

Reliable atomic data for fusion research and astrophysics:

Benchmarking calculations for highly charged ions



José R. Crespo López-Urrutia
*Max-Planck-Institut für Kernphysik
Heidelberg*



HCI as resource for fundamental physics

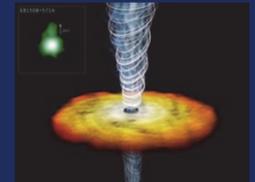
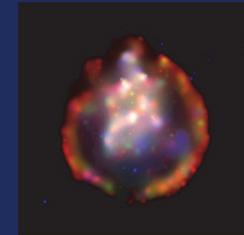
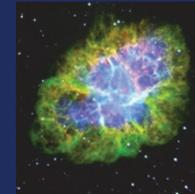
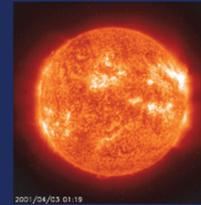
- Atoms are key assets in fundamental studies:
 - universally reproducible
 - spectroscopic frequency references from MW to VUV
 - mass references for nuclear, neutrino physics, etc.
 - EDM searches for interactions beyond the SM
 - atomic interferometric probes of space-time, relativity
- Limitation: Unstable at high interaction energies
- Using HCI expands these possibilities:
 - high intrinsic stability against perturbations
 - stable at high photon energies up to the 0.1 MeV
 - in greater variety than atoms or singly charged ions

Review of Modern Physics coming up:

(arXiv, Kozlov, Safronova, JRC, Schmidt 2018)

In the Universe, elements are mostly highly ionized: **Highly charged ions (HCI)**

- Interior of the Sun (15 MK)
- Solar corona (2 MK)
- Solar wind (MK)
- Supernova remnants
- Active galactic nuclei (100 MK)
- Warm-hot intergalactic medium (0.1-1 MK)



In the laboratory:

- Fusion machines (50 MK)
- Accelerators, laser produced plasmas (1 MK)
- Electron beam ion traps (e. g. in Heidelberg)

State of the art in the field of HCl

- X-ray photon energies 1.5 ppm
- VUV photon energies 4 ppm
- Optical photon energies 0.3 ppm
- Lifetimes (ns... ms) 0.15 %
- Natural linewidths X-rays: resolved

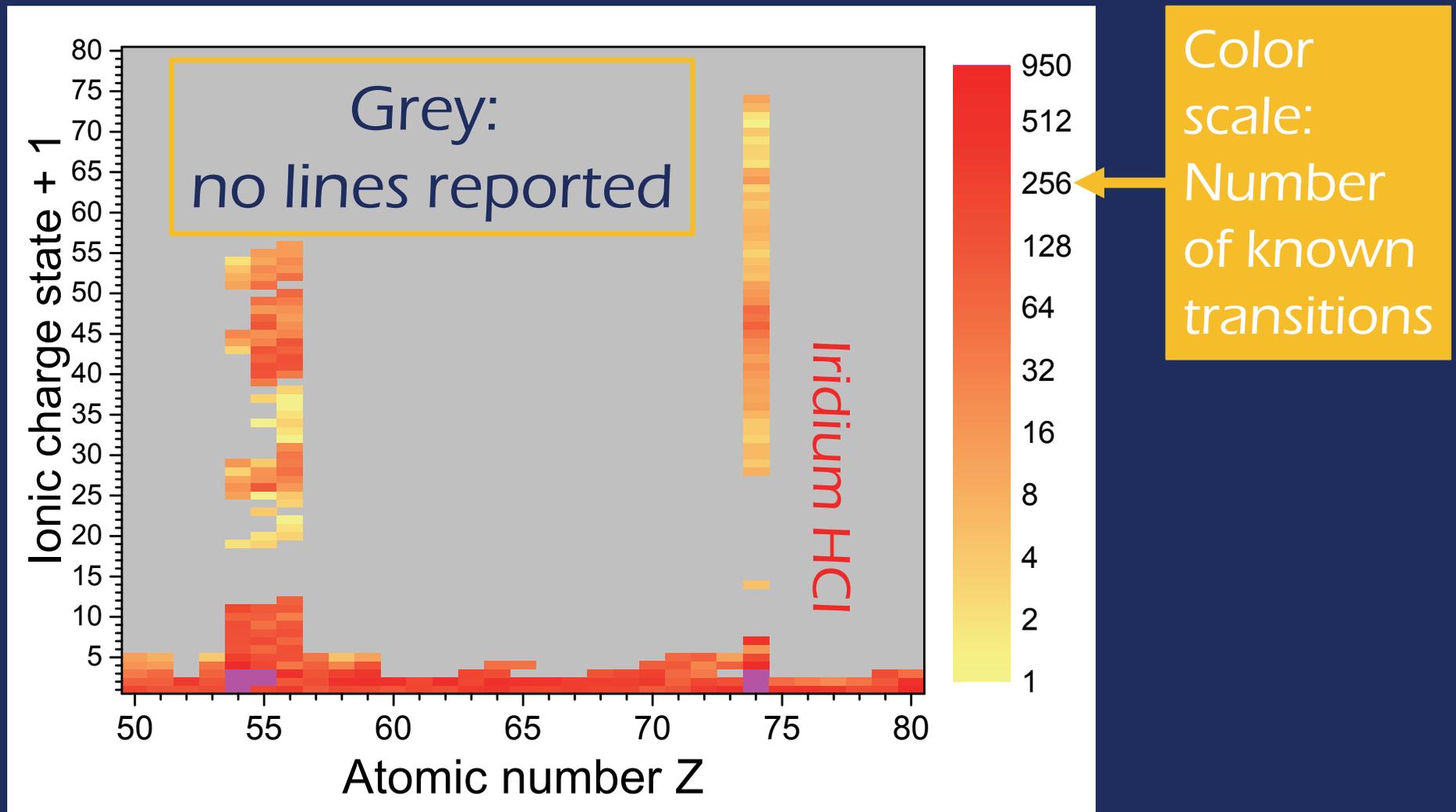
Accuracy is 12 orders of magnitude lower than in frequency metrology

Stone-age spectroscopy at the 10^{-6} level

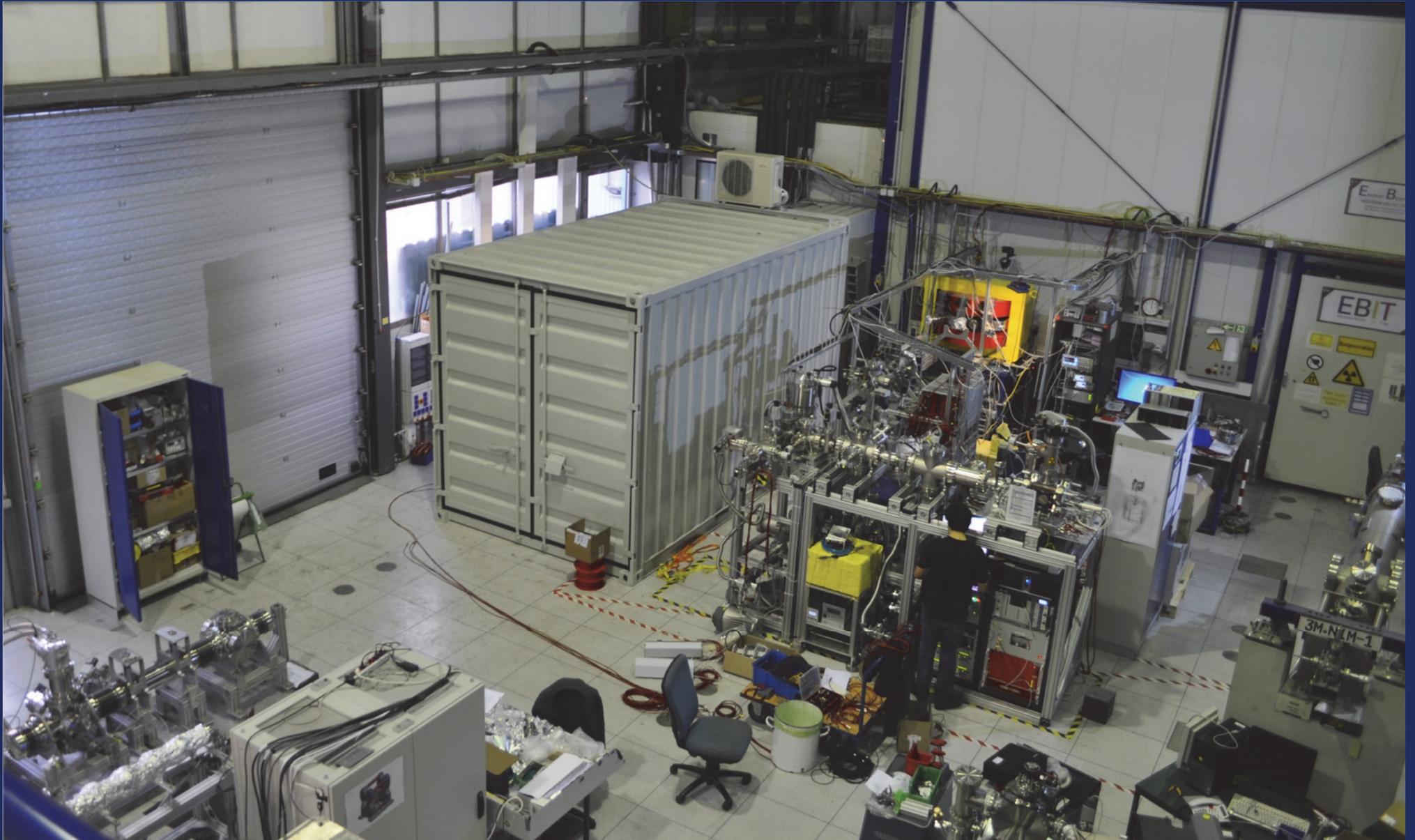


HCI: Under way in the “spectral desert”

- No reports about the ions of interest and no transition data available for most ions!
- HCI production in EBIT easy, identification much harder



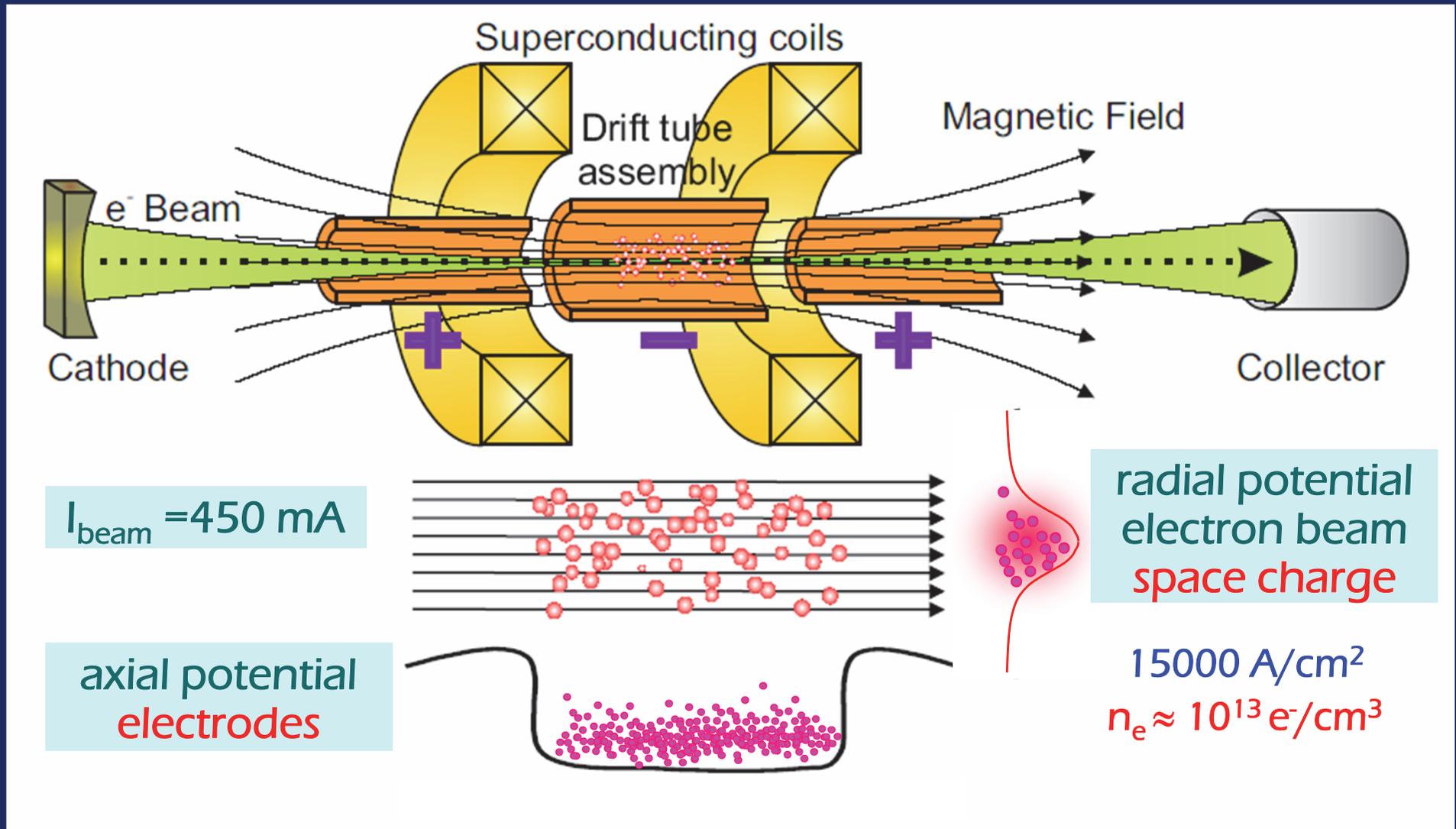
EBIT facility at MPIK



Overview

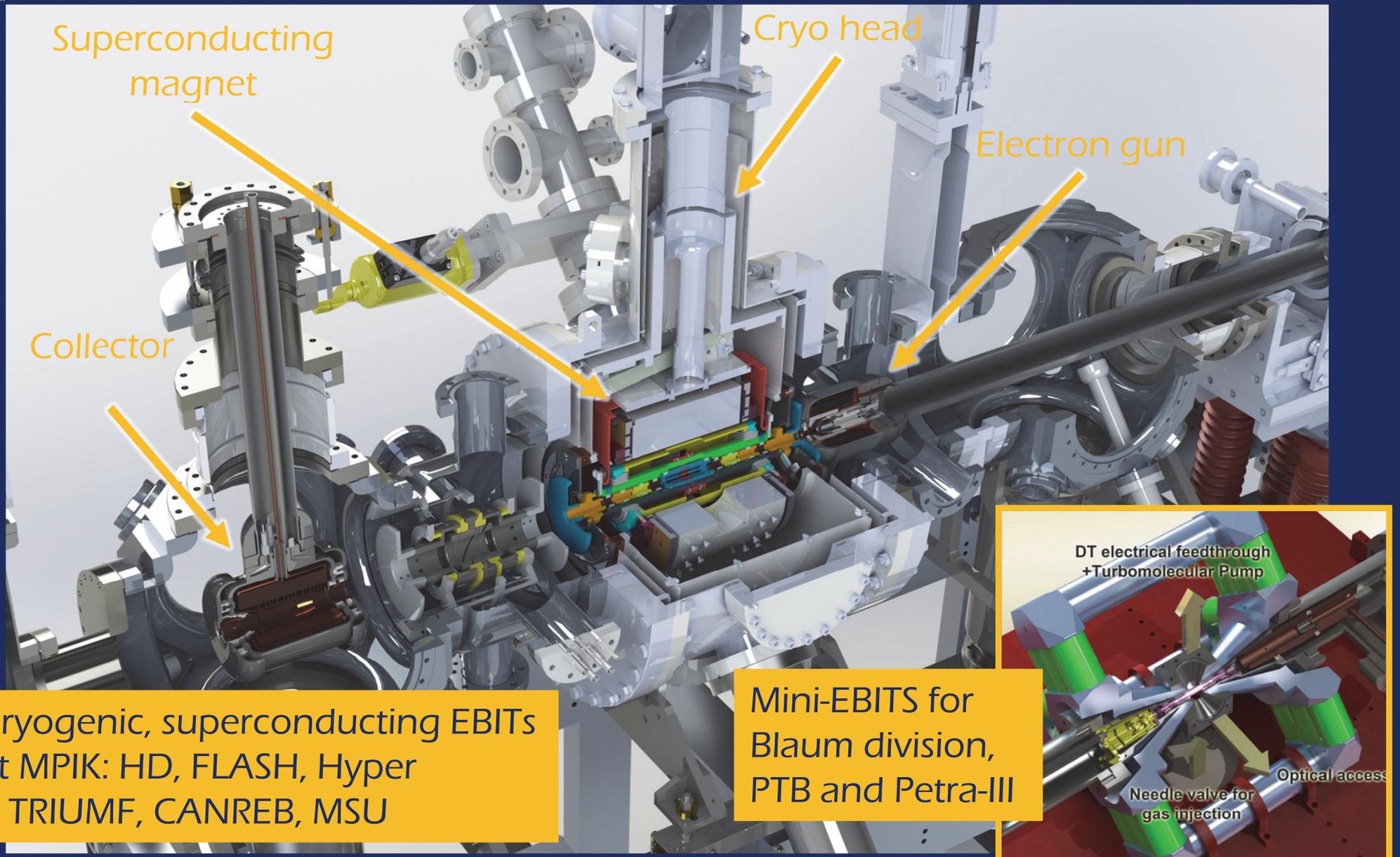
- Electron beam ion traps
- Photon excitation studies
- Electron excitation studies
- Optical and EUV spectroscopy
- Charge exchange
- Frequency metrology

HCl production with electron beam ion trap



Electron beam drives ionization, excites and traps the ions inside a cylindrical volume

Electron beam ion traps big and small

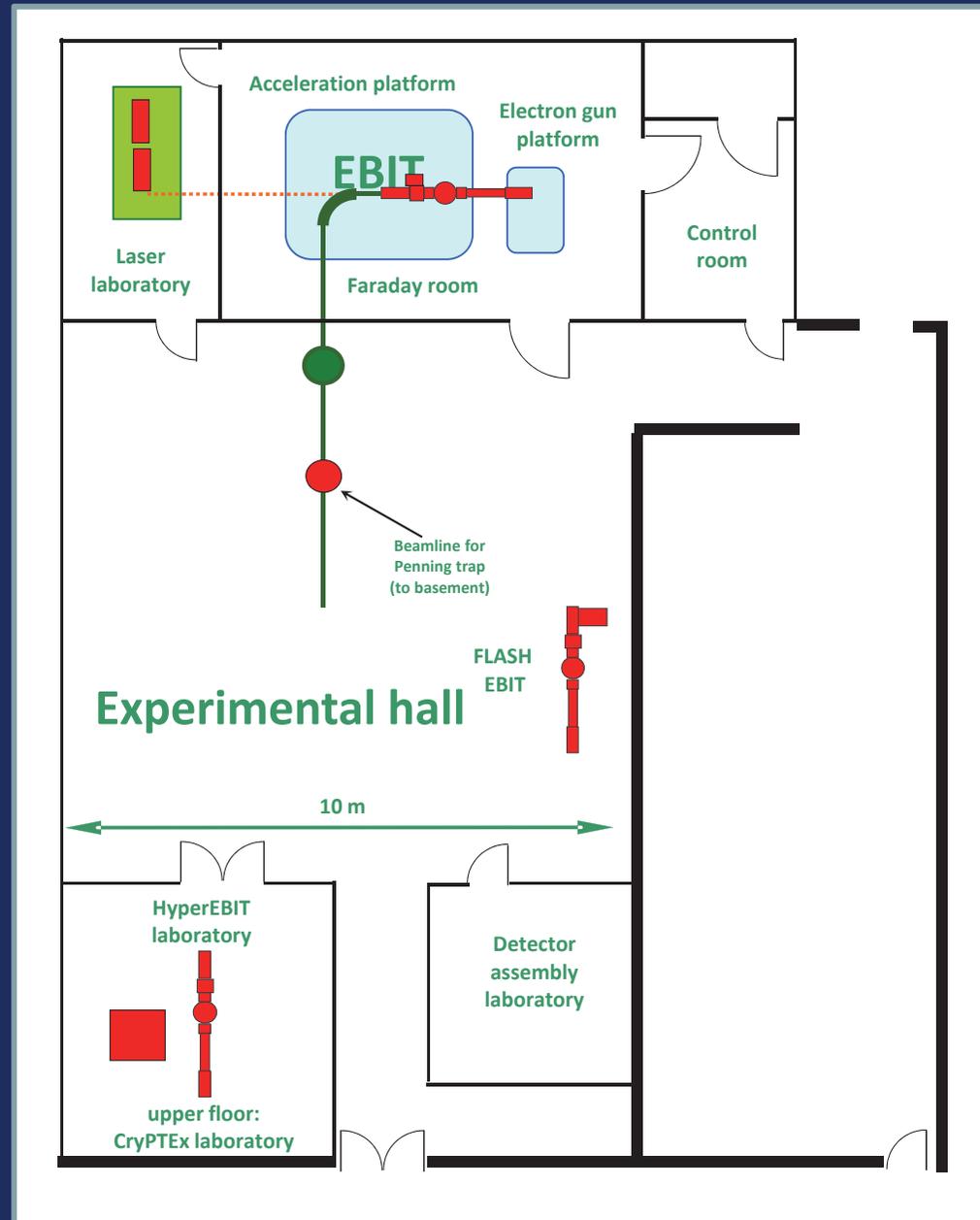


Cryogenic, superconducting EBITs at MPIK: HD, FLASH, Hyper + TRIUMF, CANREB, MSU

Mini-EBITS for Blaum division, PTB and Petra-III

- Unique facility at MPIK, supporting Pfeifer and Blaum division
- Out of ~20 research EBITs worldwide, 10 are at or come from MPIK

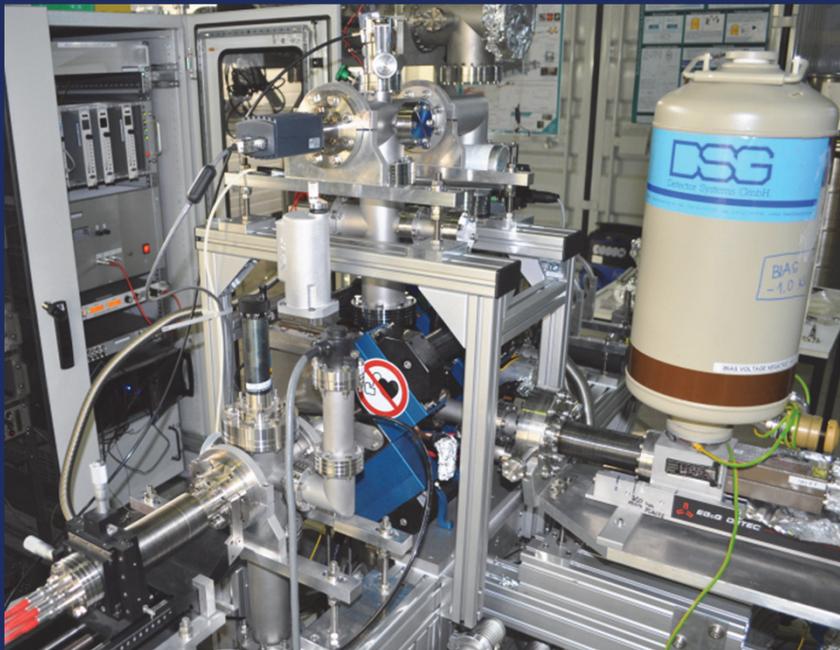
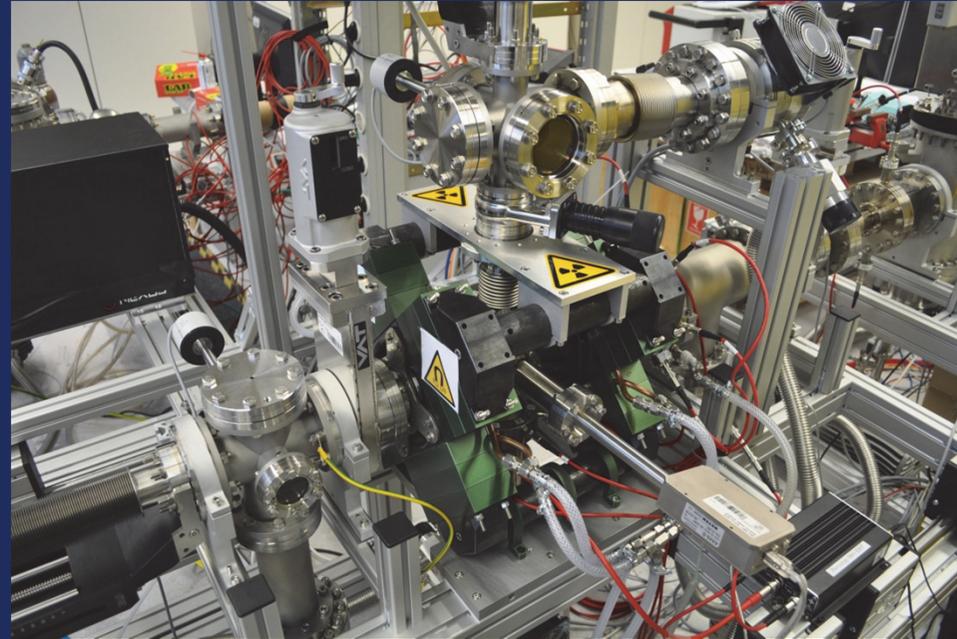
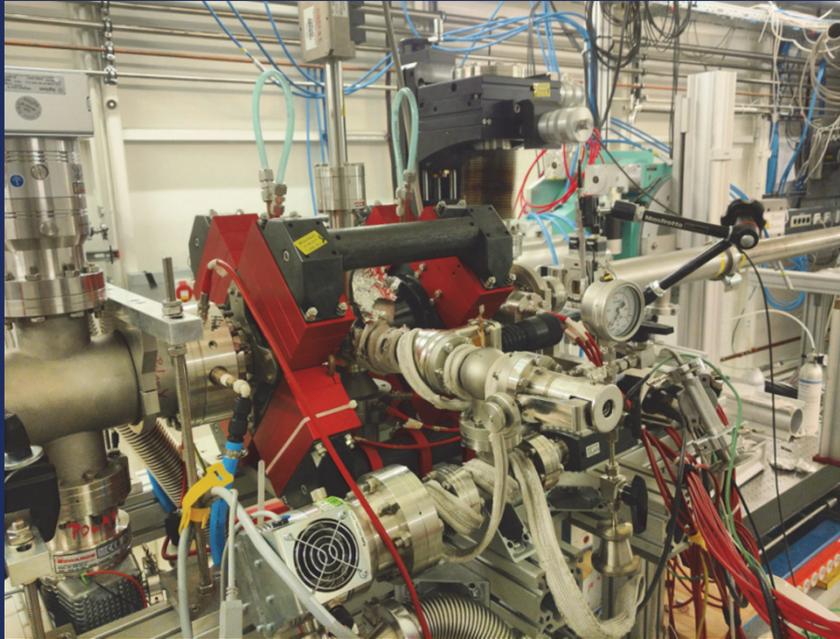
EBIT facility at MPIK





