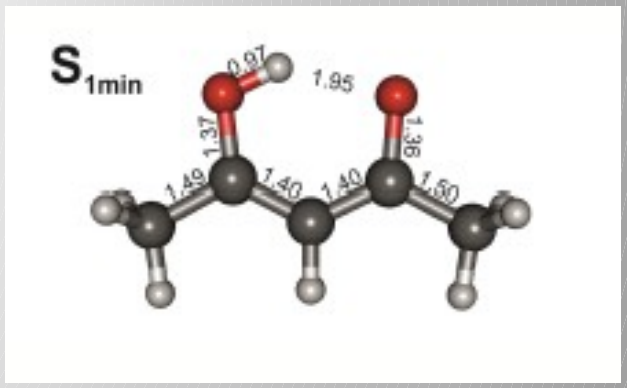
GS

ππ*

CI



CI



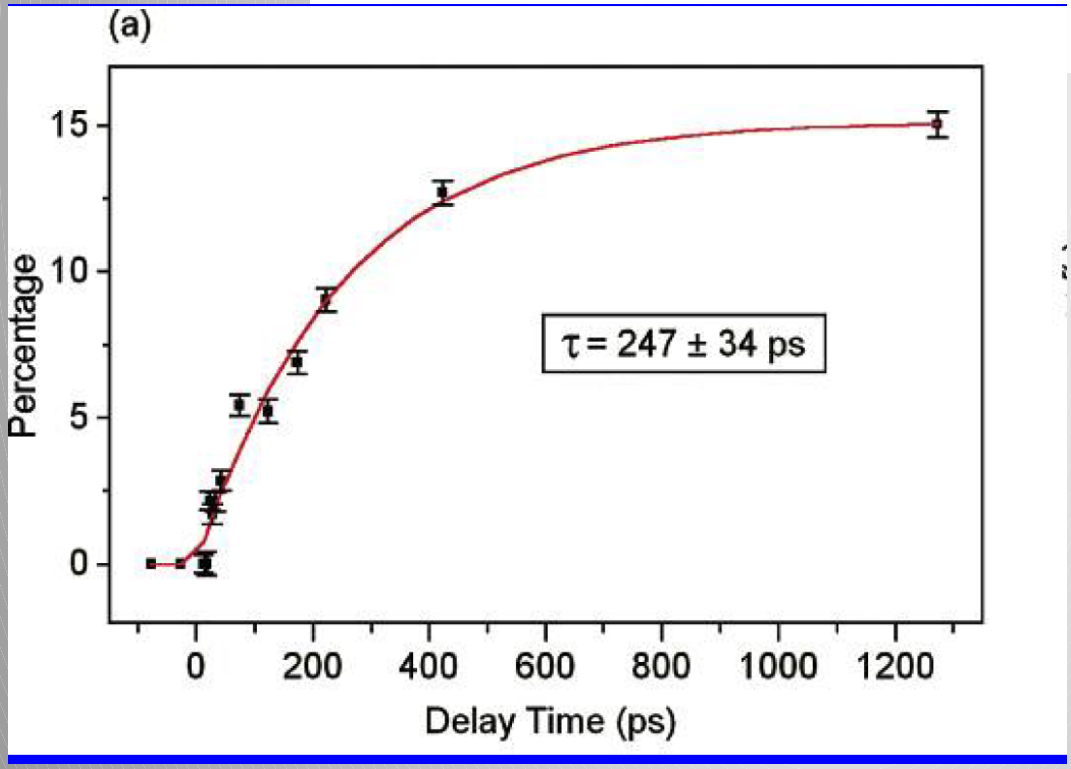