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Some compac EBITs





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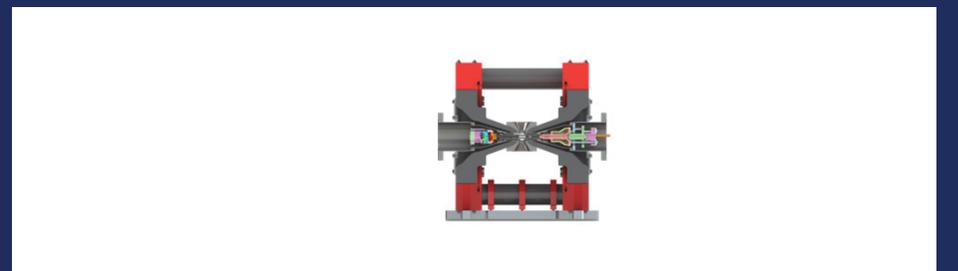
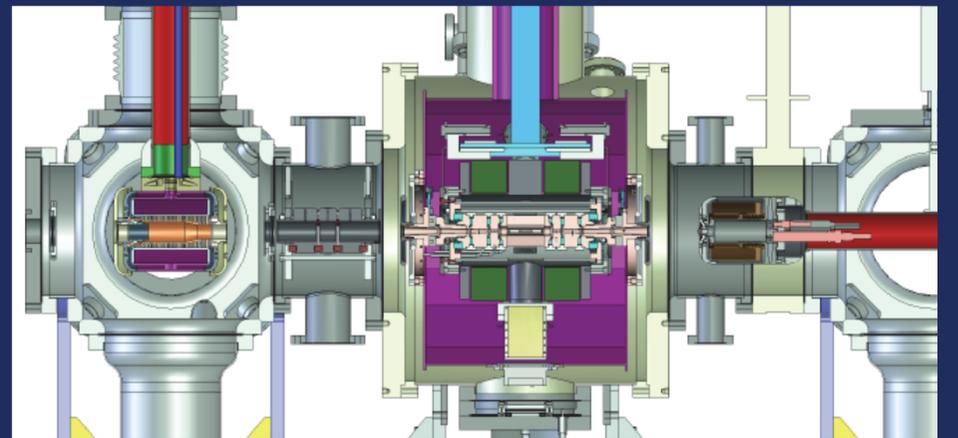
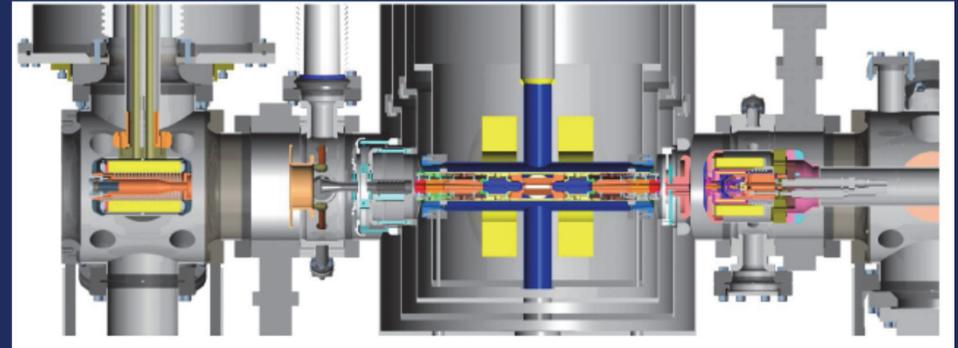
Electron beam ion traps at MPIK

Cryogenic devices:

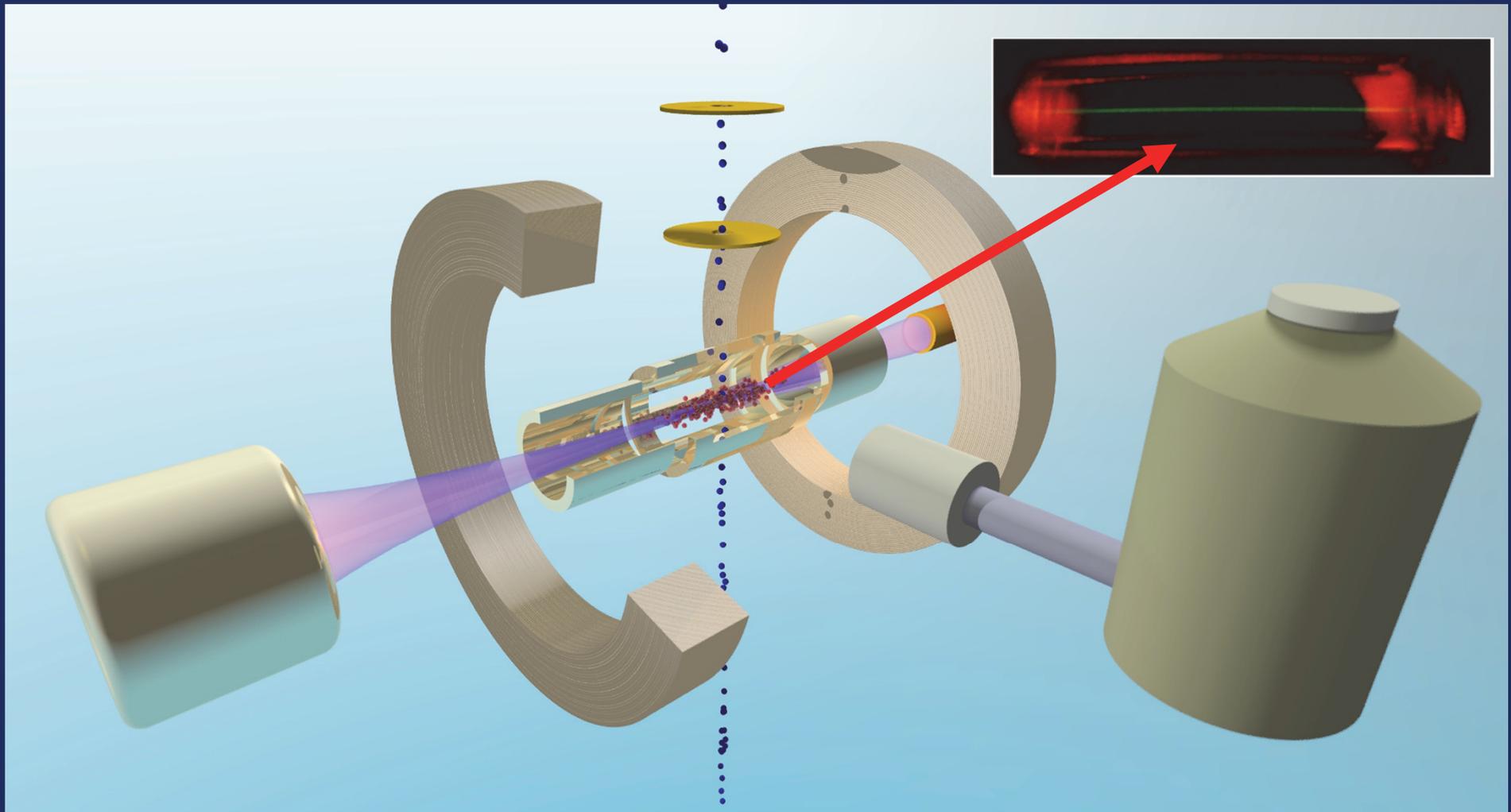
- HD EBIT: stationary machine built in 1999 (former FreEBIT)
- FLASH EBIT: transportable for beamtimes at FLASH, BESSY, LCLS and PETRAIII
- Hyper EBIT

Miniature:

- Polar-X EBIT (at PETRAIII)
- Tip-EBIT (Blaum division)
- TT-EBIT (Blaum division)
- CryPTEx-II-EBIT

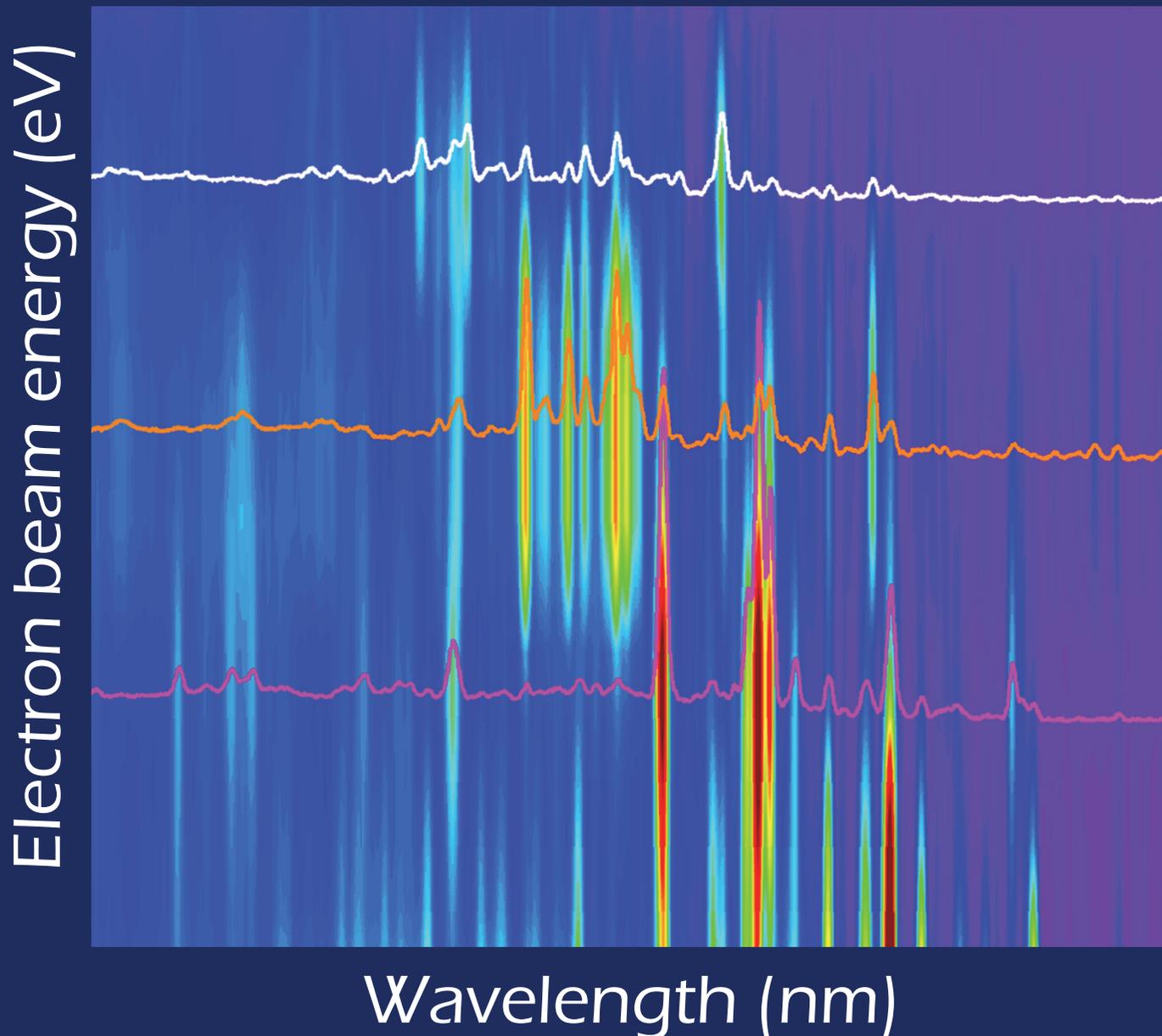


Strong excitation by electron impact and resonant photorecombination



Ge, Si detectors, crystal and grating spectrometers, microcalorimeters, etc., for X-ray diagnostics

Choice of charge state by dialing electron beam energy



What we do with EBITs

- Photorecombination processes: **radiative + dielectronic, trielectronic and quadruelectronic recombination**,
- **Photoionization of HCl** with synchrotron radiation, from N^{3+} (from 60 eV) to Kr^{33+} (at 14 keV)
- High-resolution spectroscopy **from optical to X-rays**
- **Free-electron laser soft x-ray spectroscopy** (<800 eV)
- High-resolution x-ray metrology with synchrotron radiation (<14.4 keV)
- **Laser spectroscopy** of forbidden optical lines in HCl
- **Sympathetic cooling of HCl** for frequency metrology
- **Charge-exchange** studies

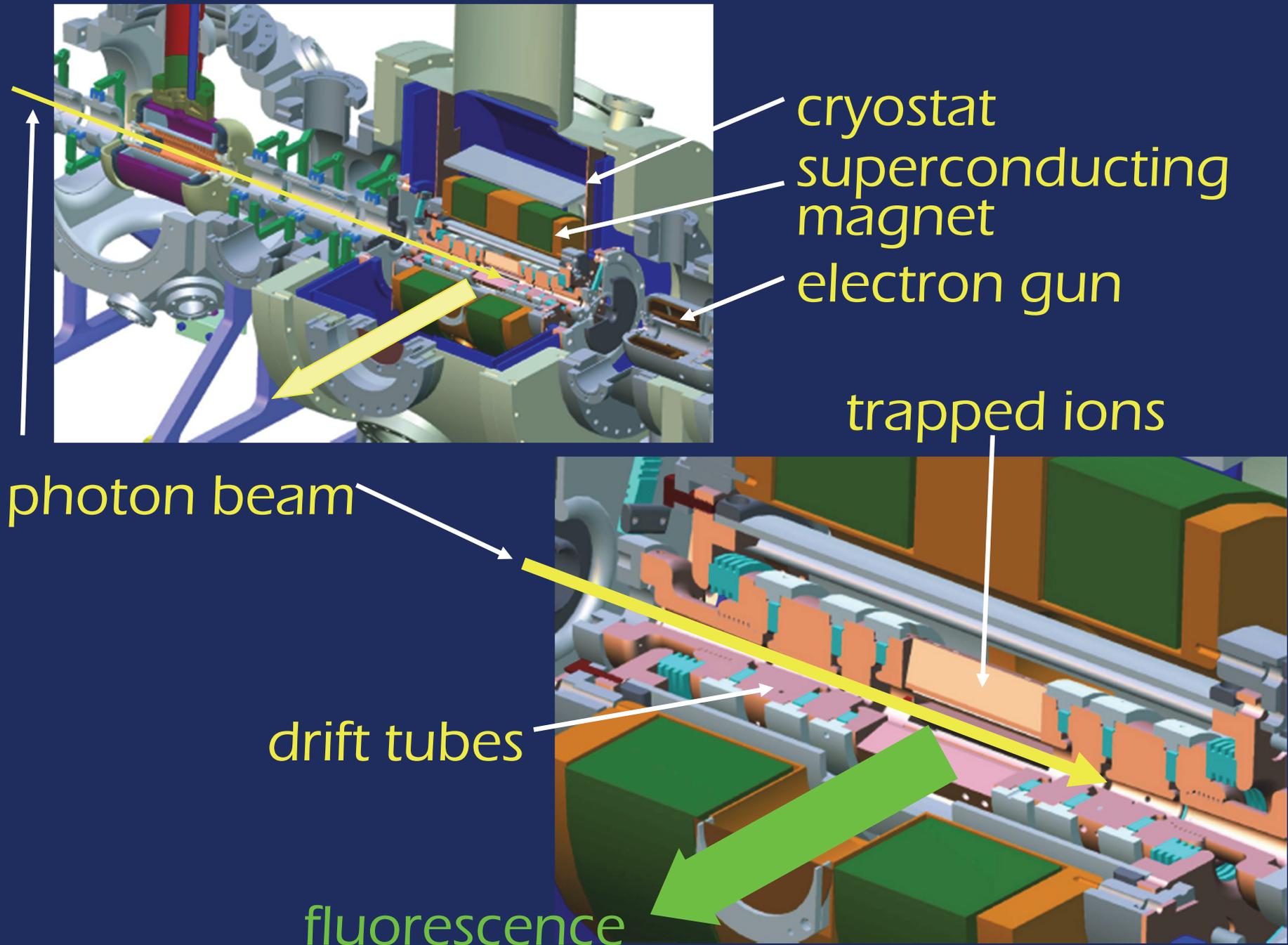
Free-electron laser and synchrotron-radiation excitation and photoionization of highly charged ions

Photonic interactions with HCI

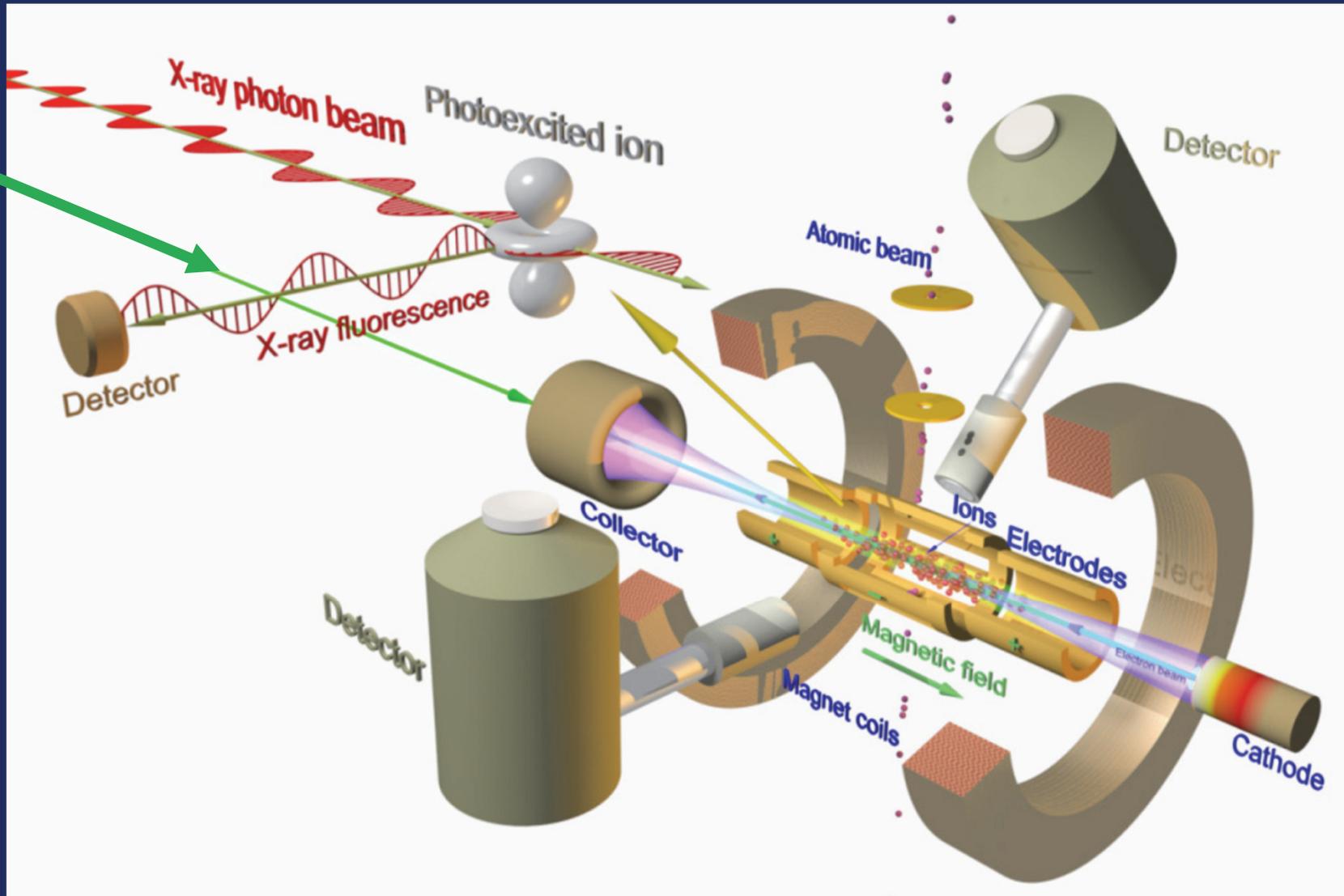
Combine novel X-ray sources (free-electron lasers, synchrotrons) with electron beam ion trap (EBIT)

- to measure **excitation energies** beyond current accuracy limits
- to determine **cross sections** and **line profiles** for photoexcitation, photoionization HCI benchmarking atomic theory

Interaction with photon beams



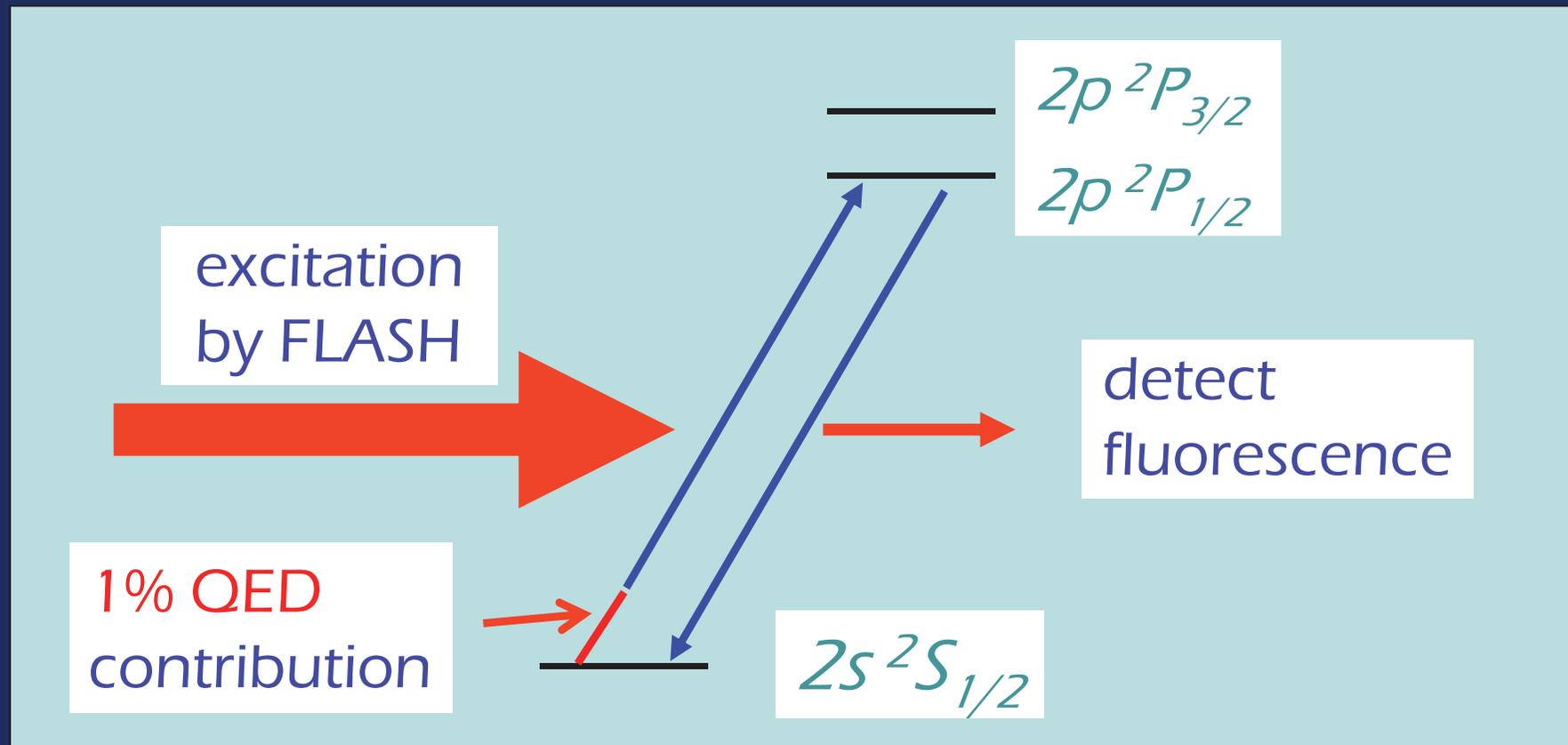
Resonant **photon excitation** in EBIT



- Synchrotron radiation (PETRAIII),
 - Free-electron lasers (LCLS) ,
- provide **X-rays with high power and energy resolution**

Soft X-ray laser spectroscopy at FLASH

FEL 50 eV beam excites resonantly
the $2s-2p$ transition in **Li-like Fe^{23+}** at 50 eV



S. W. Epp *et al.*, Phys. Rev. Lett. 98 (2007) 183001



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LCLS: Linac Coherent Light Source



last km
of SLAC

300 m of
undulators

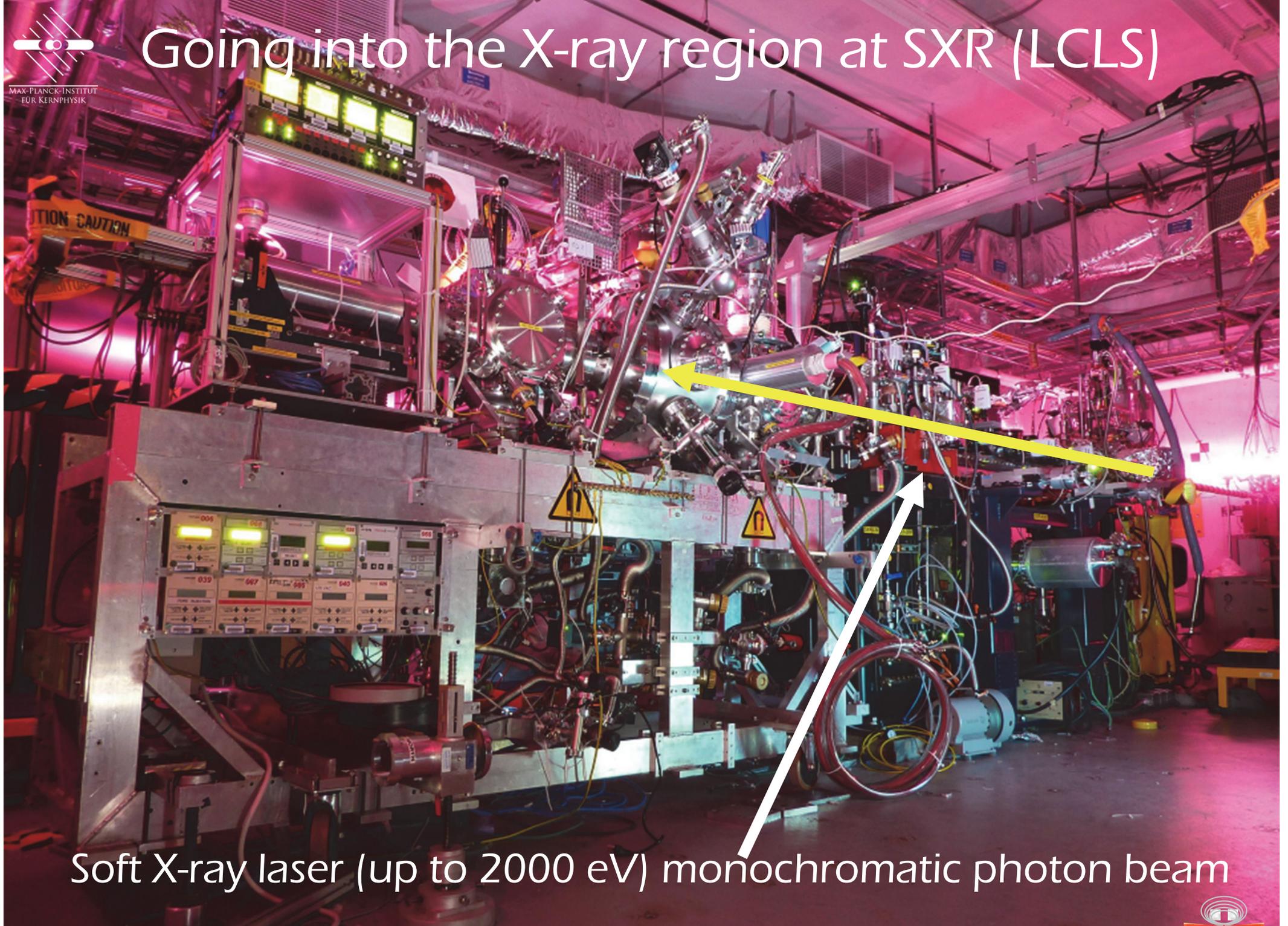
Photon bunches:

- 2 mJ
- 10...300 fs
- 120 Hz
- 550 eV...11000 eV

EBIT at SXR

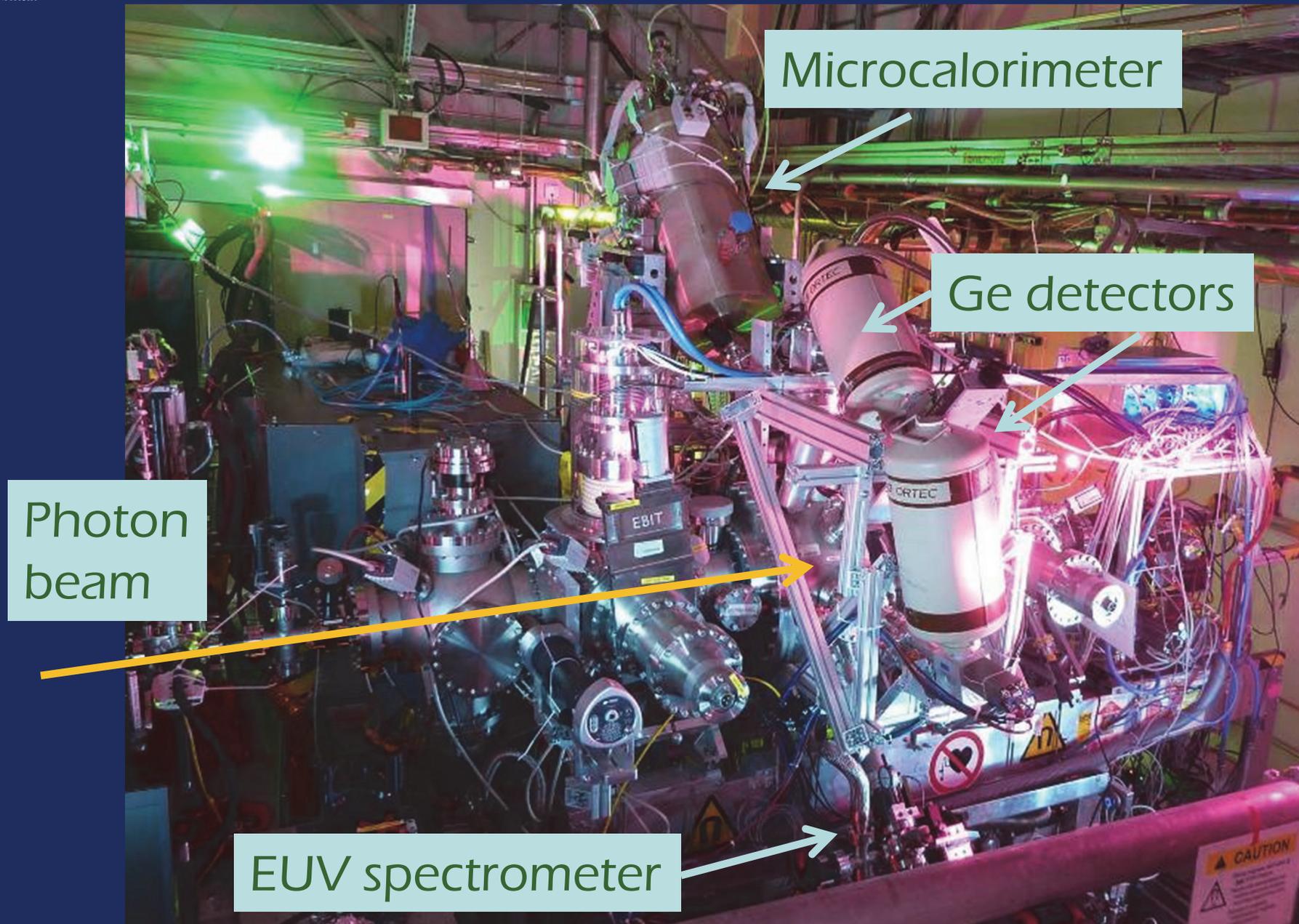


Going into the X-ray region at SXR (LCLS)

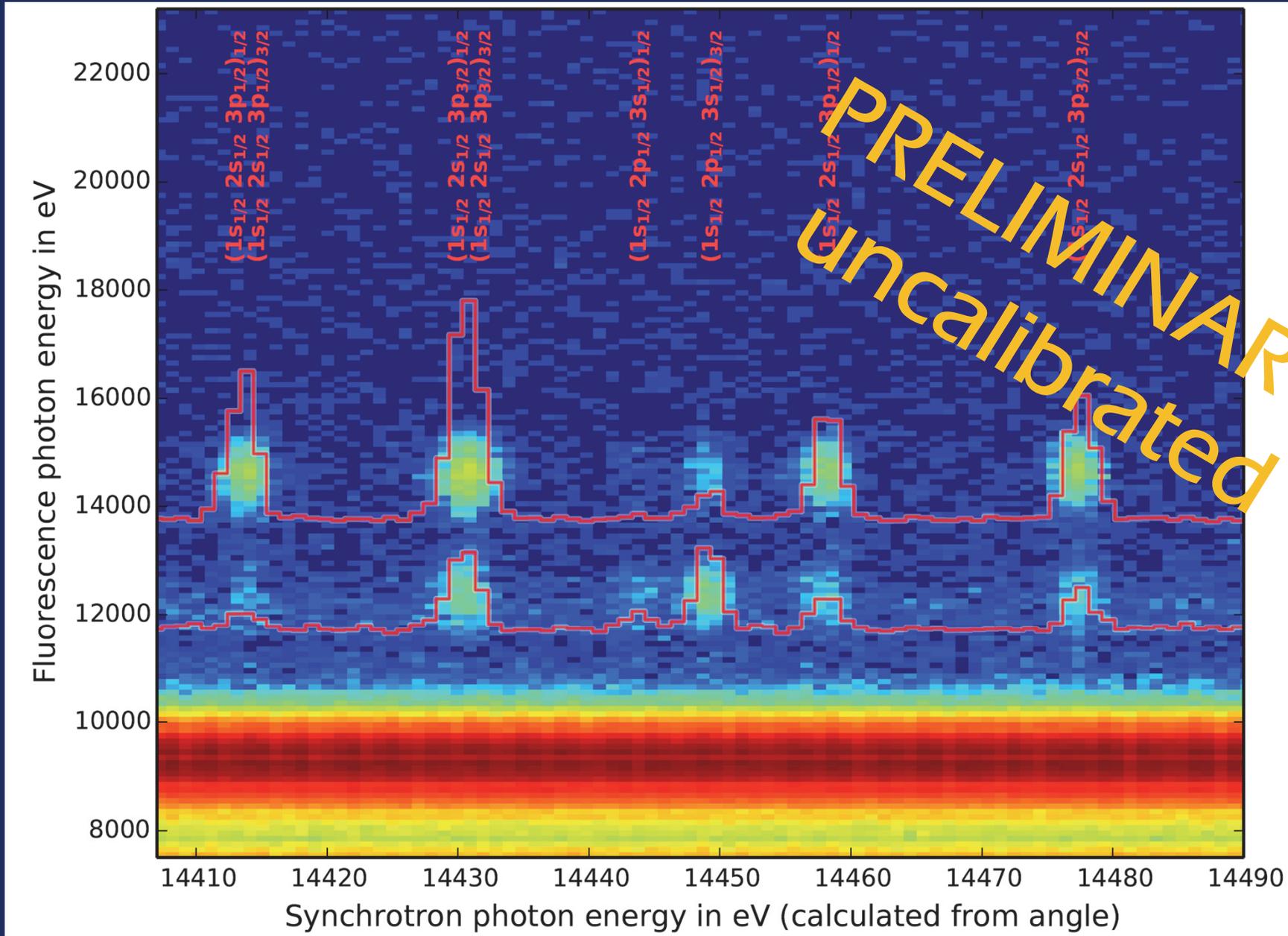


Soft X-ray laser (up to 2000 eV) monochromatic photon beam

Adding X-ray fluorescence detectors

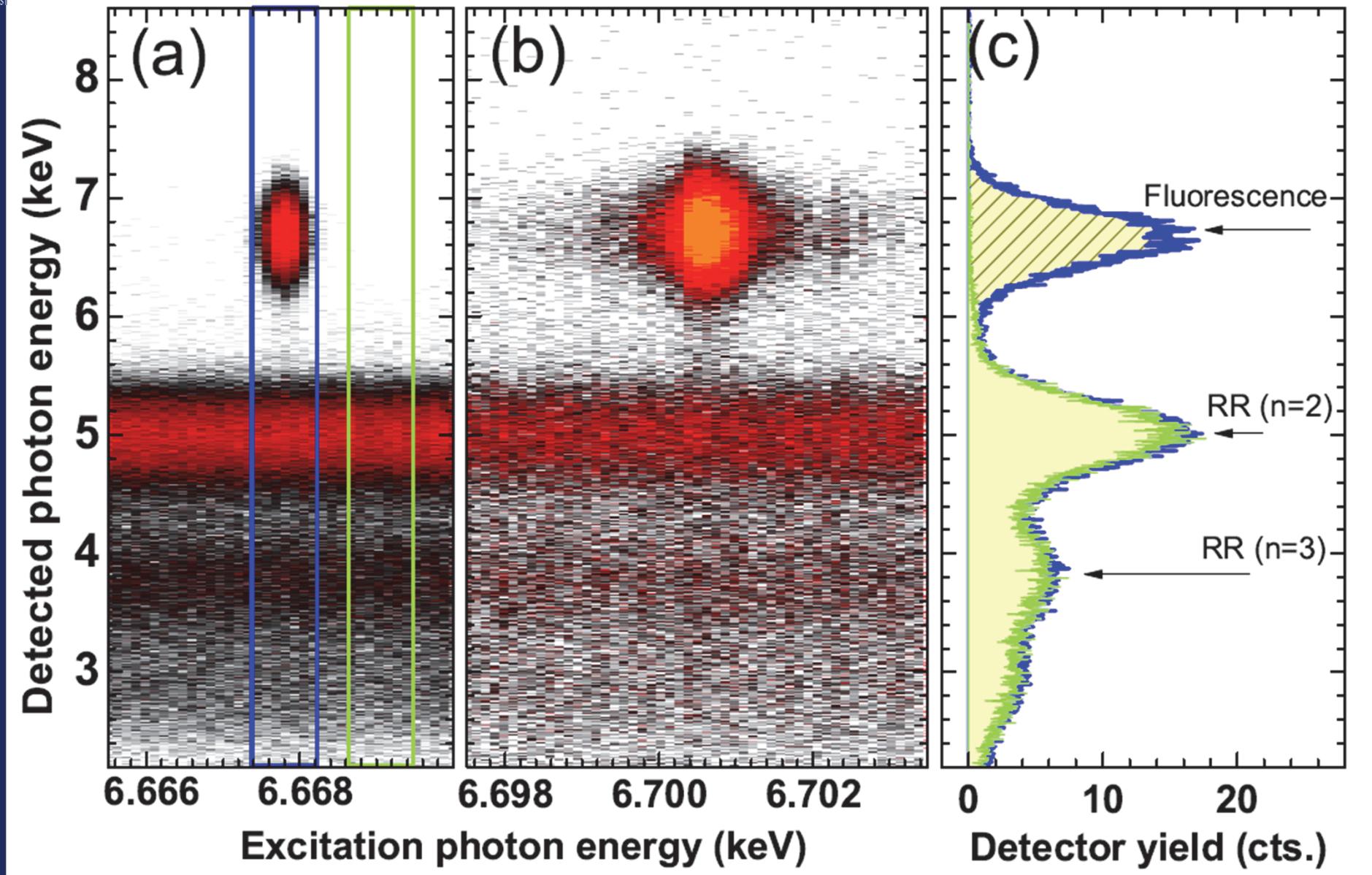


New results: Overview spectra of Br^{33+} (Li-like)



S. Bernitt, MPIK (2016)

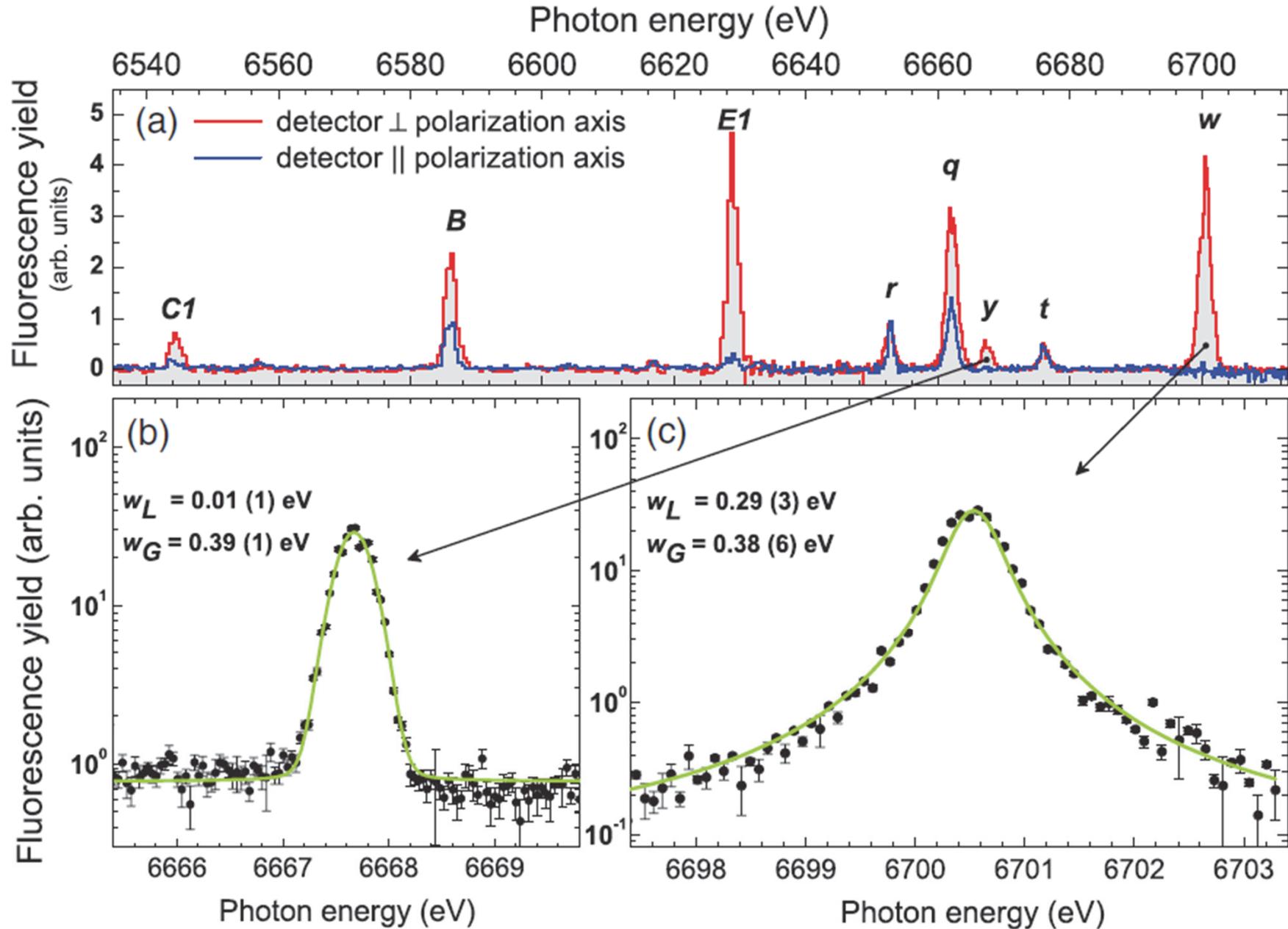
High resolution scans show line widths



X-ray energy scanned by monochromator



Overview and detailed scans



Linewidth determinations in Fe^{23+} and Fe^{24+}

Line	Experiment	Theory	MCDF		
			Radiative	Auger	Total
<i>w</i>	311 (10)	301 [49] 301 [35] 303 [33] 315 [50]	301	0	301
<i>q</i>	255 (31)	310 [33]	312	0.081	312
<i>r</i>	250 (11)	226 [33]	208	32	241
<i>t</i>	131 (29)	167 [33]	112	52	163
<i>E1</i>	437 (12)	382 [33]	292	95	387
<i>E2</i>	178 (34)	149 [33]	31	136	167
<i>C1</i>	524 (12)	499 [33]	218	334	552
<i>C2</i>	385 (207)	611 [33]	412	135	547
<i>N1</i>	565 (45)	498 [33]	146	400	546
<i>N2</i>	594 (50)	504 [33]	164	338	502
<i>N3</i>	570 (109)	505 [33]	155	360	515
<i>O1</i>	859 (229)	756 [33]	264	529	793
<i>O2</i>	772 (228)	785 [33]	304	518	822
<i>F</i>	998 (203)	989 [33]	351	651	1020

Natural linewidths w_L of $1s \rightarrow 2p$ transitions (in meV)

J. K. Rudolph et al., PRL 111, 103002 (2013)

Transition energies

TABLE I. X-ray transitions of heliumlike to fluorinelike iron ions resonantly excited from the ground state with synchrotron radiation. X-ray fluorescence was detected as a function of photon energy. Energies are given in units of eV. The calibration is based on the absorption edge technique. The experimental uncertainties are shown as (statistical)(systematic). Relative energies are not affected by the systematic uncertainty which accounts for a shift of the absolute scale. Angle brackets enclose results affected in their accuracy by line blends.

Ion	Line	Initial state	Final state	This experiment	Theory	Theory	Experiment
Fe ²⁴⁺	w	1s ² 1S ₀	1s 2p 1P ₁	6700.549 (5) (70)	6700.4347 (11) [32] 6700.490 [34]	6700.4 [33] 6700.4 [35]	6700.8 [22] 6700.4 [23] 6700.9 [36]
Fe ²⁴⁺	y	1s ² 1S ₀	1s 2p 3P ₁	6667.671 (3) (69)	6667.5786 (12) [32] 6667.629 [34]	6667.6 [33] 6667.6 [35]	6667.9 (4) [22] 6667.5 [23] 6667.5 [36]
Fe ²³⁺	t	1s ² 2s ² S _{1/2}	1s 2s 2p ² P _{1/2}	6676.202 (3) (69)	6676.129 (47) [37] 6675.8 [38]	6676.4 [33]	⟨6676.8 (7)⟩ [22] 6676.3 [23]
Fe ²³⁺	q	1s ² 2s ² S _{1/2}	1s 2s 2p ² P _{3/2}	6662.240 (6) (69)	6662.188 (11) [37] 6661.9 [38]	6661.9 [33]	6662.1 (5) [22] 6662.2 [23]
Fe ²³⁺	r	1s ² 2s ² S _{1/2}	1s 2s 2p ² P _{1/2}	6652.826 (3) (69)	6652.776 (25) [37] 6652.6 [38]	6653.5 [33]	⟨6654.2 (7)⟩ [22] 6652.5 [23]
Fe ²³⁺	u	1s ² 2s ² S _{1/2}	1s 2s 2p ⁴ P _{3/2}	6616.629 (4) (68)	6616.559 (11) [37]	6616.7 [33]	⟨6617.9 (1.2)⟩ [22] 6616.6 [23]
Fe ²²⁺	E1	1s ² 2s ² 1S ₀	1s 2s ² 2p 1P ₁	6628.804 (5) (68)	6631.057 [39] 6627.4 ^a /6628.3 ^b	6628.7 [33] 6627.39 [40]	6628.9 (3) [22] 6628.7 [23]
Fe ²²⁺	E2	1s ² 2s ² 1S ₀	1s 2s ² 2p ³ P ₁	6597.858 (3) (67)	6596.55 [40] 6596.1 ^a /6597.7 ^b	6595.8 [33]	
Fe ²¹⁺	B	1s ² 2s ² 2p ² P _{1/2}	1s 2s ² 2p ² P _{1/2} 1s 2s ² 2p ² D _{3/2}	⟨6586.085 (7) (67)⟩ ⟨6586.085 (7) (67)⟩	6586.3 ^a /6585.1 ^b 6587.0 ^a /6585.8 ^b (6587.2) [41]	6586.3 [33] 6586.5 [33]	⟨6585.9 (5)⟩ [22] ⟨6585.7⟩ [23]
Fe ²⁰⁺	C1	1s ² 2s ² 2p ² 3P ₀	1s 2s ² 2p ³ 3D ₁	6544.225 (4) (66)	6544.8 ^a /6544.0 ^b	6543.6 [33]	⟨6544.6 (9)⟩ [22] ⟨6544.4⟩ [23]
Fe ²⁰⁺	C2	1s ² 2s ² 2p ² 3P ₀	1s 2s ² 2p ³ 3S ₁	6556.879 (16) (66)	6557.3 ^a /6556.3 ^b	6555.0 [33]	
Fe ¹⁹⁺	N1	1s ² 2s ² 2p ³ 4S _{3/2}	1s 2s ² 2p ⁴ 4P _{5/2}	6497.067 (5) (65)	6497.5 ^a /6497.2 ^b	6496.6 [33]	⟨6497.7 (1.4)⟩ [22] 6497.3 [23]
Fe ¹⁹⁺	N2	1s ² 2s ² 2p ³ 4S _{3/2}	1s 2s ² 2p ⁴ 2P _{3/2}	6506.845 (7) (65)	6507.3 ^a /6506.9 ^b	6506.0 [33]	⟨6509.6 (1.4)⟩ [22] ⟨6509.1⟩ [23]
Fe ¹⁹⁺	N3	1s ² 2s ² 2p ³ 4S _{3/2}	1s 2s ² 2p ⁴ 4P _{1/2}	6509.133 (14) (65)	6509.6 ^a /6509.1 ^b	6508.1 [33]	⟨6509.6 (1.4)⟩ [22] ⟨6509.1⟩ [23]
Fe ¹⁸⁺	O1	1s ² 2s ² 2p ⁴ 3P ₂	1s 2s ² 2p ⁵ 3P ₂	6466.900 (14) (64)	6467.4 ^a /6466.5 ^b 6466.3 [41]	6564.4 [33]	6467.6 (1.7) [22] ⟨6466.5⟩ [23]
Fe ¹⁸⁺	O2	1s ² 2s ² 2p ⁴ 3P ₂	1s 2s ² 2p ⁵ 3P ₁	6474.318 (33) (64)	6474.9 ^a /6473.9 ^b 6473.7 [41]	6473.0 [33]	⟨6472.7 (2.7)⟩ [22] ⟨6474.7⟩ [23]
Fe ¹⁷⁺	F	1s ² 2s ² 2p ⁵ 2P _{3/2}	1s 2s ² 2p ⁶ 2S _{1/2}	6435.239 (14) (63)	6435.7 ^a /6434.6 ^b	6434.8 [33]	6436.1 (2.0) [22] 6434.8 [23]

^aOur theoretical results obtained in the framework of the multiconfiguration Dirac-Fock (MCDHF) method [29]

^bOur theoretical results using the Flexible Atomic Code (FAC) of Gu with the standard configuration-interaction package [42].