ππ*

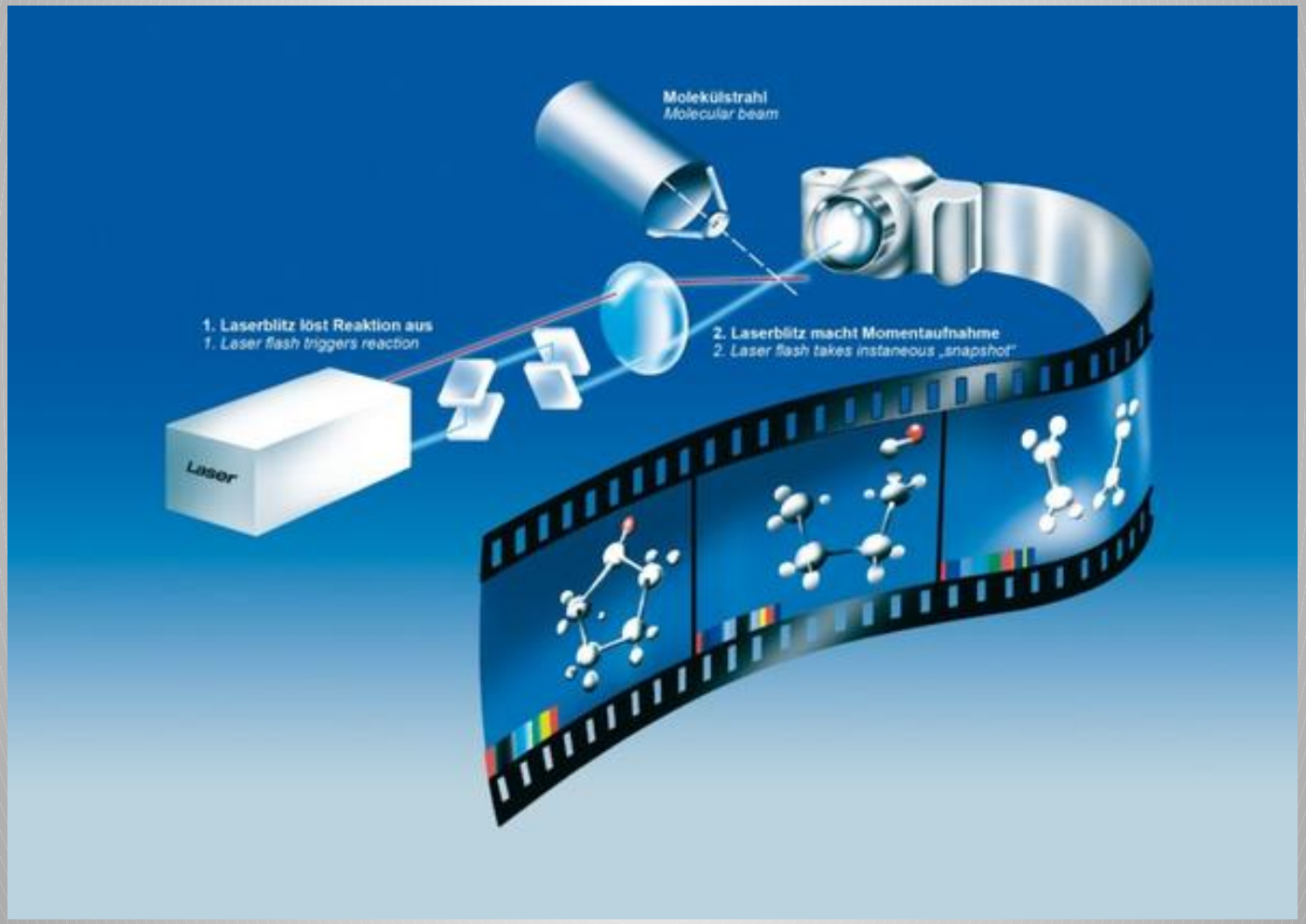
nπ*

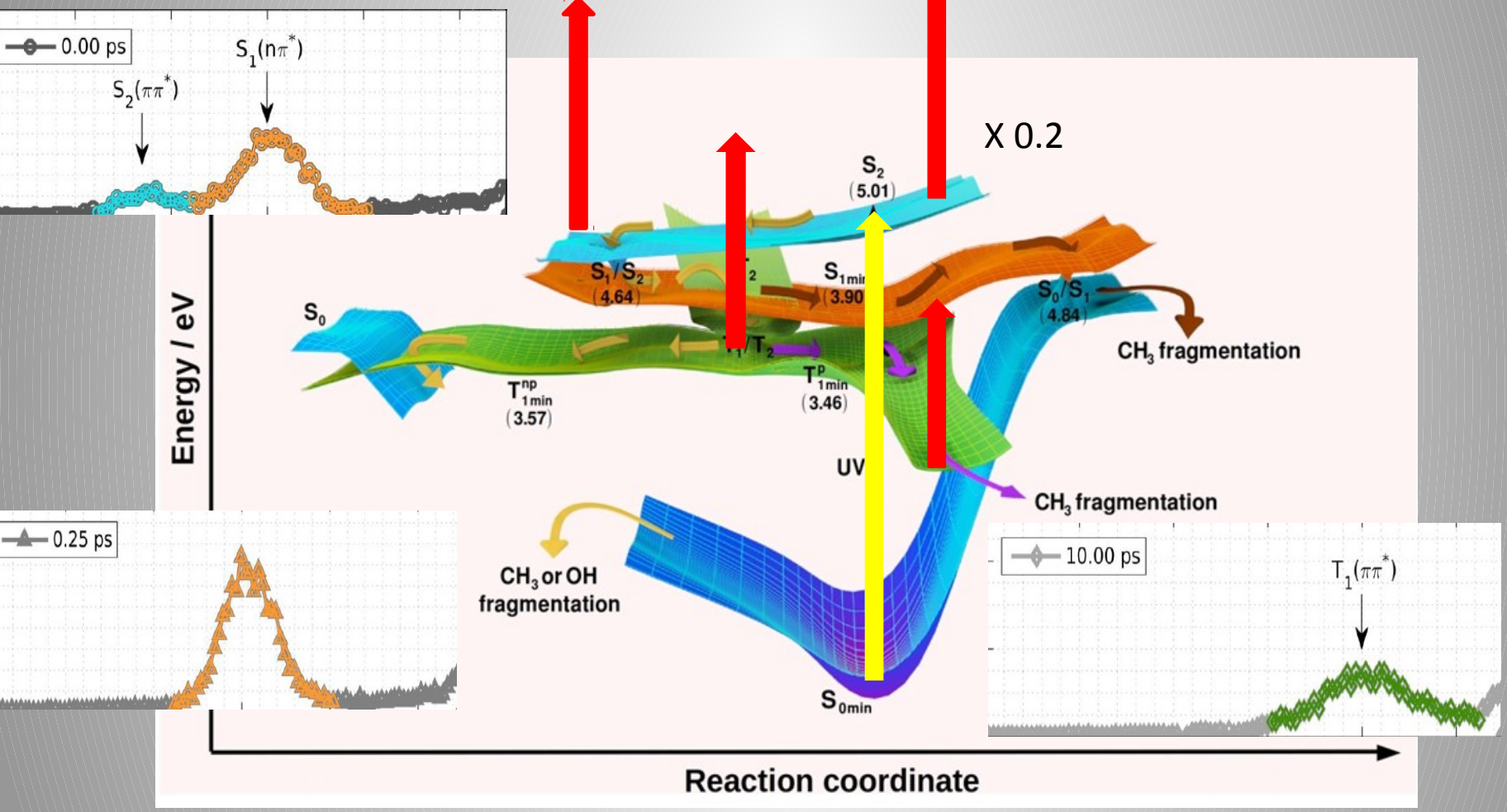
Ultrafast Electron Diffraction: Structural Dynamics of the Elimination Reaction of Acetylacetone