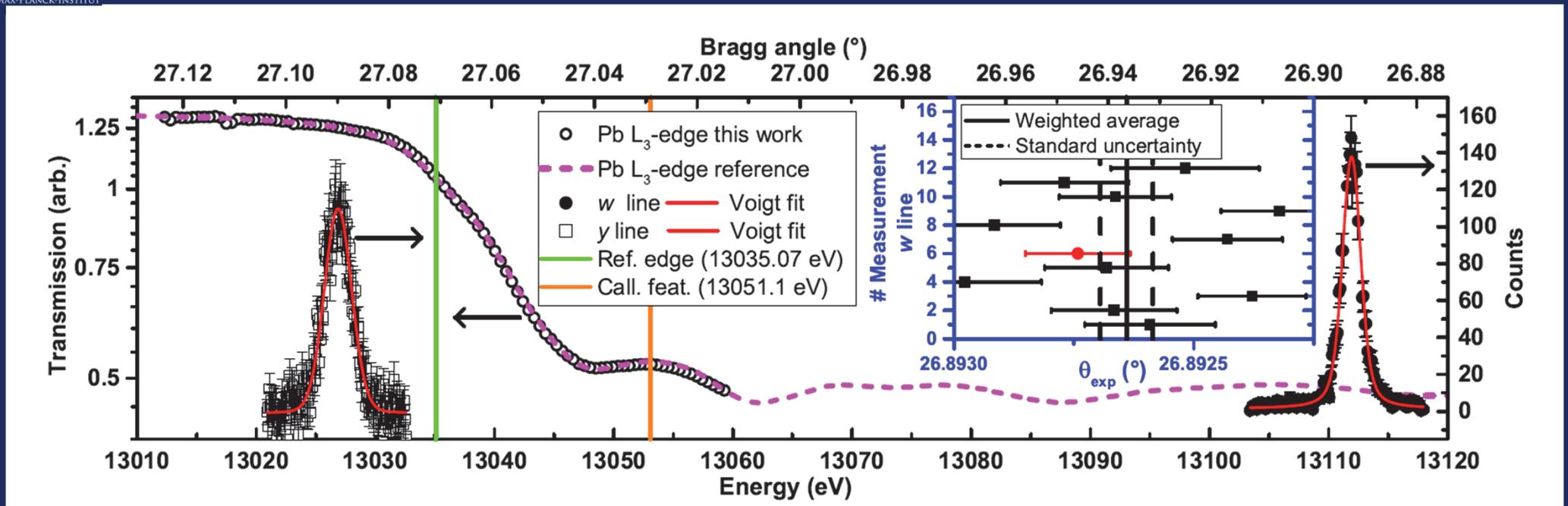
16 dominant
transitions
measured
with high
precision

J. K. Rudolph et al.,
PRL 111, 103002
(2013)



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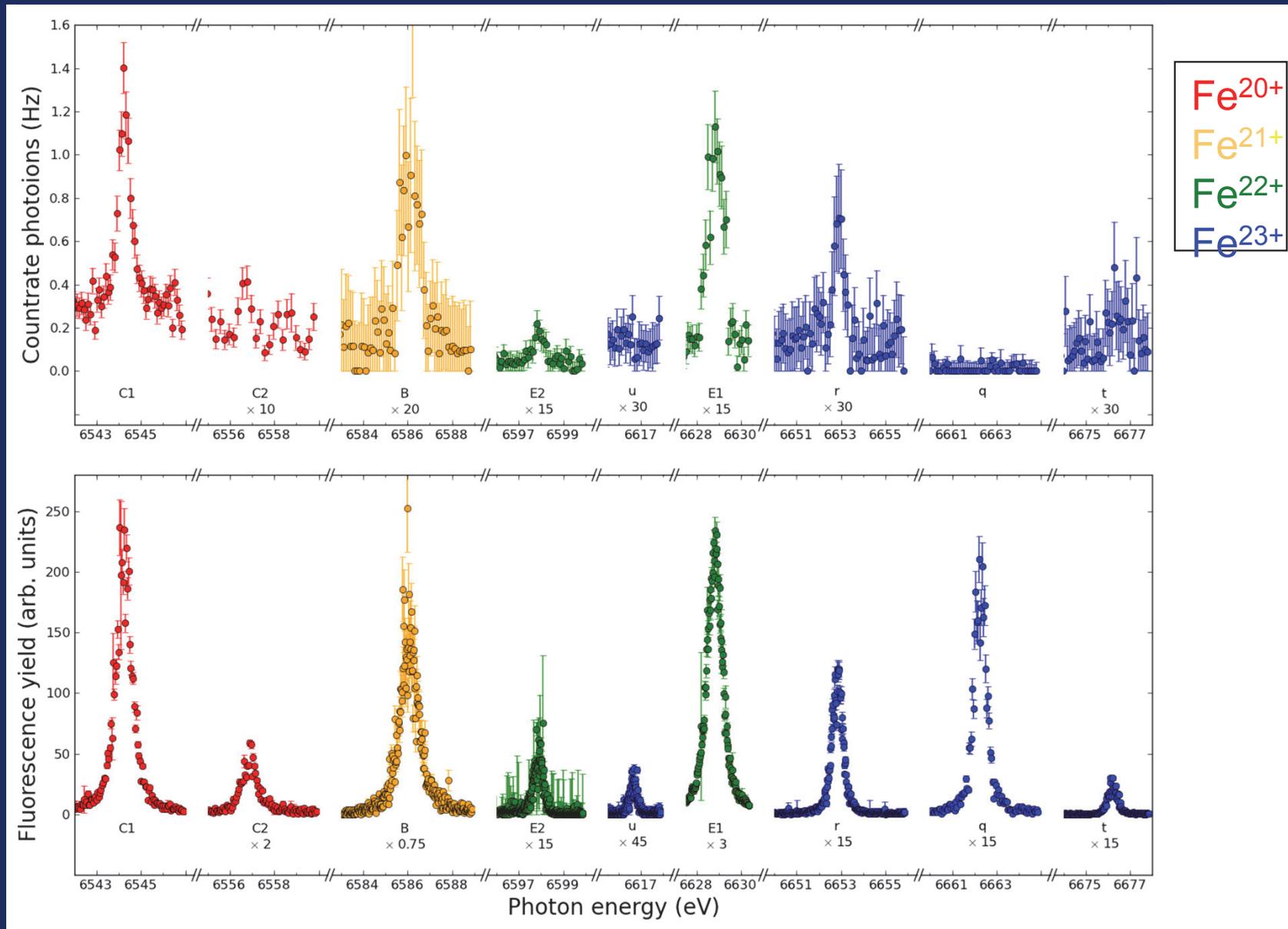
Petra III: Kr³⁴⁺ resonant excitation



Experimental raw data (Si(333)) of the w and y line along with the Pb L₃-edge absorption spectrum (PbL) for energy calibration. The w data points show a result from a single scan (15 minutes). Fitted Bragg angle is 26.89274(4) degrees. The y line is an overlay of 25 single scans. PbL (open circles): our data scaled to the (dashed) reference data. Inset (blue): Centroids from 12 individual scans of w.

Epp et al, PRA 92, 020502(R) (2015)

Fluorescence vs. photoion yield

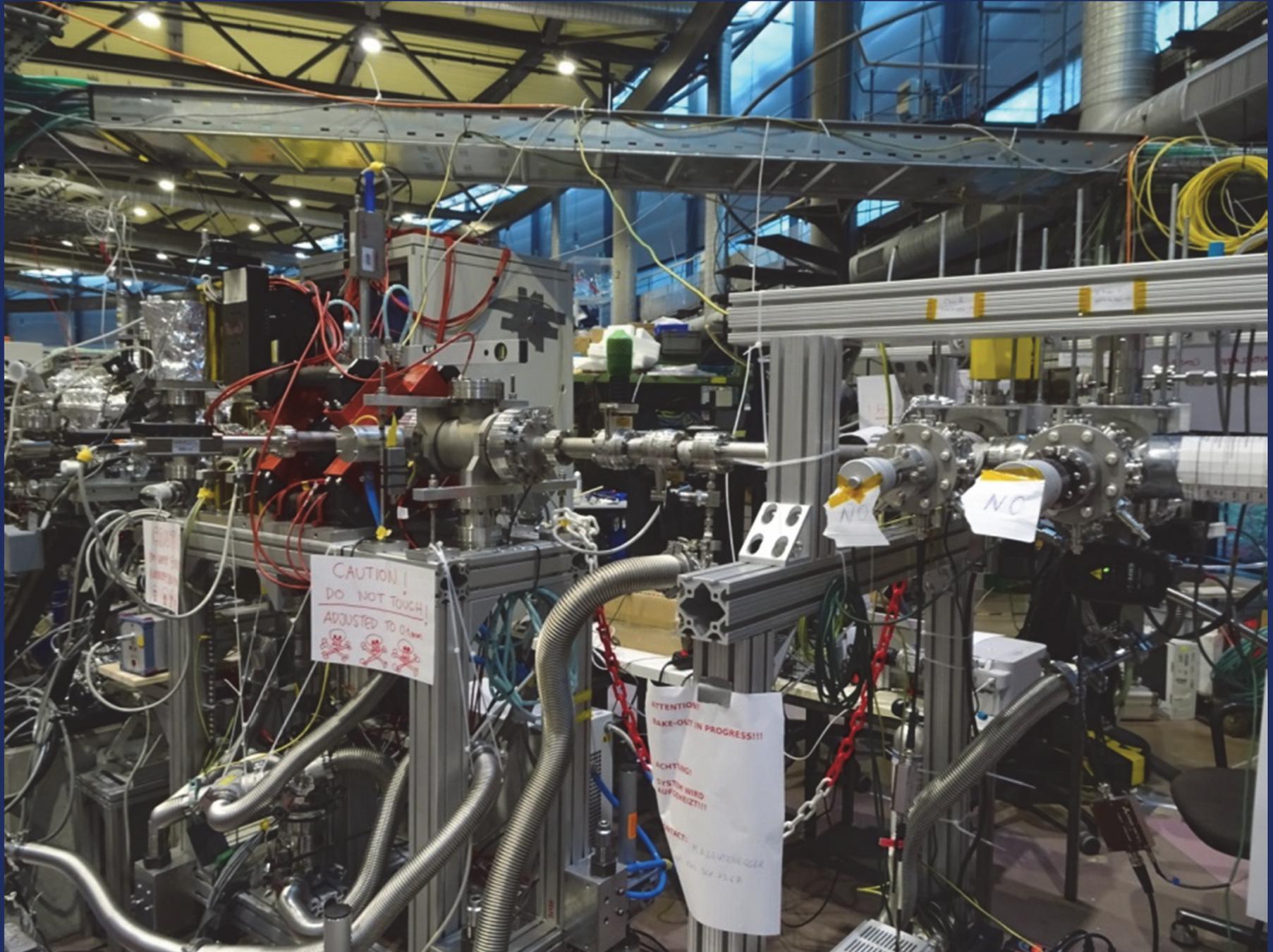


R. Steinbrügge et al., PRA 91, 032502 (2015)

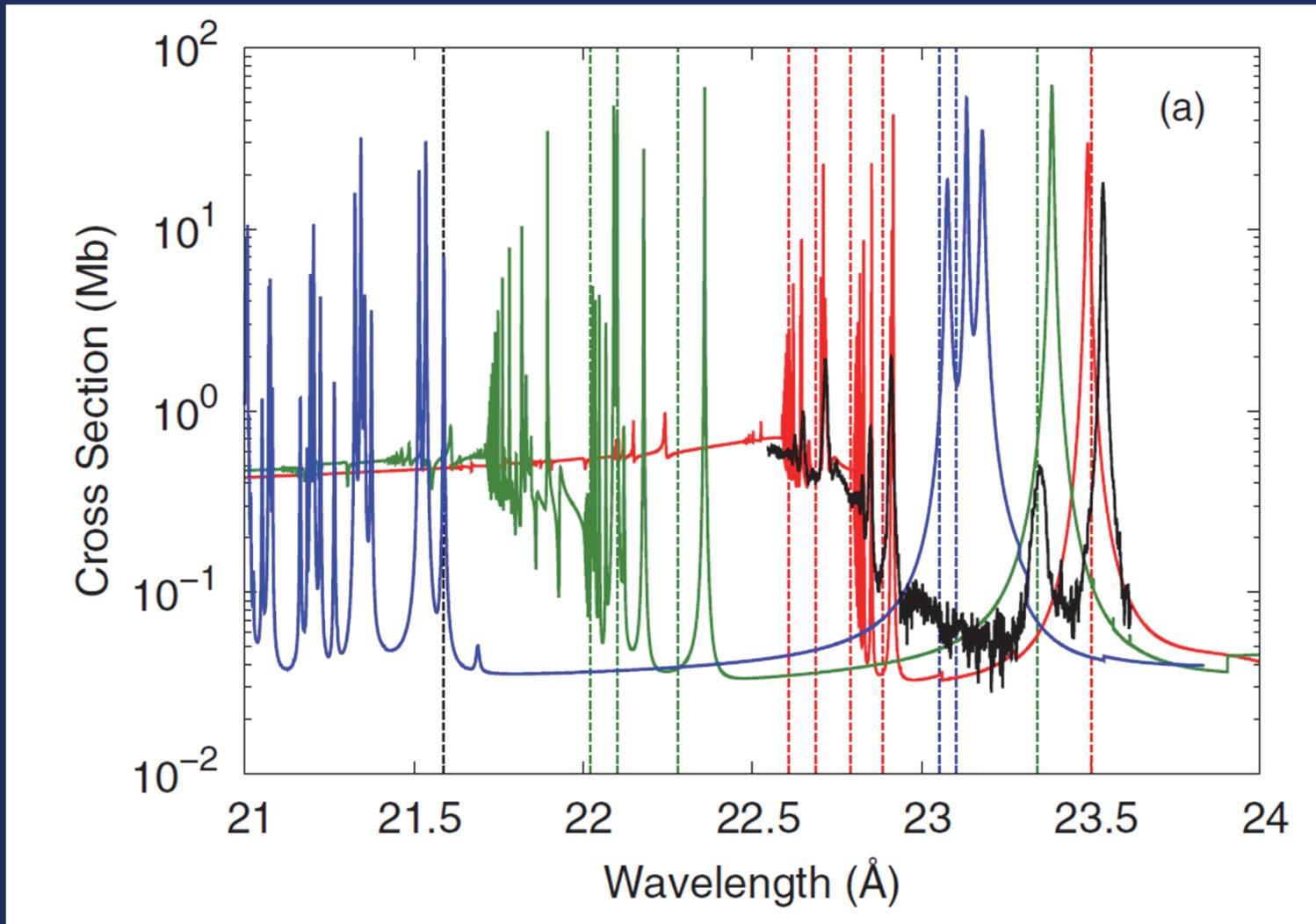
- 70 meV systematic uncertainty of the calibration
- 5 meV typical statistical uncertainties
- For $Z > 18$ never measured so precisely

J. K. Rudolph et al., PRL 111, 103002 (2013)

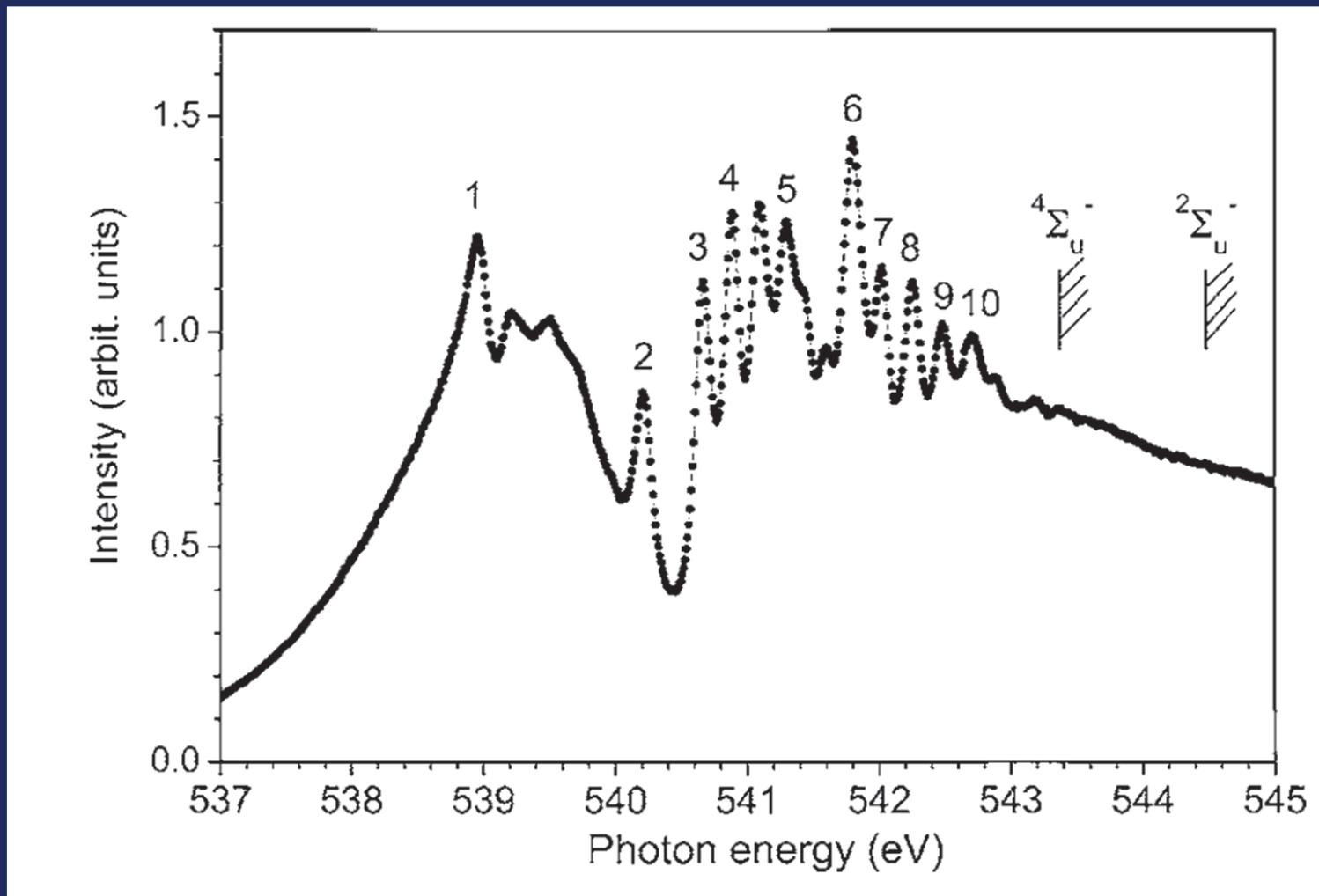
PolarX-EBIT and gas-cell setup



Some theory models vs. experiments

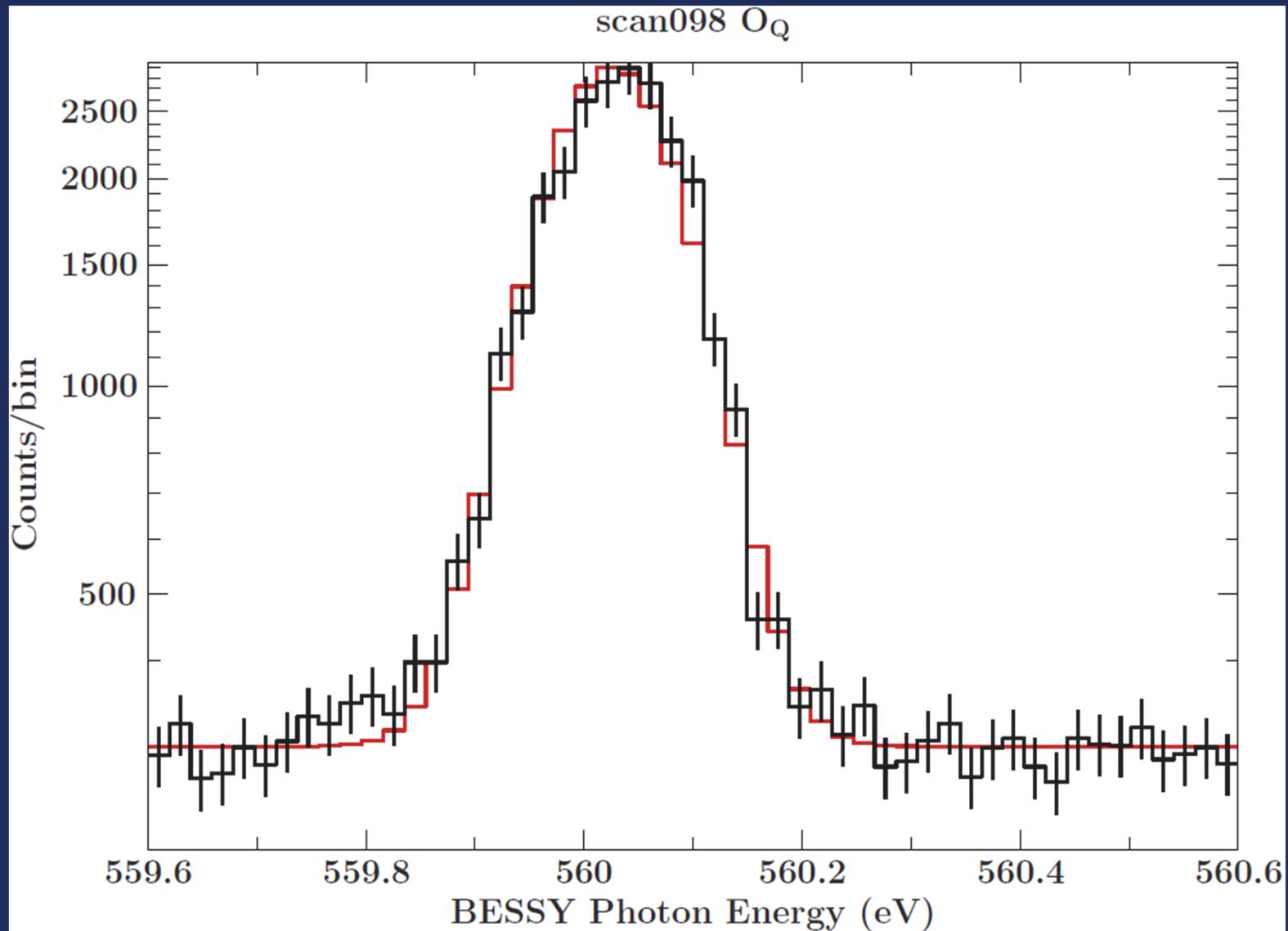


O₂ photoabsorption

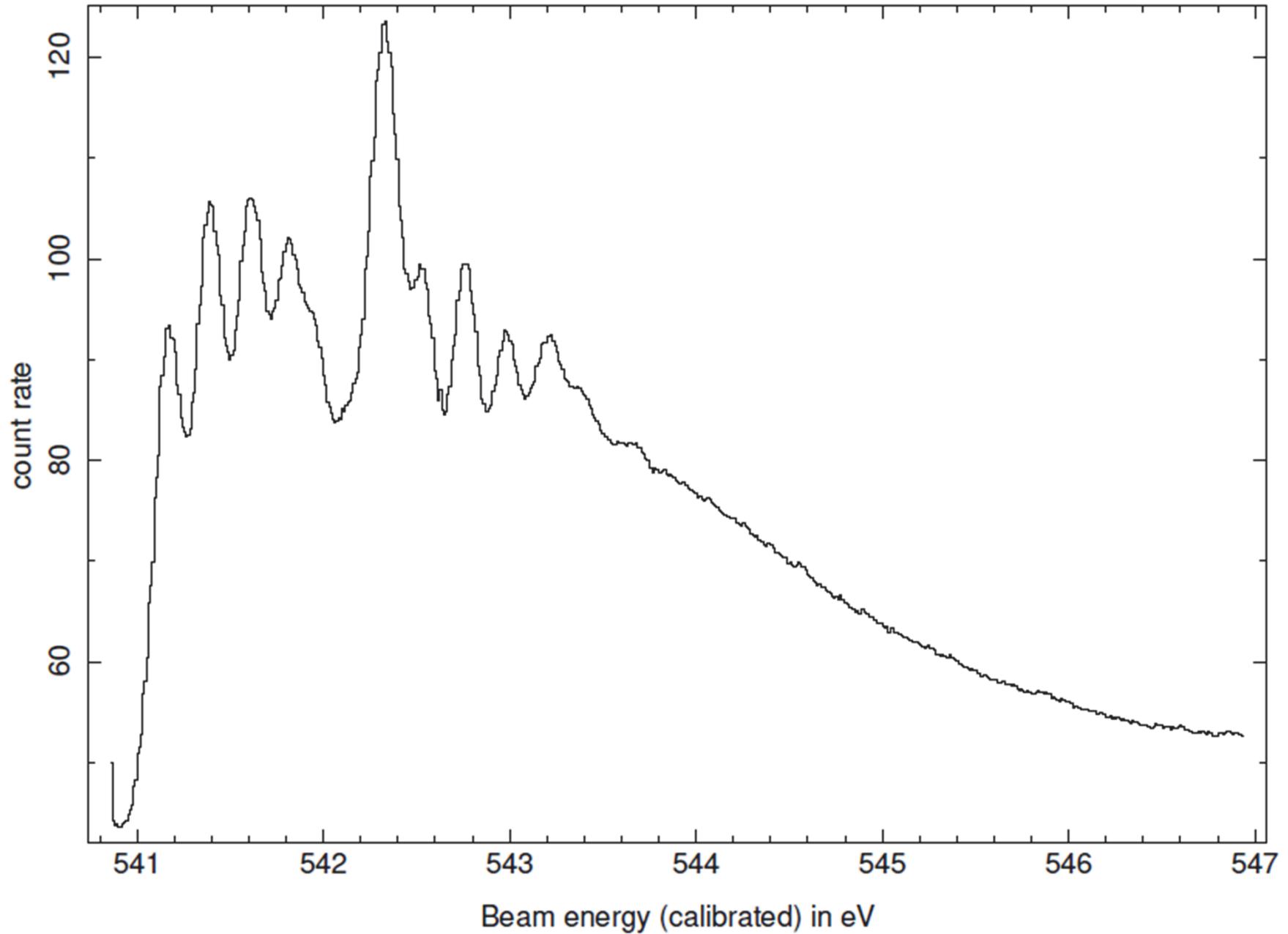


From: Feifel et al.

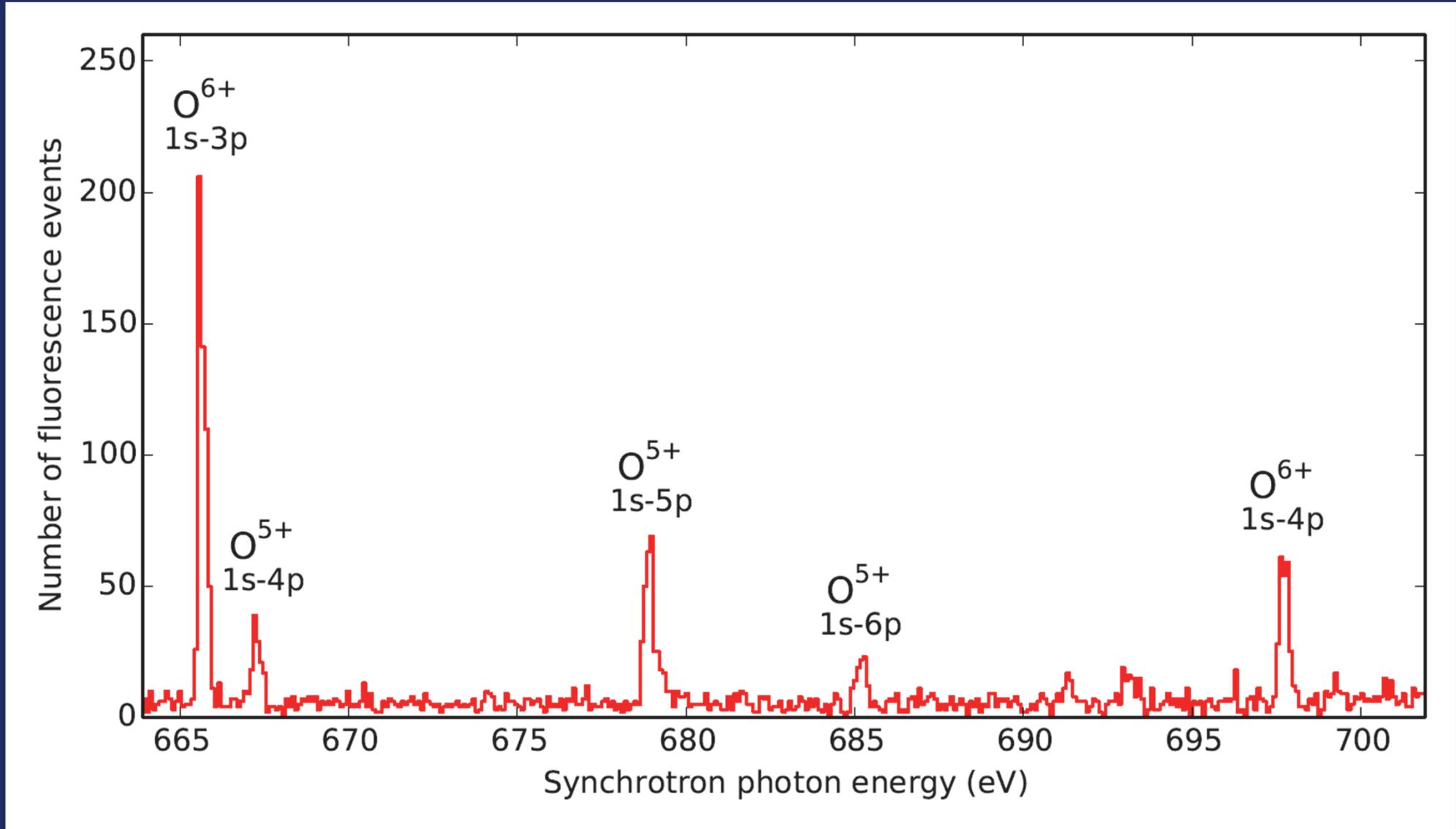
He-like O^{5+} 1s-2p (line q)



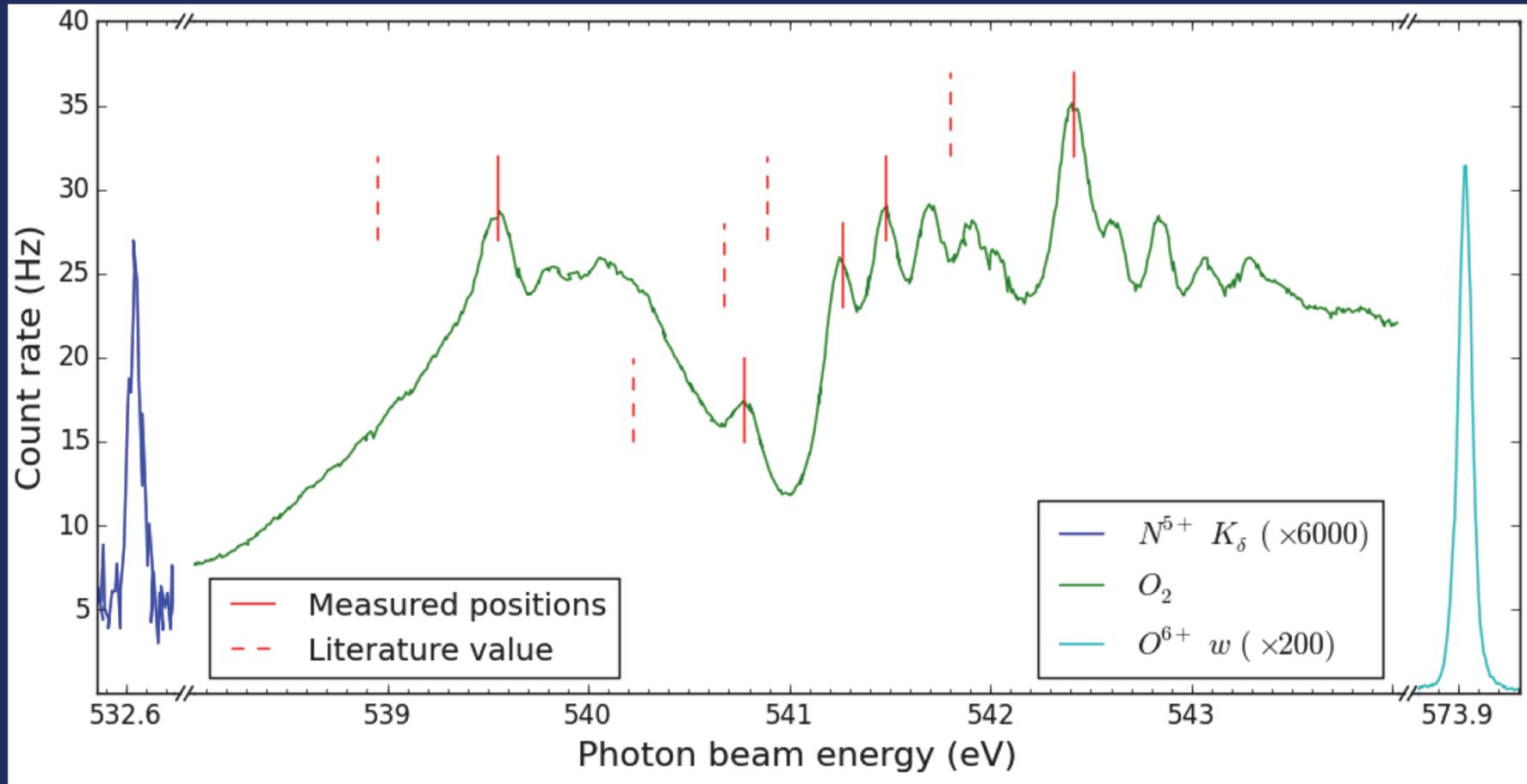
O₂ absorption edges



Overview spectrum at low resolution and statistics

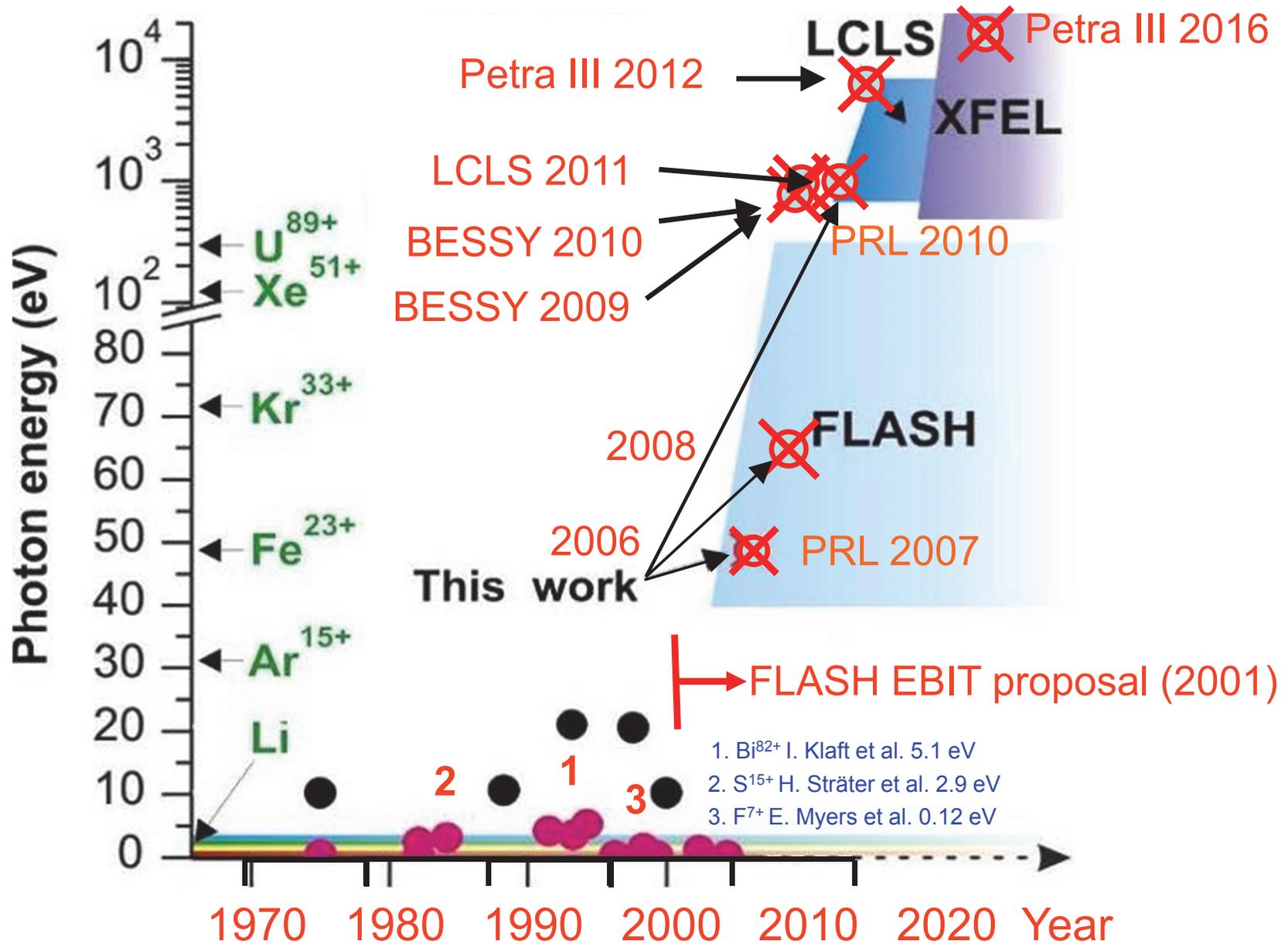


≈500 meV offset relative to old calibration!



G.V. Brown, P. Beiersdorfer, T. Lockard (LLNL); R. Kelley, C.A. Kilbourne,
M.A. Leutenegger, F.S. Porter (GSFC); J. Wilms (FAU)

Photon energy range accessed

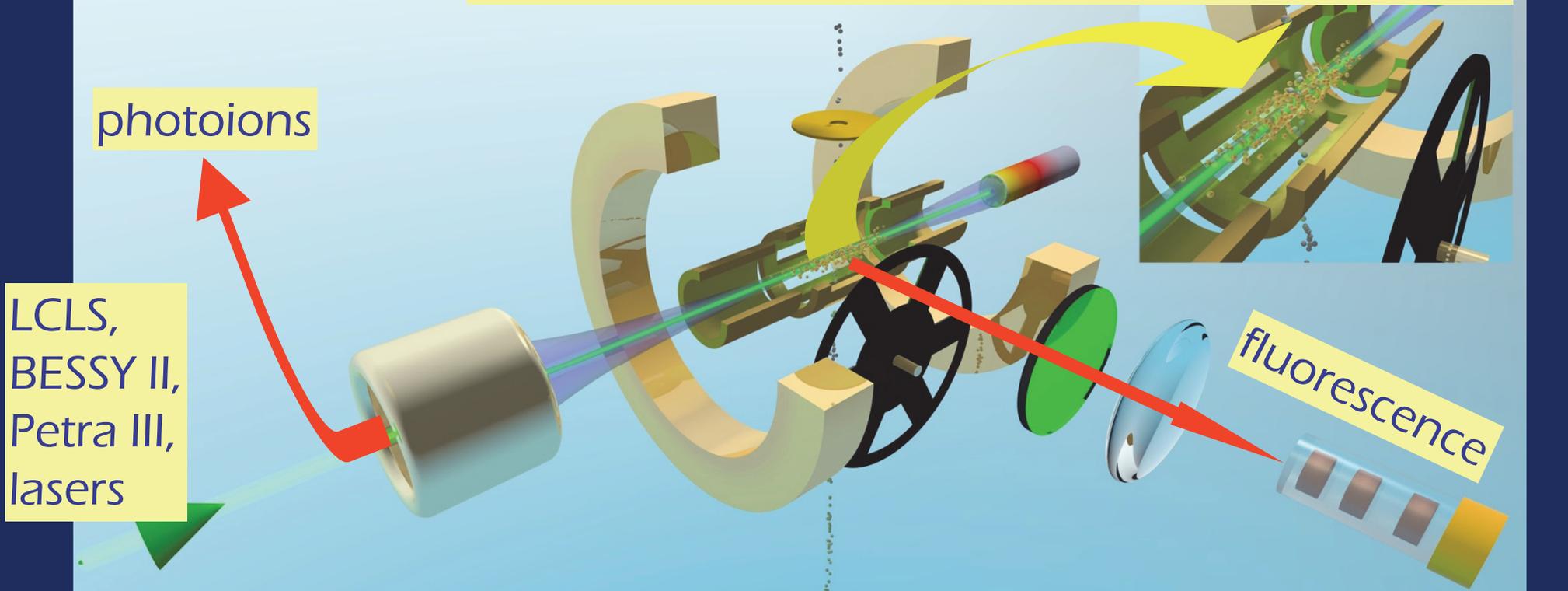




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Resonant photon excitation in EBITs

Photon beams interact with trapped ions



photoions

LCLS,
BESSY II,
Petra III,
lasers

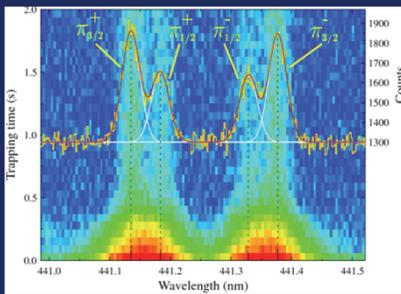
fluorescence

Visible M1
 Ar^{13+}

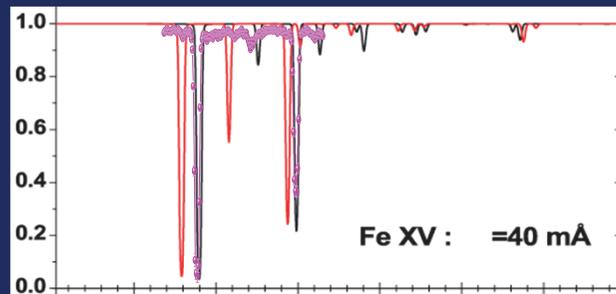
Soft X-ray photoionization
 Fe^{14+}

FEL 800 eV
 Fe^{16+}

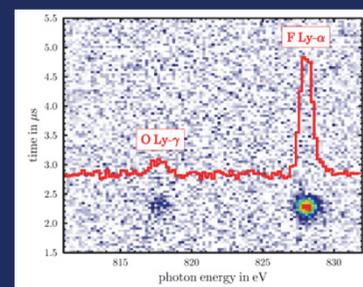
Synchrotron 6 keV
 Fe^{24+} , 13 keV Kr^{34+}



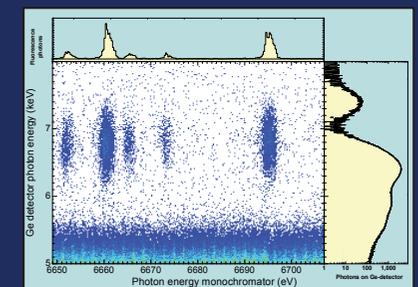
V. Mäckel et al.,
PRL 107 143002
(2011)



M. C. Simon et al.,
PRL 105 183001
(2010)



S. Bernitt et al.,
Nature 492, 225
(2012)



J. Rudolph et al.,
PRL 111, 103002
(2013)

Ar¹²⁺ : ionization potential 684 eV

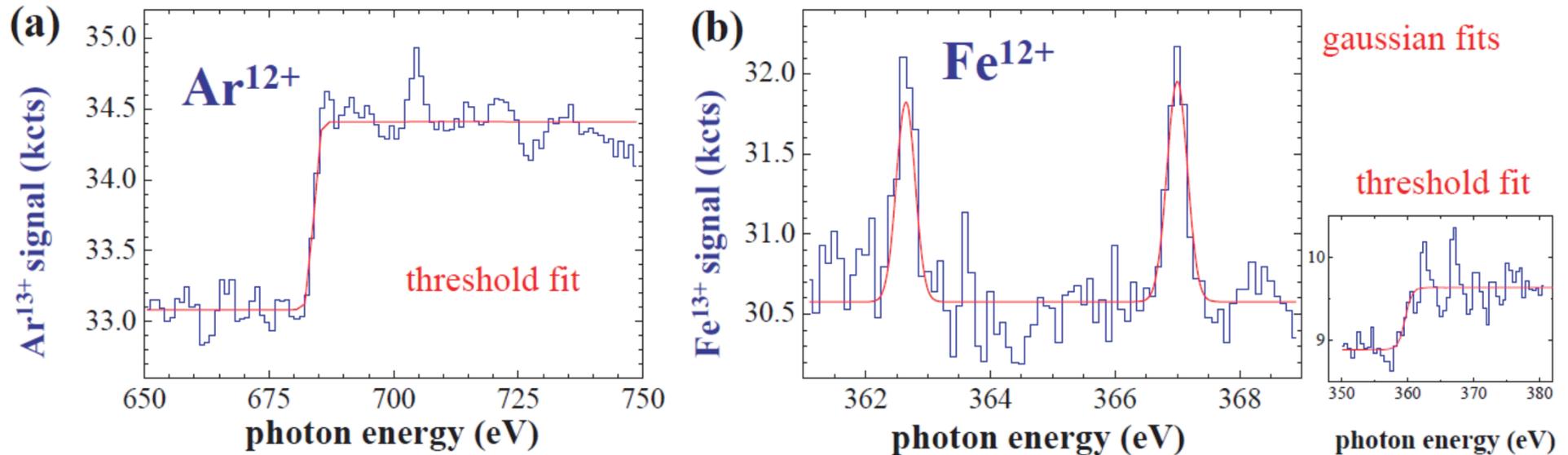
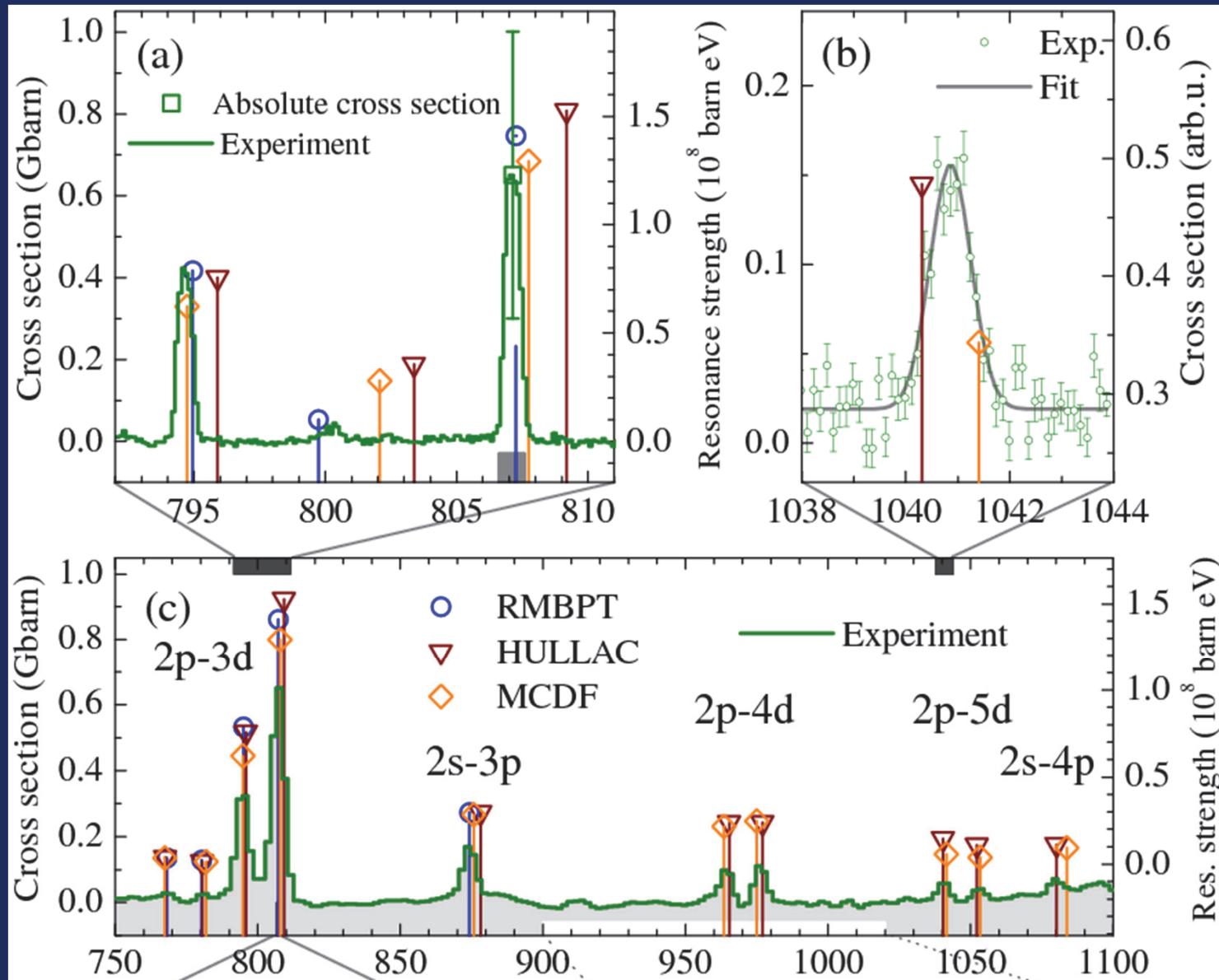


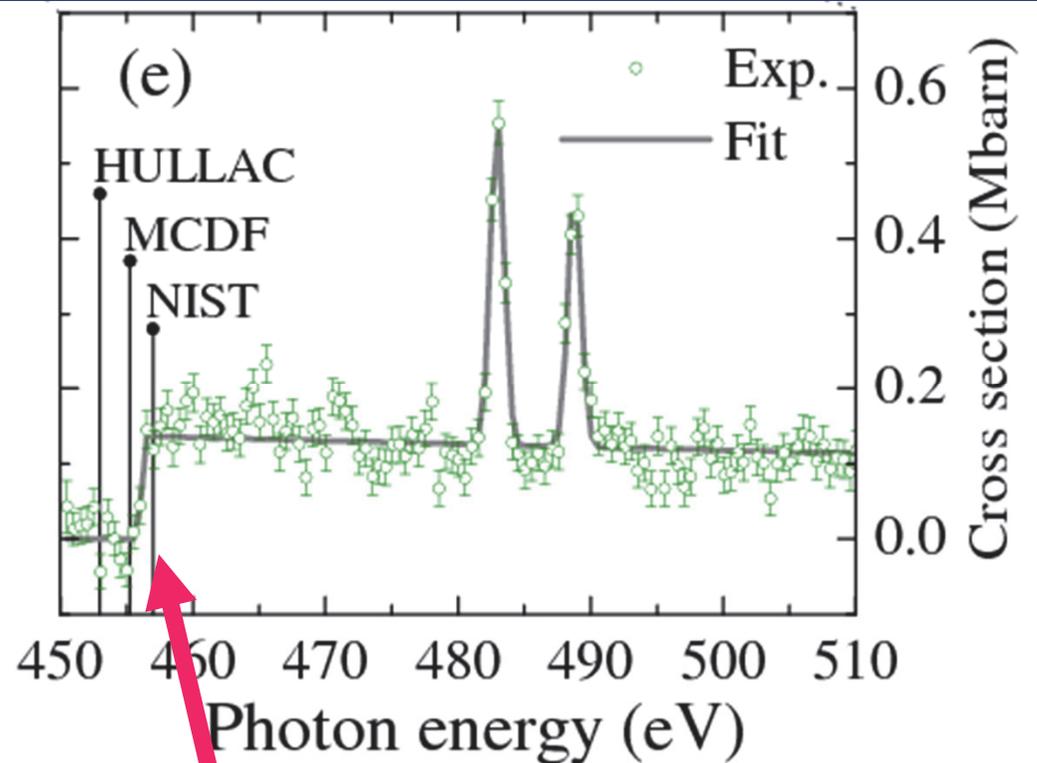
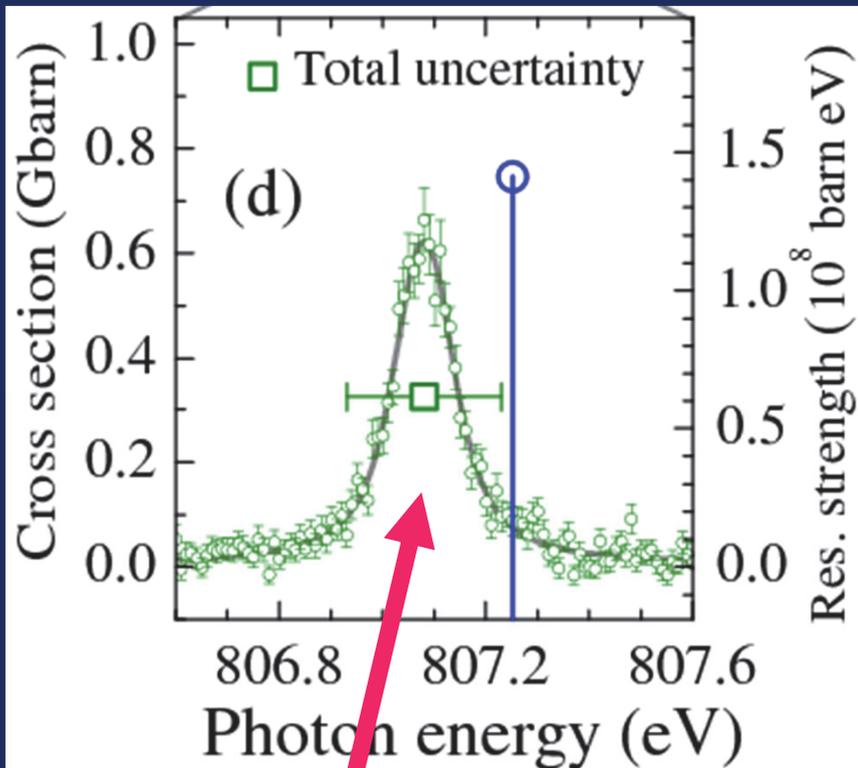
Figure 4. (color online) PI of ions in charge state $q=12$ demonstrate the ability to access HCIs by the EBIT based method. (a) PI threshold of Ar¹²⁺ at 683.93 eV, obtained by a fit to the Ar¹³⁺-signal. The strong background signal below the ionization edge is mainly caused by residual gas ions with close lying charge-to-mass ratios (O⁵⁺, C⁴⁺). (b) Near-threshold PI of Fe¹²⁺ revealing two significant resonances at 362.6 eV and 370.0 eV.