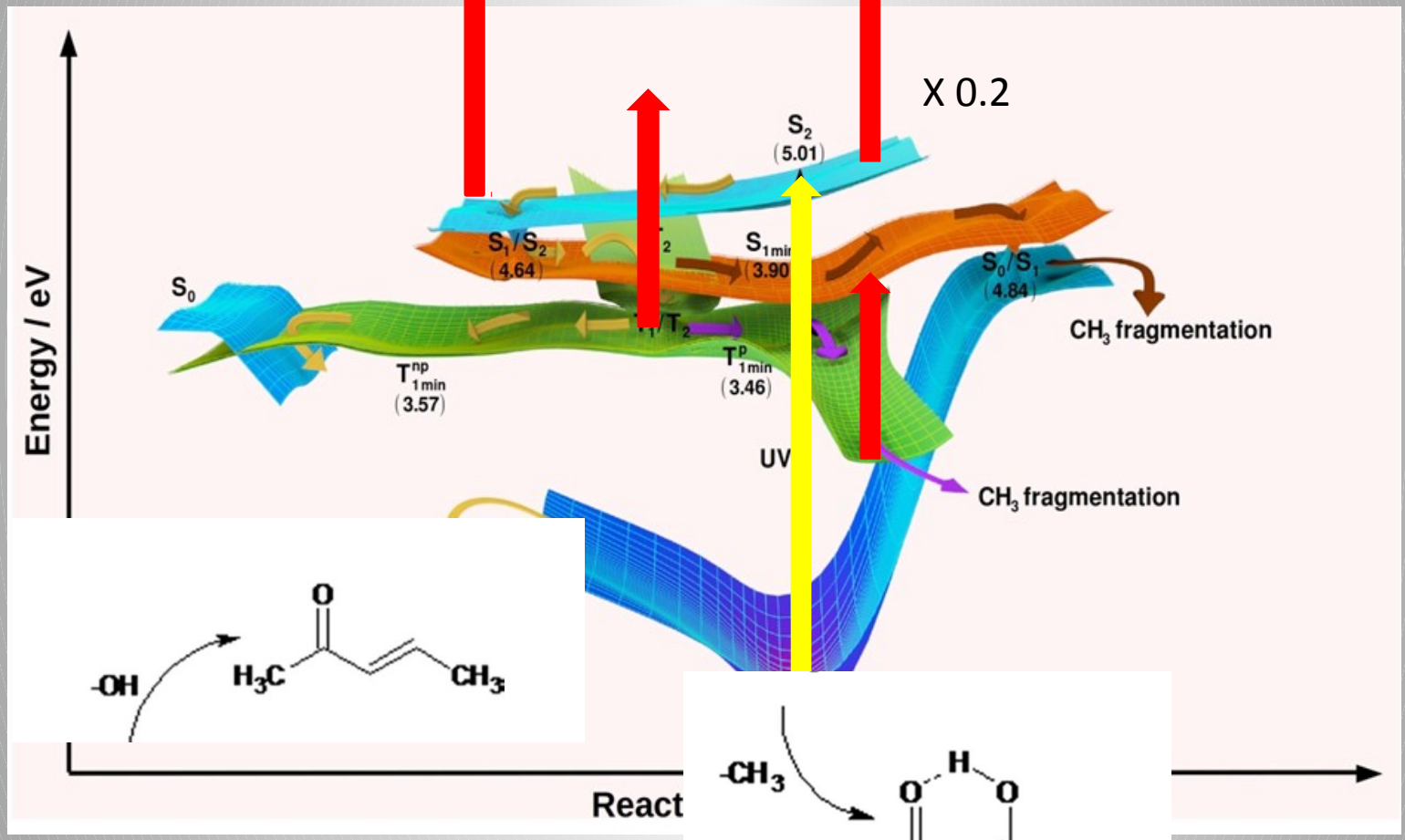
Shoujun Xu, Sang Tae Park, Jonathan S. Feenstra, Ramesh Srinivasan, and Ahmed H. Zewail*

Laboratory for Molecular Sciences, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125




Molekülstrahl
Molecular beam
1. Laserblitz löst Reaktion aus
1. Laser flash triggers reaction
2. Laserblitz macht Momentaufnahme
2. Laser flash takes instaneous „snapshot"
Laser


0.00 ps
$S_2(\pi\pi^*)$
$S_1(n\pi^*)$
X 0.2
S_2
(5.01)
S_1/S_2
(4.64)
S_{1min}
(3.90)
S_0/S_1
(4.84)
S_0
T_1/T_2
T^{np}_{1min}
(3.57)
T^{p}_{1min}
(3.46)
CH_3 fragmentation
UV
CH_3 fragmentation
CH_3 or OH
fragmentation
S_{0min}
Energy / eV
Reaction coordinate
0.25 ps
10.00 ps
$T_1(\pi\pi^*)$


X 0.2
S2
(5.01)
S1/S2
(4.64)
S1min
(3.90
S0/S1
(4.84)
S0
T1/T2
T1min np
(3.57)
T1min p
(3.46)
CH3 fragmentation
UV
CH3 fragmentation
Energy / eV
React
OH
H3C
O
CH3
CH3
H
O
O
CH3

Which is the best way to follow a chemical reaction?

X-ray diffraction

Electron diffraction

Valence photoelectron spectroscopy

Ion spectroscopy

Summary

NO isomerization

Mainly fragmentation producing CH_n^+

Very accurate way to follow a chemical reaction