Fe¹⁴⁺ photoionization



M. C. Simon et al., PRL 105 (2010) 183001

Fe¹⁴⁺ photoionization

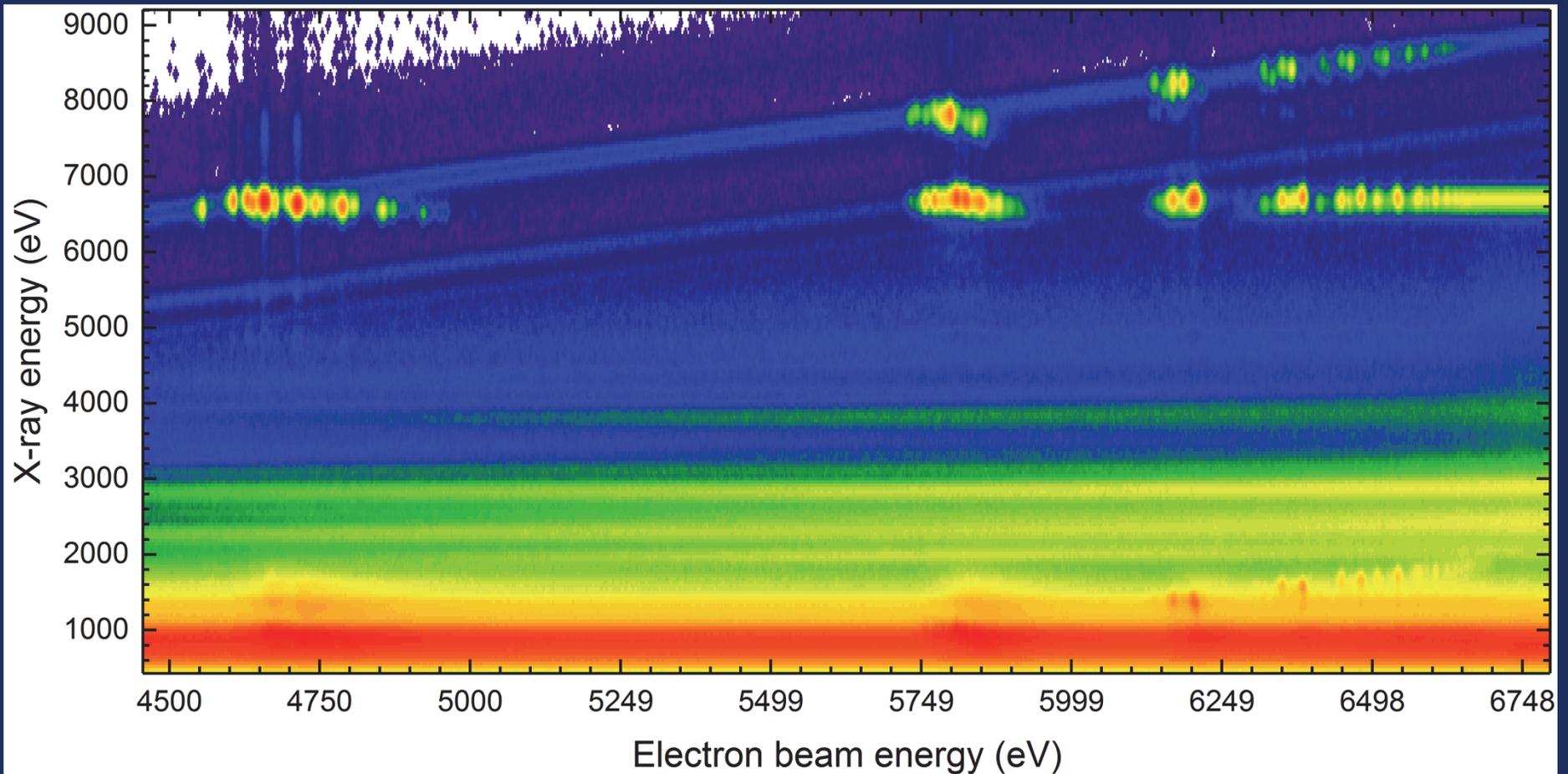


Strong resonances
allow high resolution
nearly reaching natural
line width

Current sensitivity for
non-resonant
photoionization
around 20 kbarn

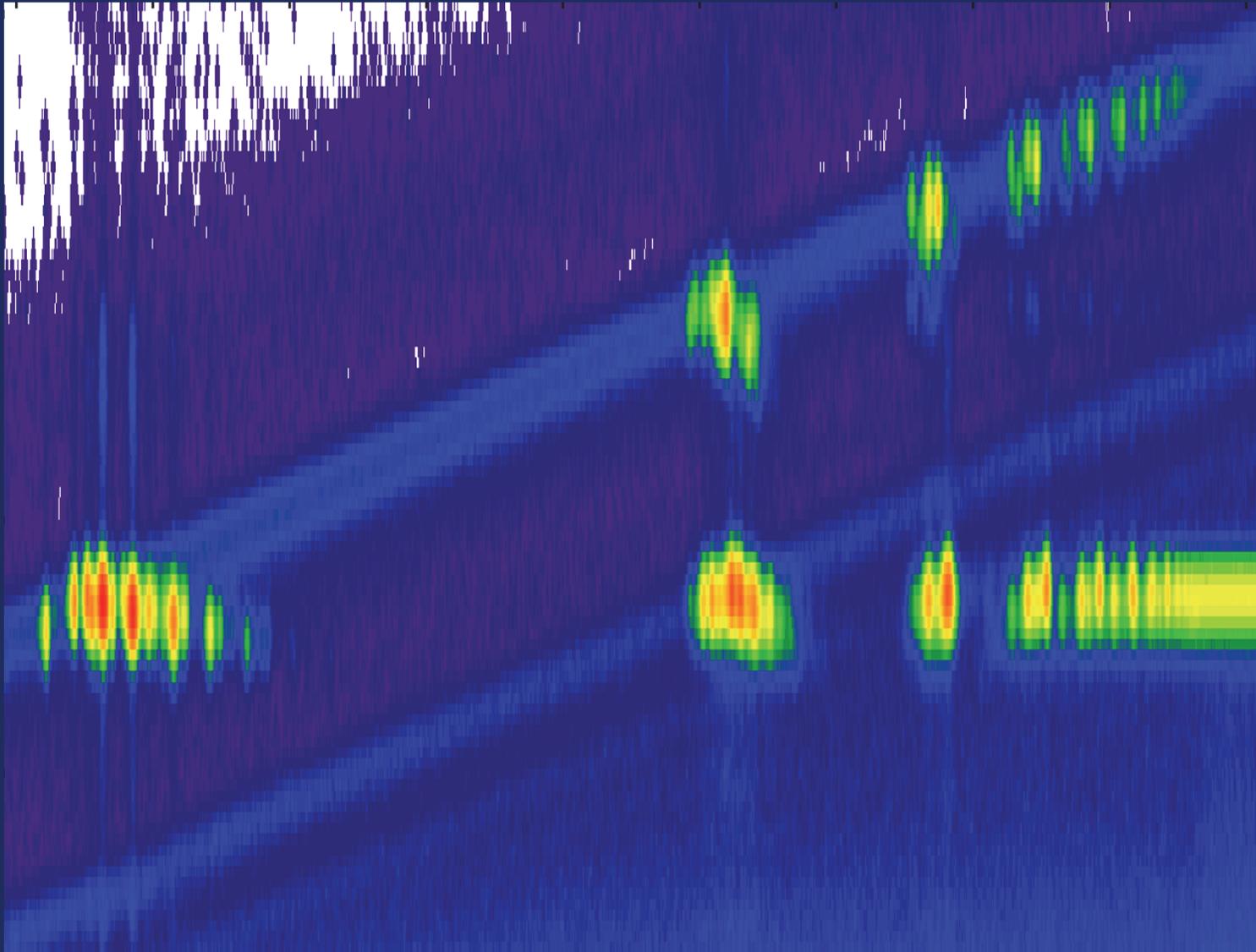
Electron-driven resonant processes

X-ray data depending on electron energy



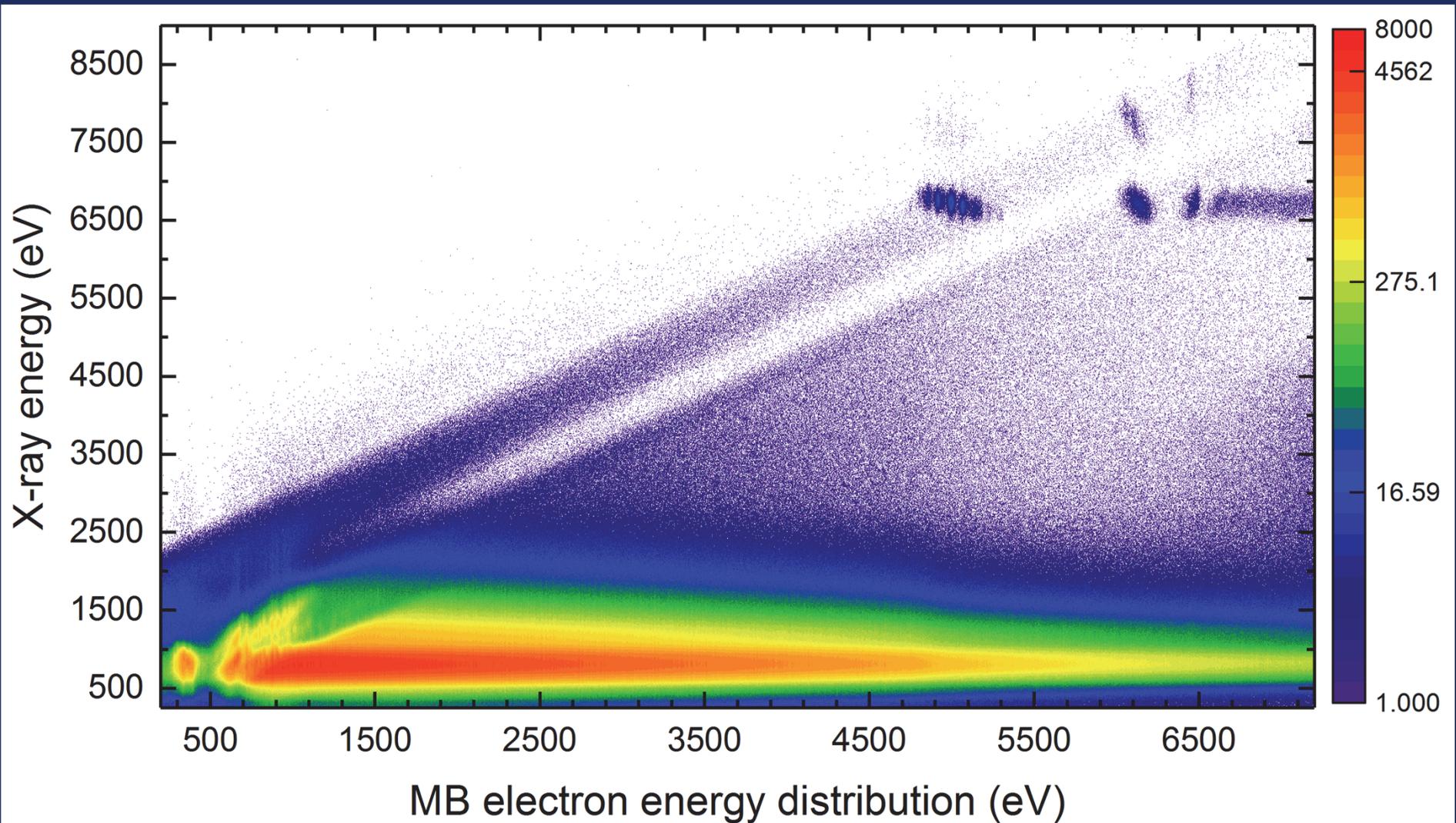
- Fe photorecombination studies
- Slow scans at high electron energy resolution

X-ray data depending on electron energy



- High energy resolution
- High statistics

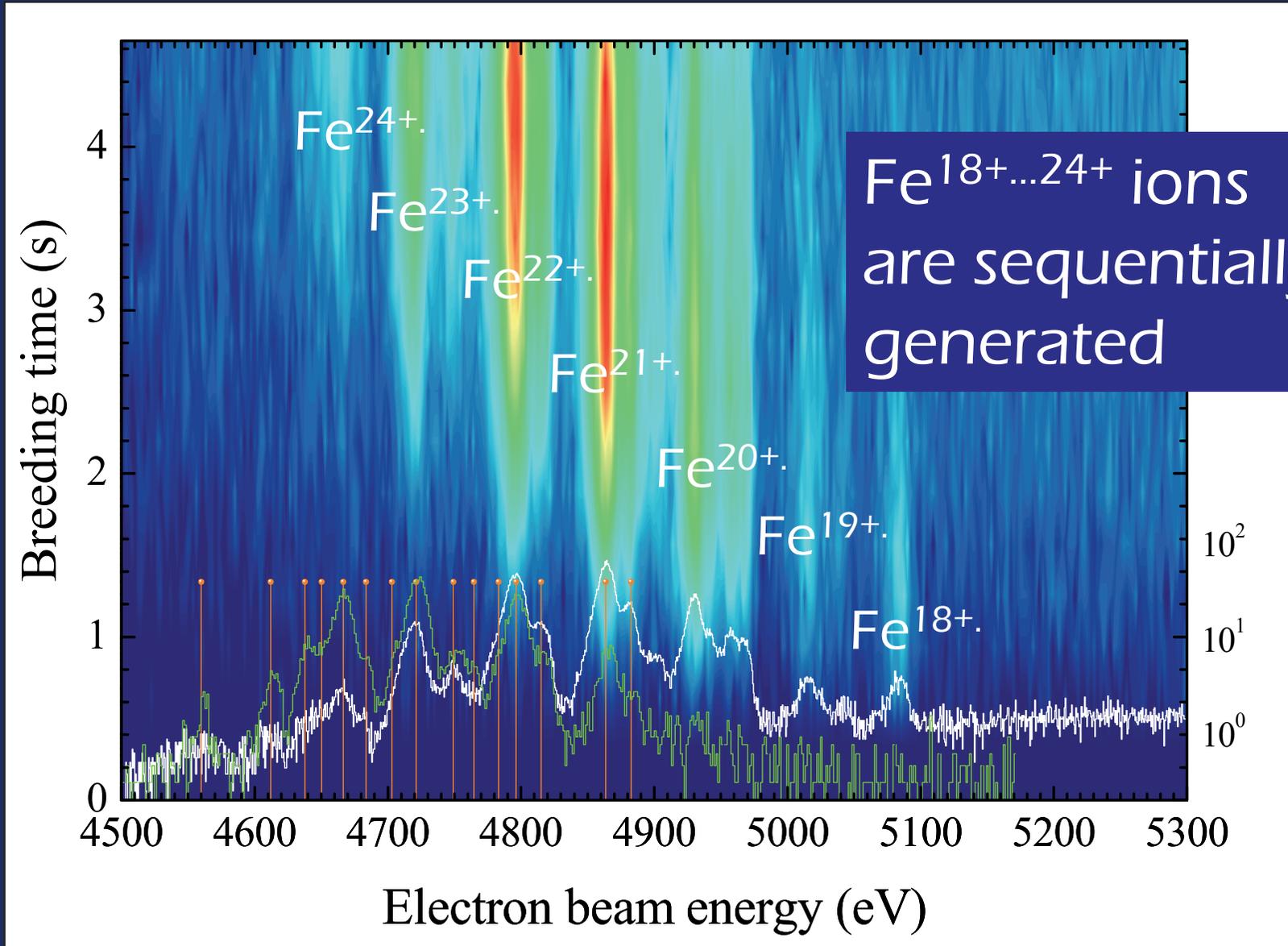
X-ray data depending on electron energy



- Fast Fe photorecombination studies
- Maxwellian electron energy distribution

X-ray data depending on electron energy

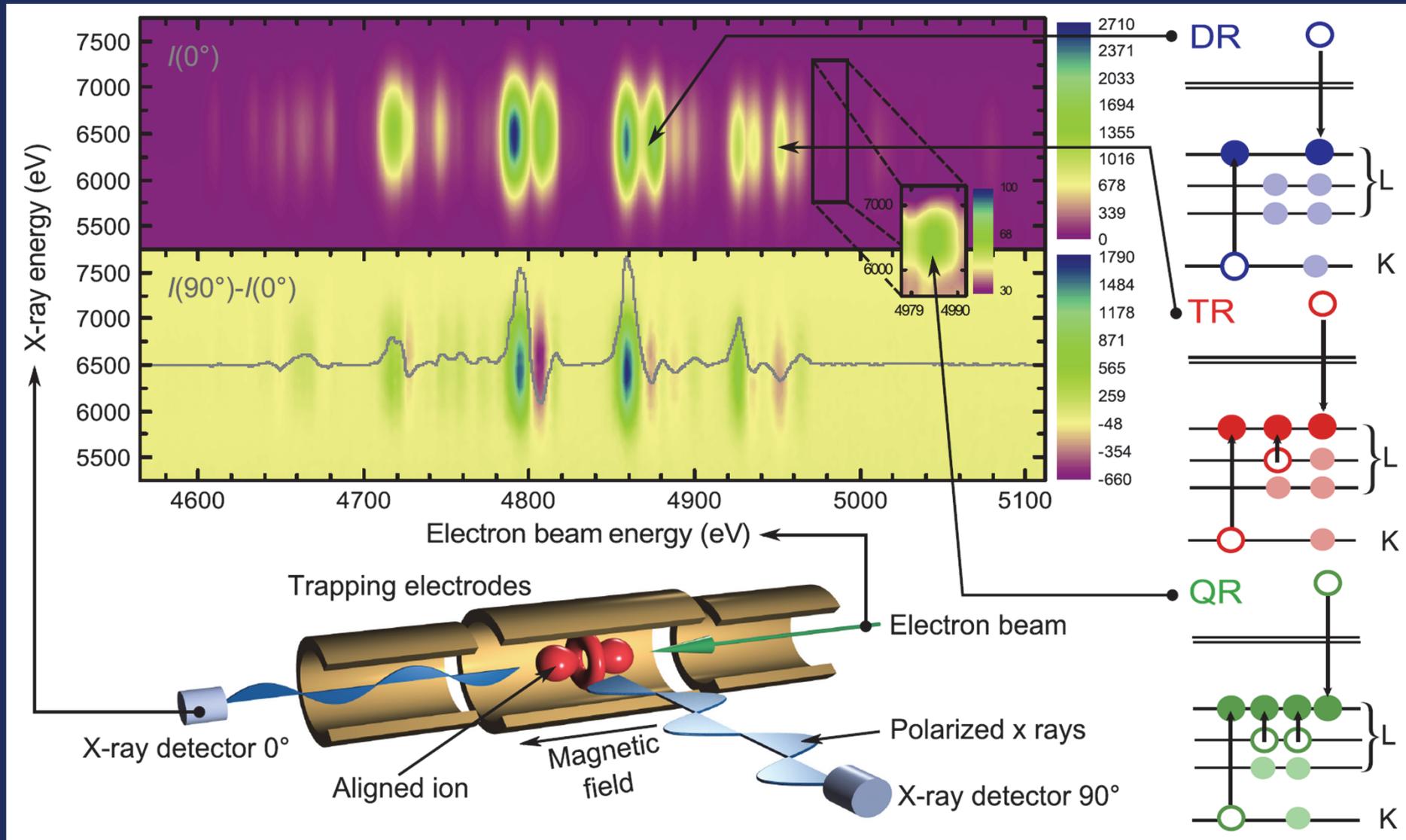
interaction time ↑



Ions in any desired charge state can be prepared, stored and spectroscopically studied

T. M. Bauman et al., PRA **90**, 052704 (2014)

Unexpected, strong contributions by many-electron resonant excitation at high resolution

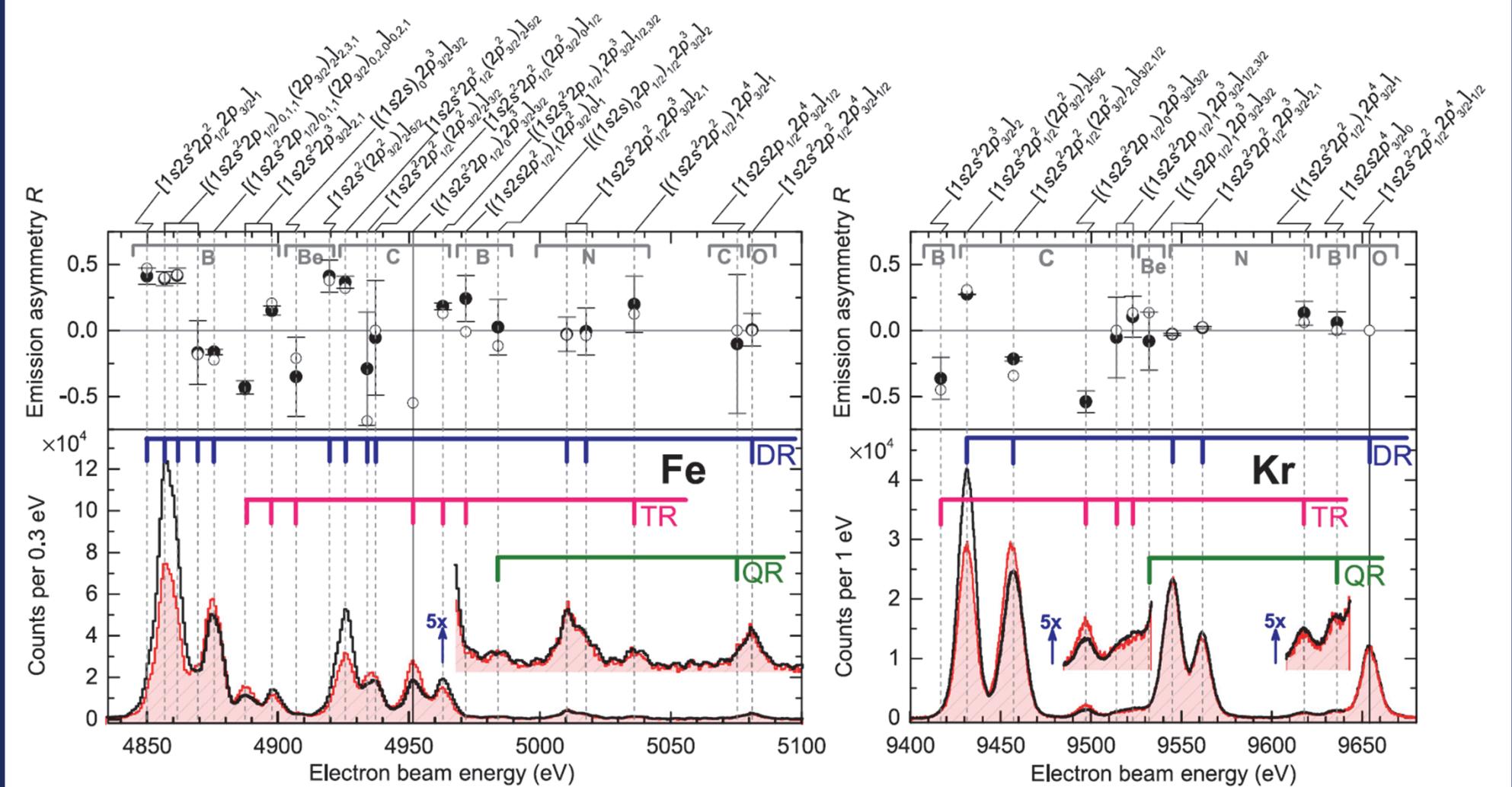


C. Shah et al., Phys. Rev. E 93, 061201(R) (2016)

C. Beilmann et al., Phys. Rev. Lett 107, 143201 (2011)

C. Beilmann et al., Phys. Rev. A 88, 062706 (2013)

Unexpected, strong contributions by many-electron resonant excitation at high resolution



C. Shah et al., Phys. Rev. E 93, 061201(R) (2016)

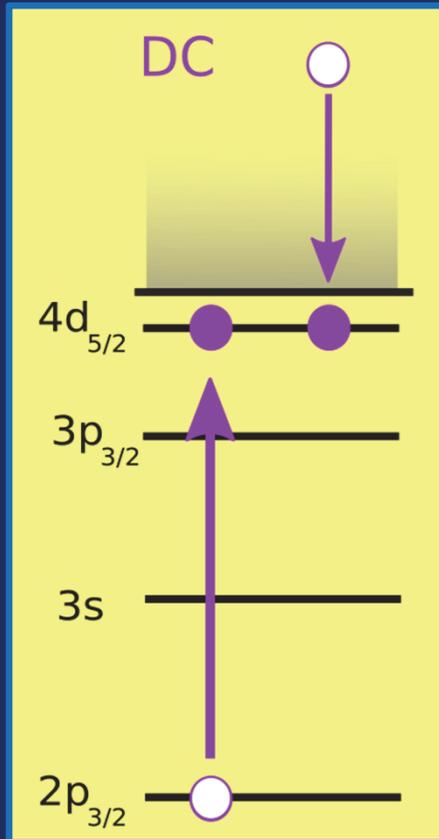
C. Beilmann et al., Phys. Rev. Lett 107, 143201 (2011)

C. Beilmann et al., Phys. Rev. A 88, 062706 (2013)

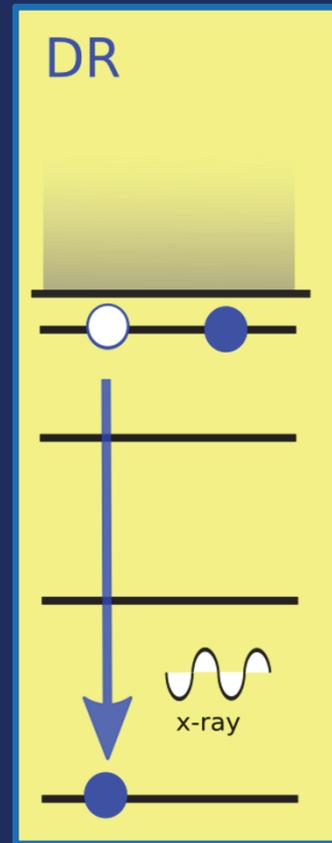
L-shell resonant excitation

Free electron capture

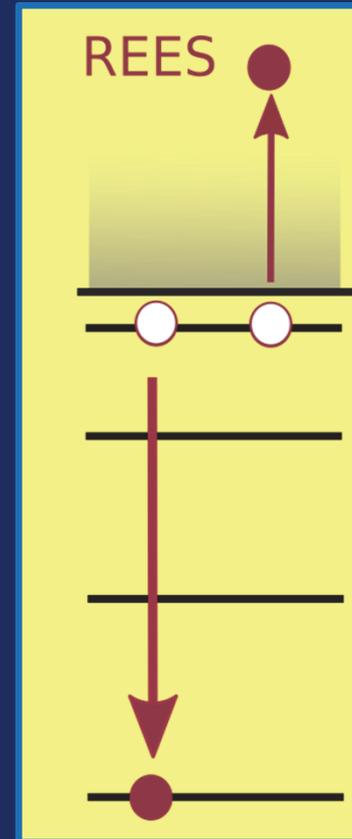
De-excitation pathways



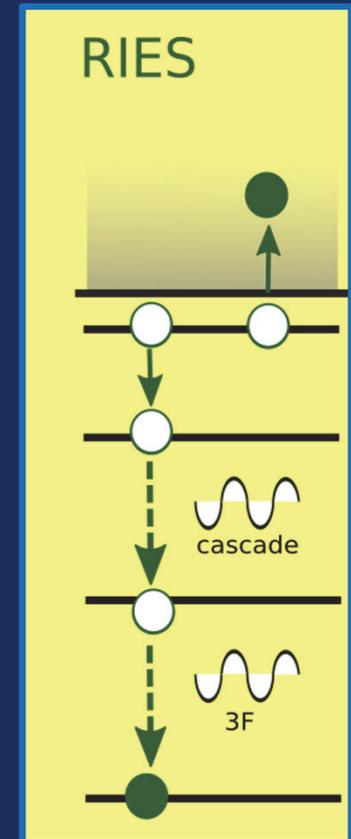
Dielectronic capture



Photon emission,
recombination

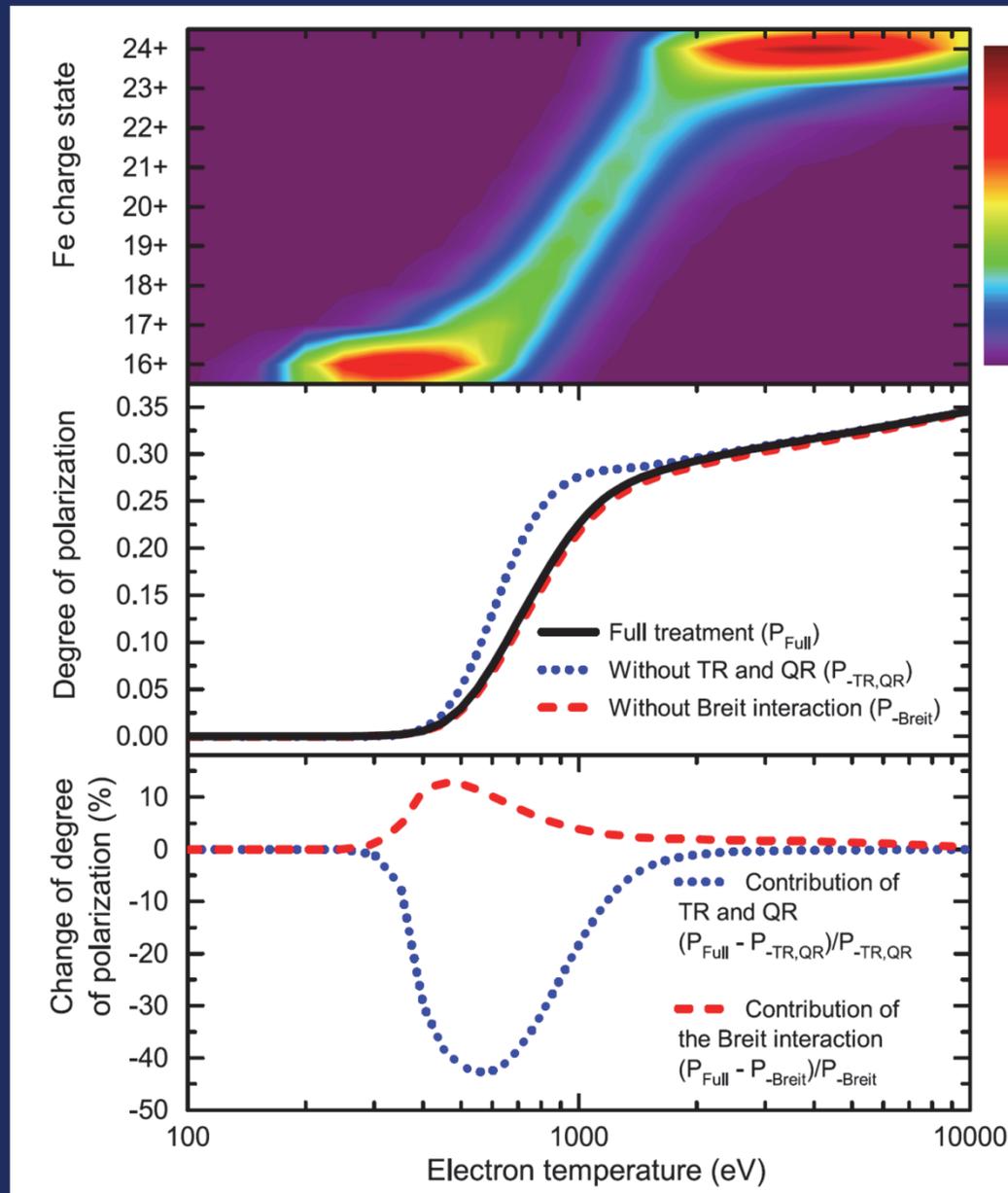


Resonant
electron scattering



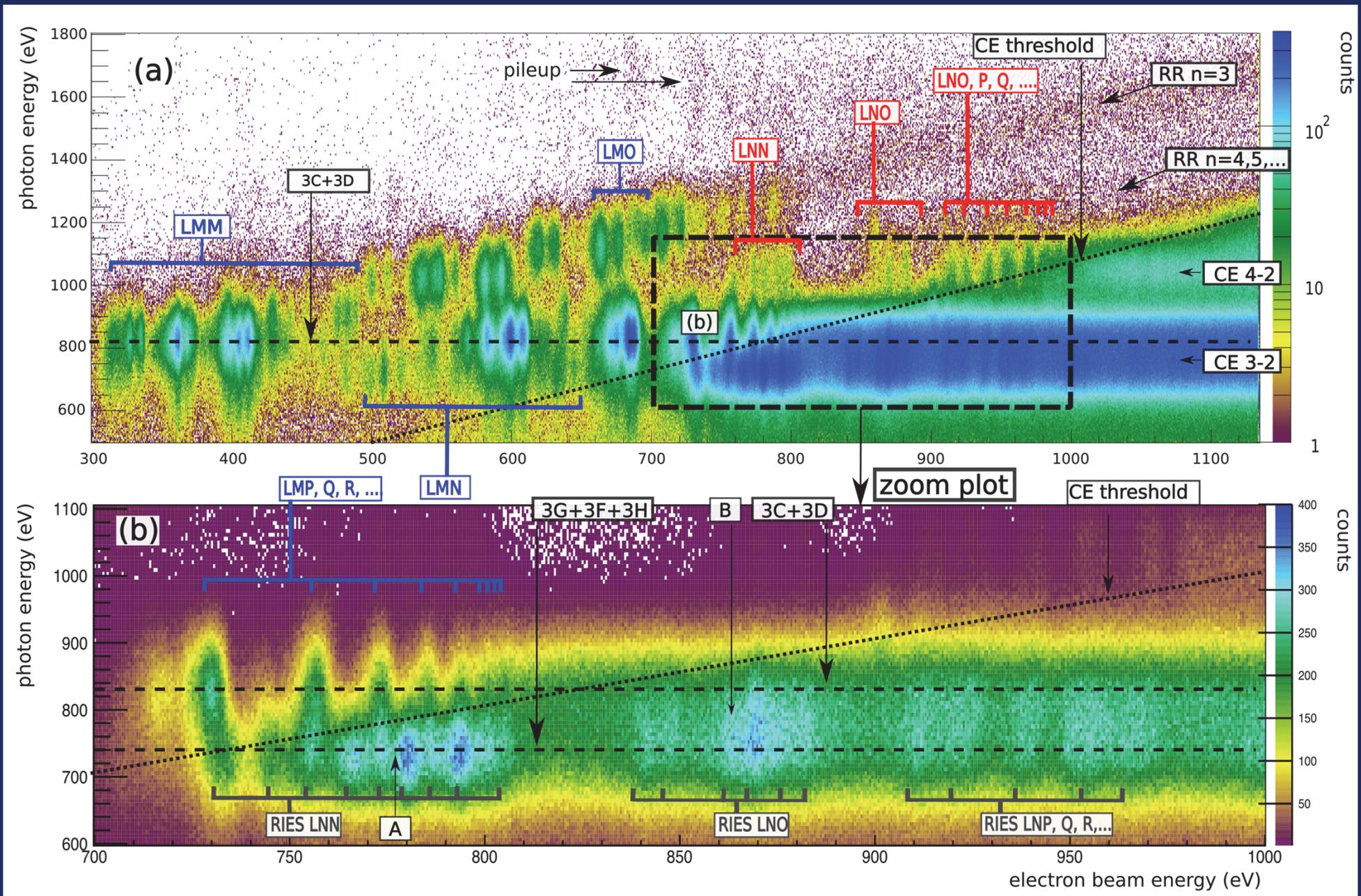
Resonant inelastic
scattering

Mean charge state of plasmas changed by many-electron resonant excitation



C. Shah et al.,
Phys. Rev. E 93,
061201(R)
(2016)

Fe L-shell resonant excitation



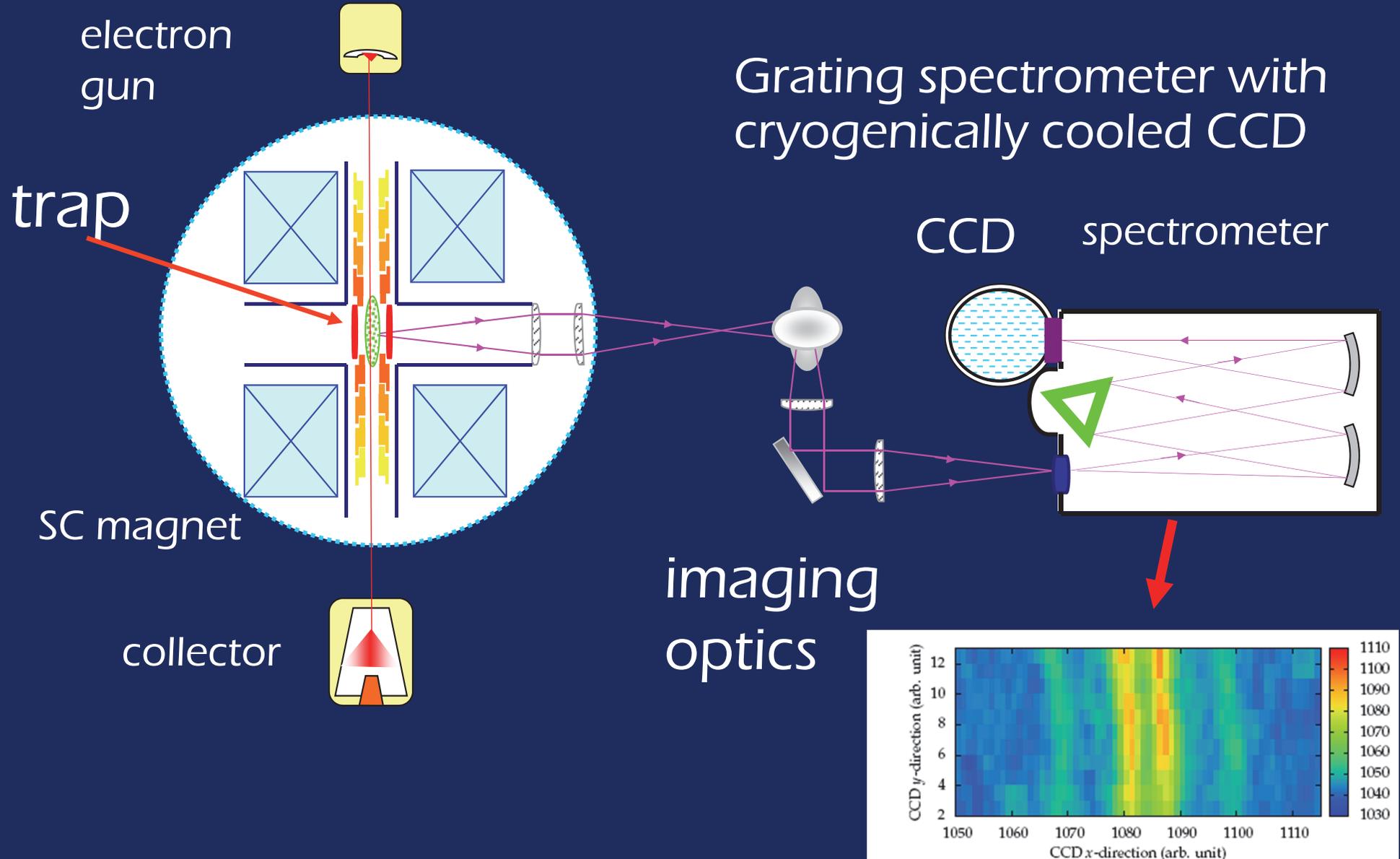
Pedro Amaro, in preparation

Conclusions from FEL, synchrotron and photorecombination studies

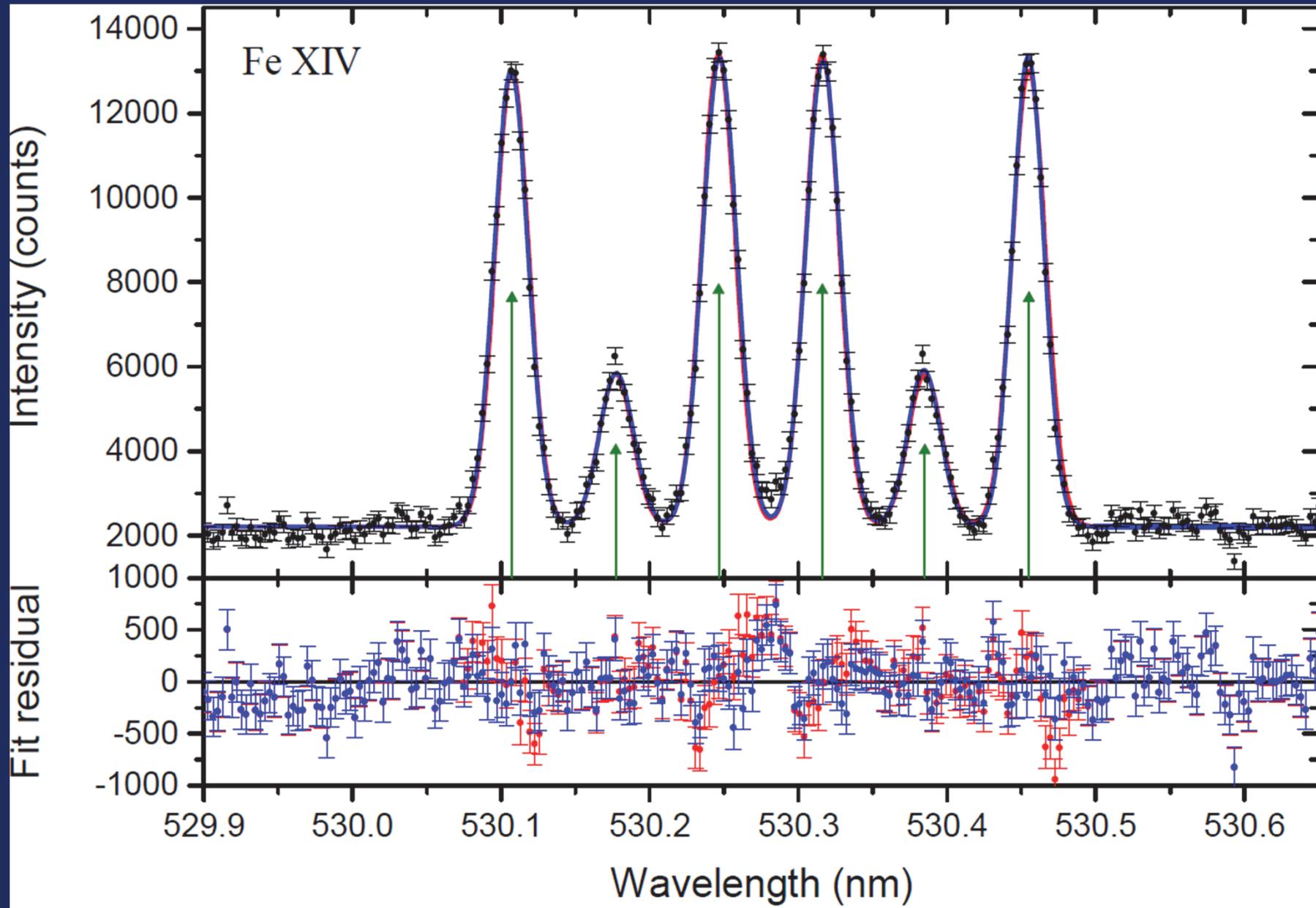
- Previously known but neglected **complex multielectron processes have experimentally shown unexpectedly strong contributions** to both photorecombination and photoionization
- Inclusion of those channels in calculations is **necessary to achieve agreement** with existing experimental data
- Even the most advanced theoretical methods are **not as accurate as the experiments**
- Achieving agreement at the 1% (energies) respectively 5% (cross sections) levels will require **more dedicated theoretical work and benchmarking experimental data**

Optical and EUV spectroscopy with EBITs

Spectroscopy of few-electron ions in the visible range

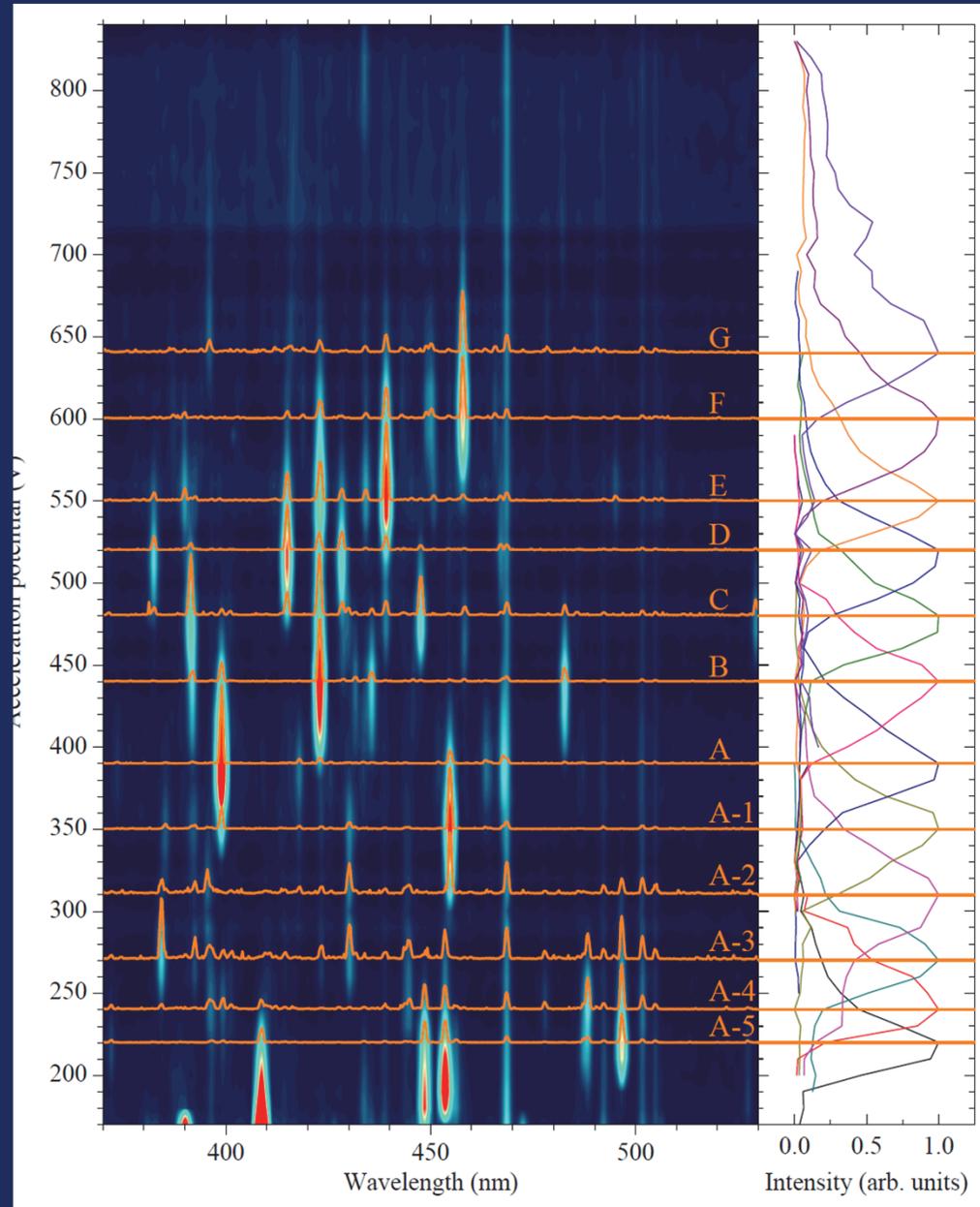


Fe^{13+} (Fe XIV): the "green coronal line"



Hendrik Bekker, accepted PRA 2018

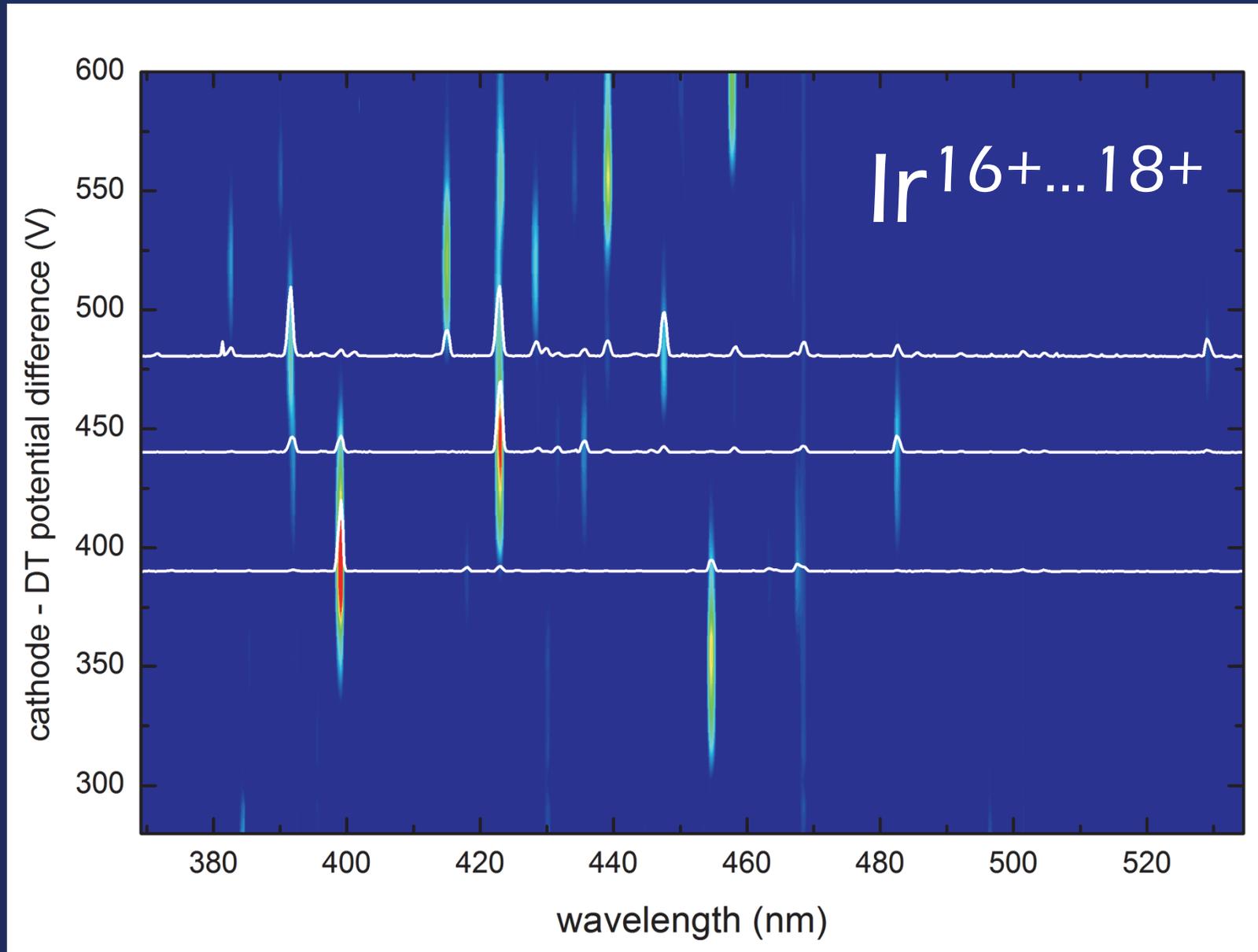
Level crossings at Ir^{17+} provide α sensitivity



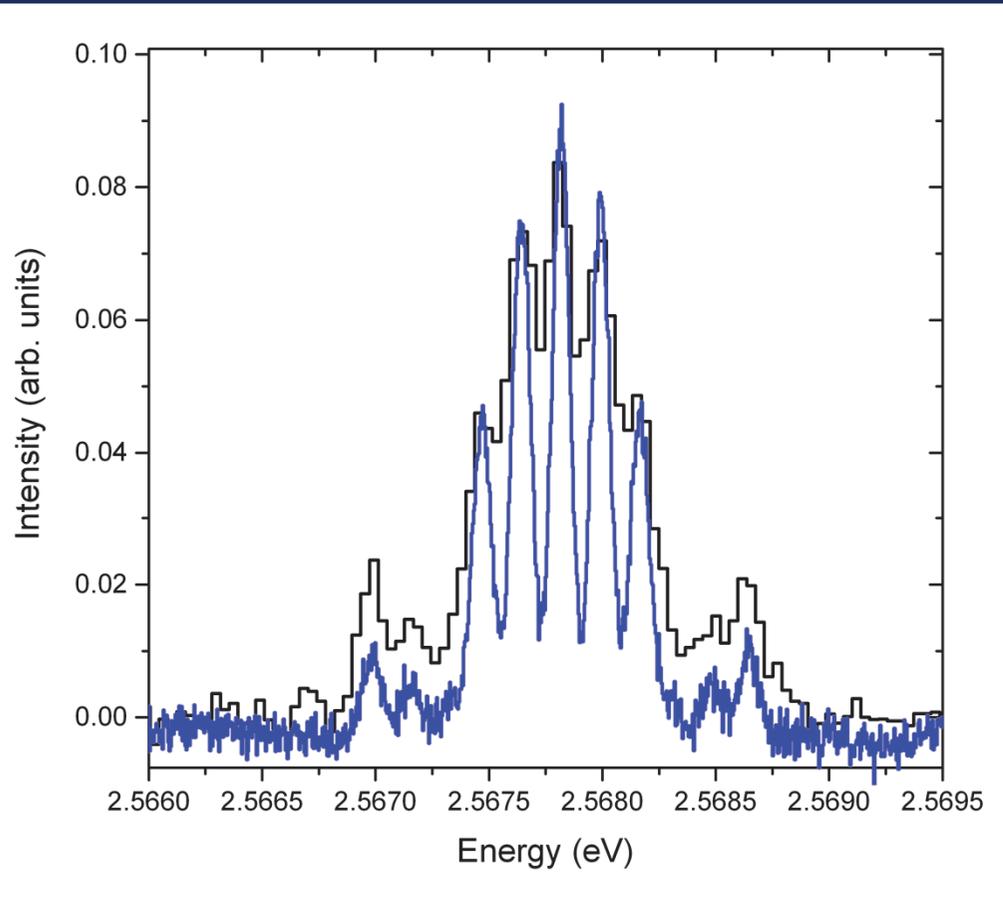
- At certain charge state levels change order
- $4f$ goes below $5s$ in Ir^{17+}
- Opposite parities degenerate: $4f^{12} 5s^2$, $4f^{13} 5s$, $4f^{14}$
- Many slow M1, E1, E2, M2, M3 transitions become possible
- Several long lived „ground states“ available

Windberger et al., PRL 114, 150801 (2015)

Visible spectra of M1 lines in Ir ions



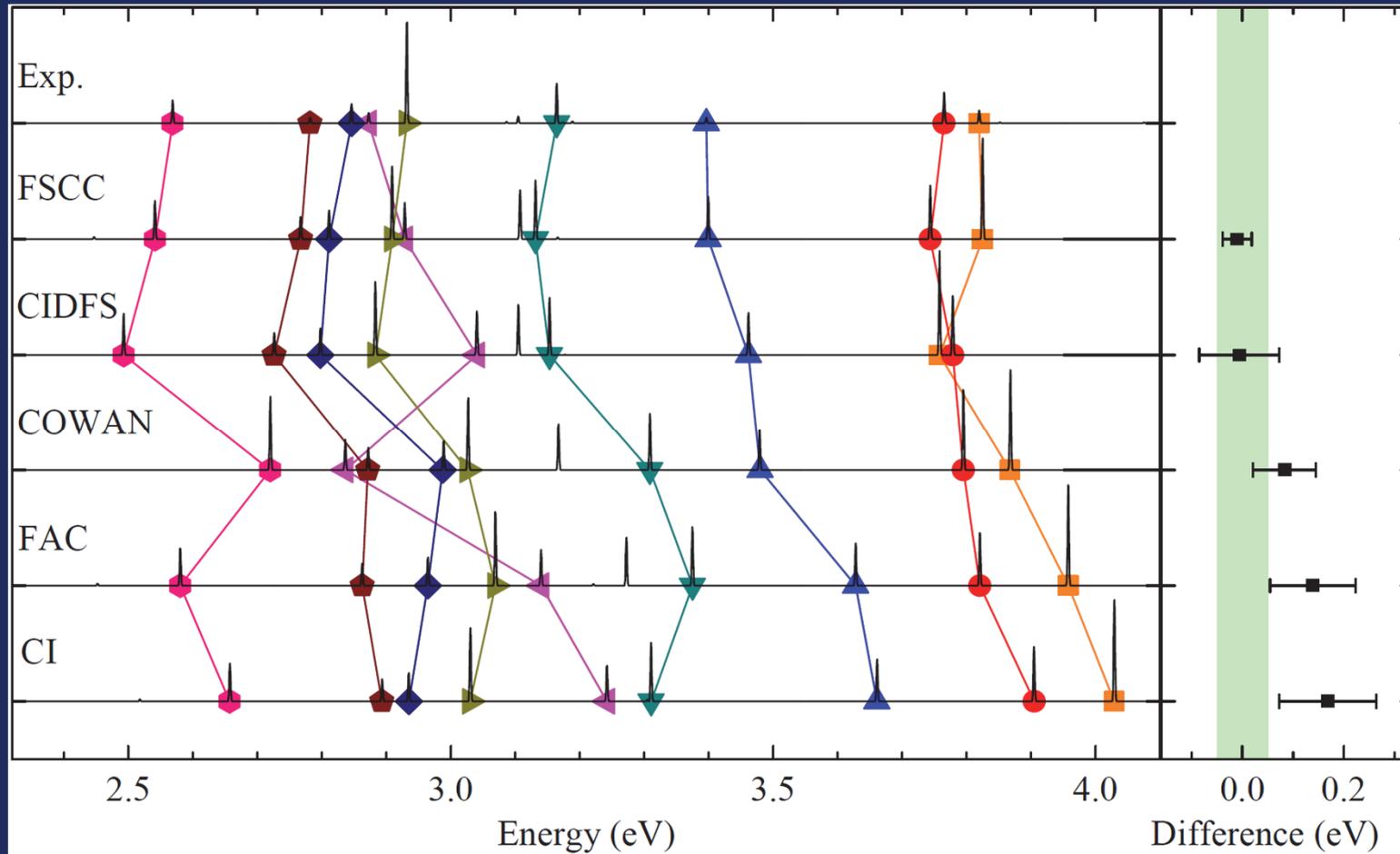
First observations; line identification difficult



Transition	Wavelength (nm)	Updated
${}^3P_1 - {}^3F_2$	226.63(2)	
${}^3F_3 - {}^3F_3^o$	240.098(1)	
${}^1G_4 - {}^3F_3^o$	255.8684(3)	
${}^3H_4 - {}^3H_5$	324.6113(4)	
${}^1F_3^o - {}^3F_4^o$	329.3025(4)	329.3028 (2)
${}^1D_2 - {}^3F_2$	365.0318(10)	365.03230(14)
${}^1F_3^o - {}^3F_3^o$	390.7408(9)	
${}^3F_3 - {}^3F_4$	391.8220(3)	391.82393(16)
${}^3P_2 - {}^1D_2$	399.4702(3)	
${}^3H_5 - {}^3H_6$	422.8950(3)	422.89512(17)
${}^1D_2 - {}^3F_3$	431.6044(3)	431.60376(8)
${}^1G_4 - {}^3F_4$	435.6348(5)	435.7595 (2)
${}^3H_4 - {}^1G_4$	445.7057(9)	445.70825(17)
${}^3F_2^o - {}^3F_3^o$	482.7039(7)	482.70386(8)
${}^3H_4 - {}^3F_3$	503.423(2)	
${}^3P_1 - {}^1D_2$	597.65(2)	

H. Bekker et al., in preparation

Comparison between theories

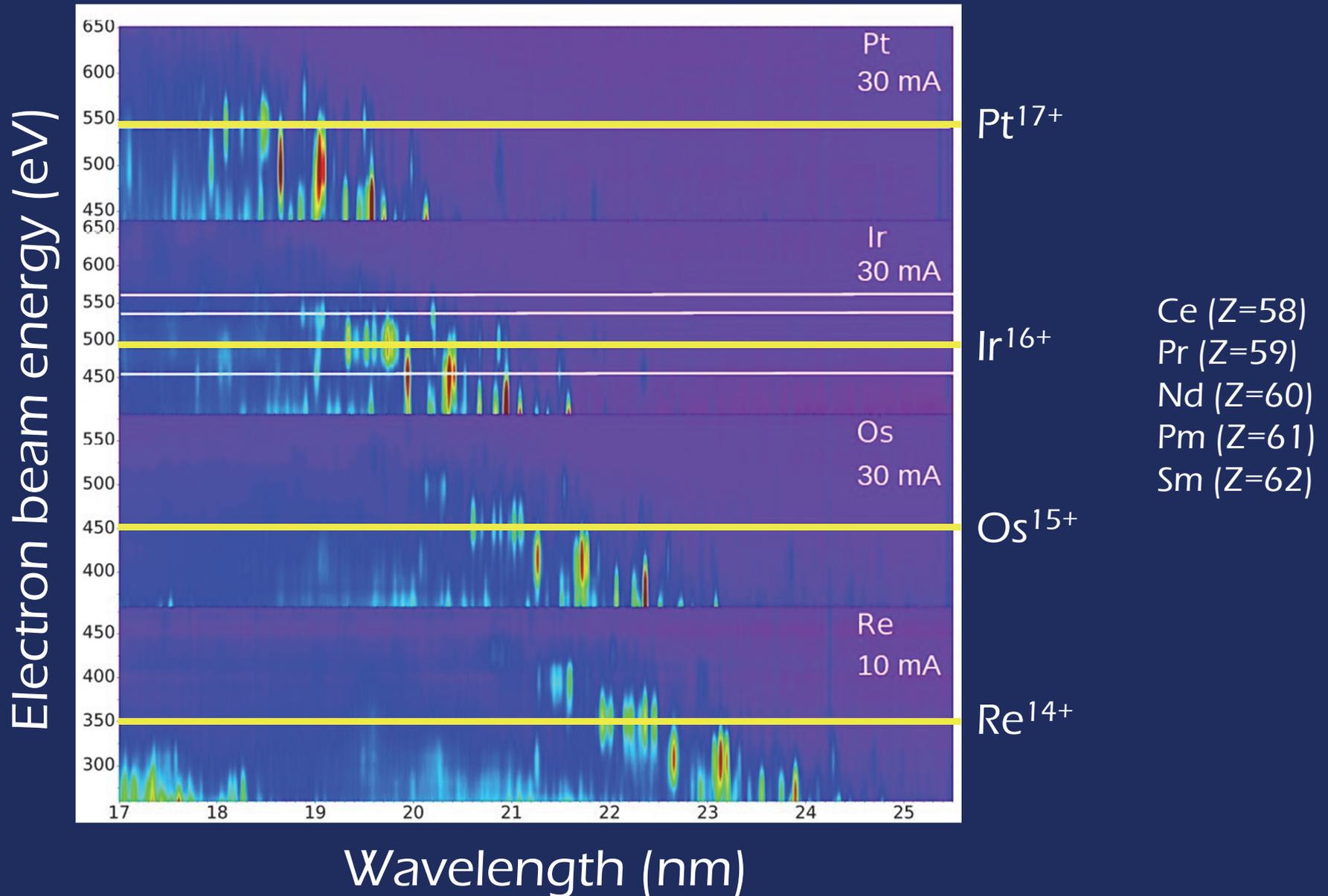


*

- Fock-space coupled cluster calculation (A. Borschevski) shows agreement with experimental result at a level suitable for identification.
- Its deviations from experiment are smaller than the average separation between spectral lines (as given by the green band).

* Berengut *et al.*, PRL 106, (2011) Windberger *et al.*, PRL 114, 150801 (2015)

Pm-like (61 electrons) isoelectronic sequence

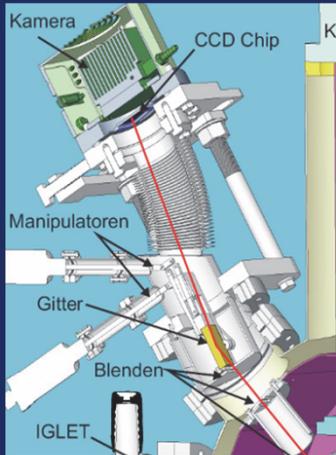


Isoelectronic sequence studied in detail to find analogies



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Electron beam ion trap diagnostics

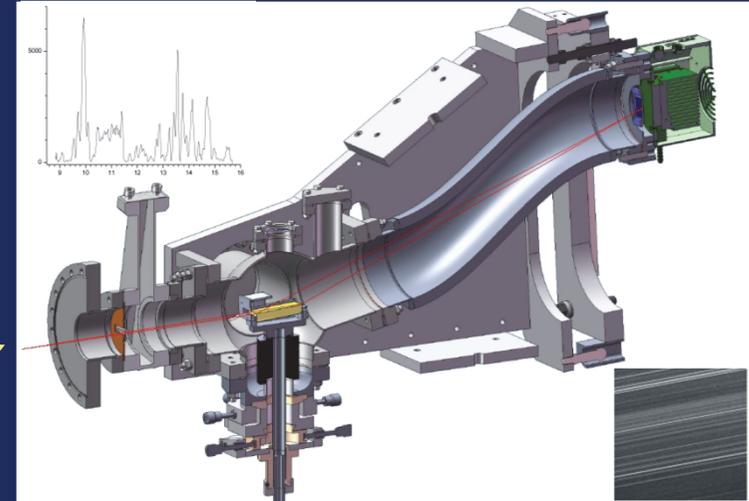


EUV grating spectrometer 1

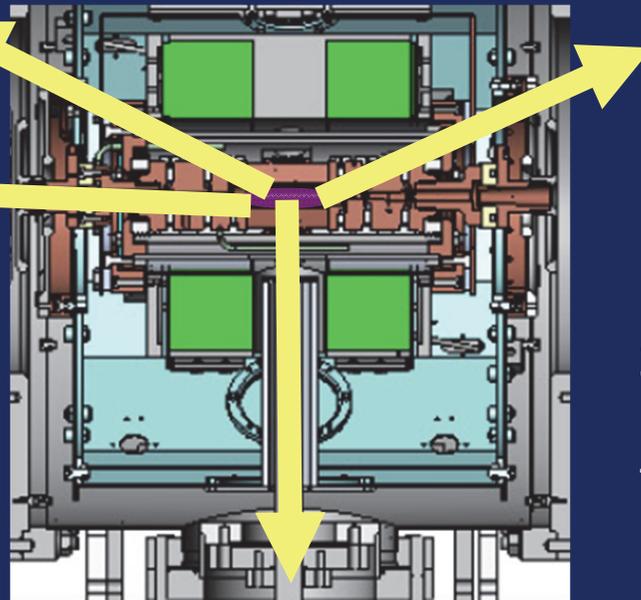
EUV to
soft X-ray

EUV

EUV grating spectrometer 2



X-ray

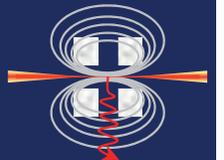
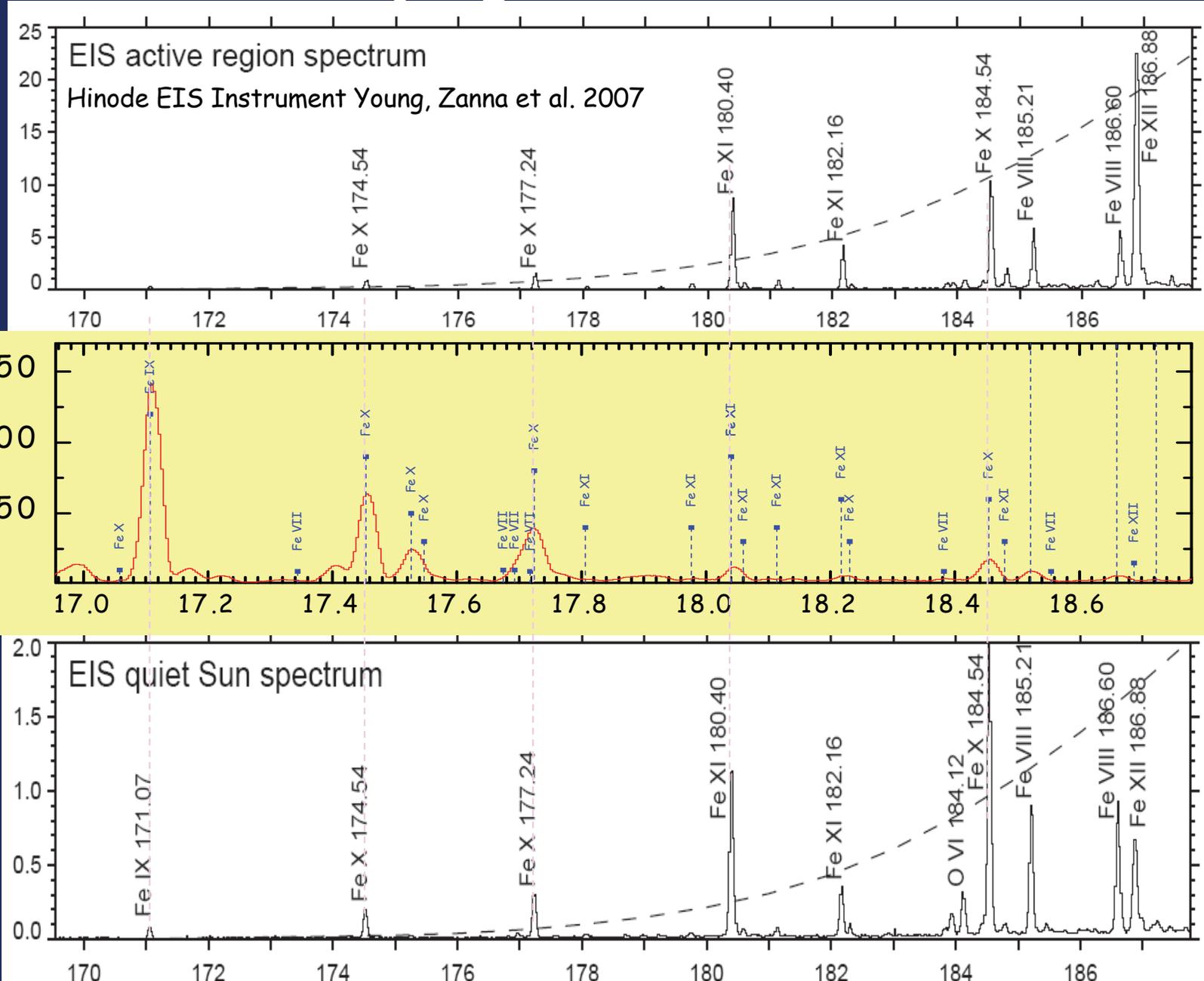


X-ray

Silicon drift detector
Germanium detector

Si drift detector, Ge detector
X-ray photons 1 to 30 keV
Two grating spectrometers
EUV photons 40 eV to 1 keV
Metallic magnetic microcalorimeter
X-ray photons 2 to 8 keV

Hinode ("sunrise"): space telescope (2006) studying the solar corona



Comparison of new data

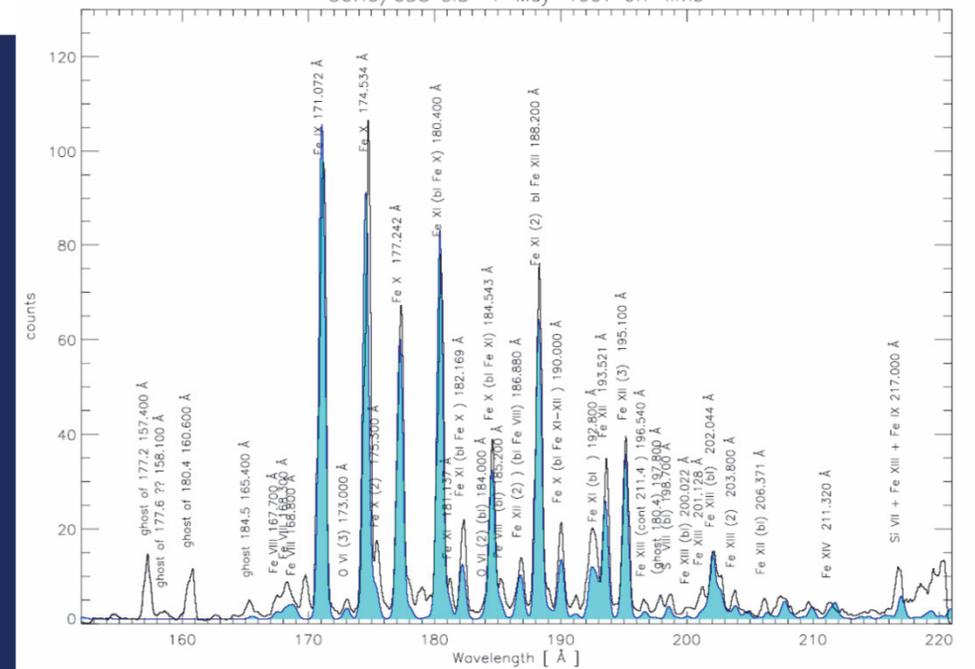
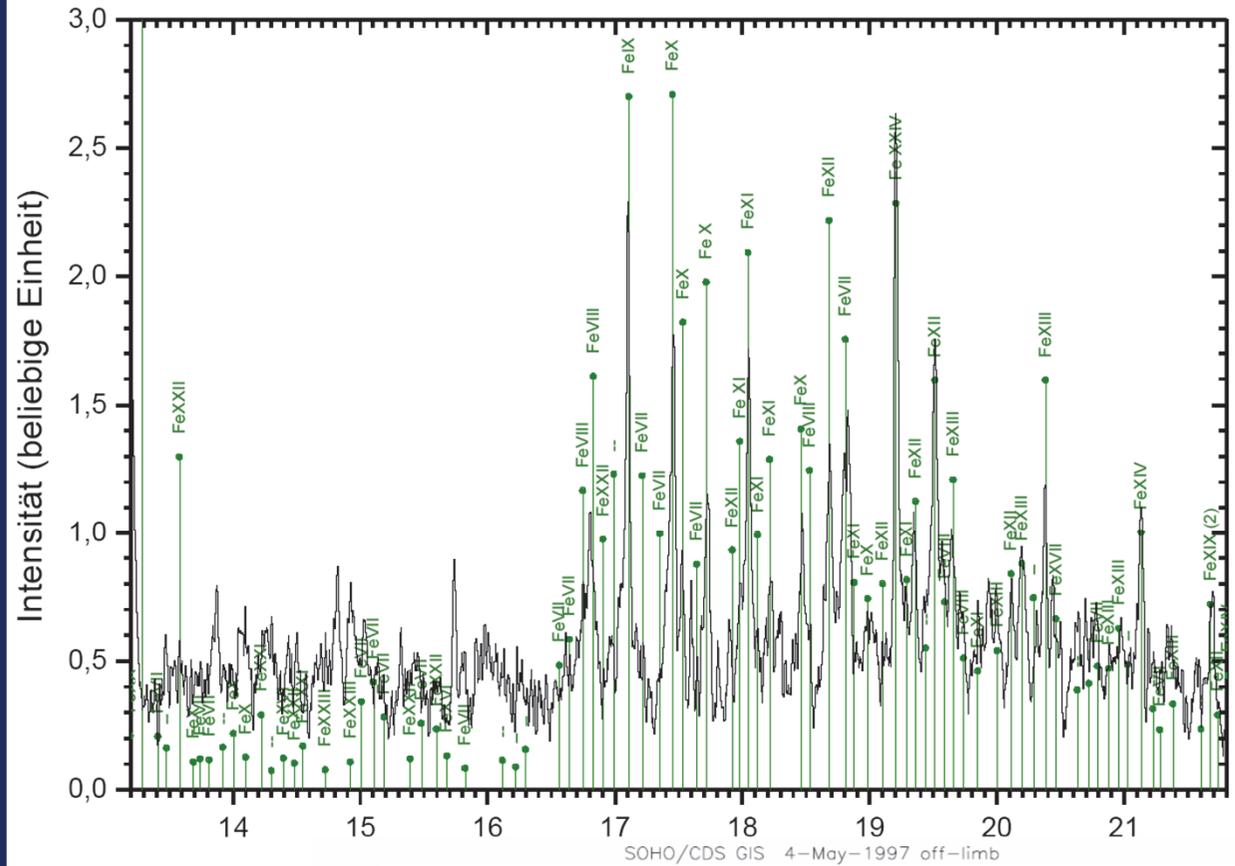


with

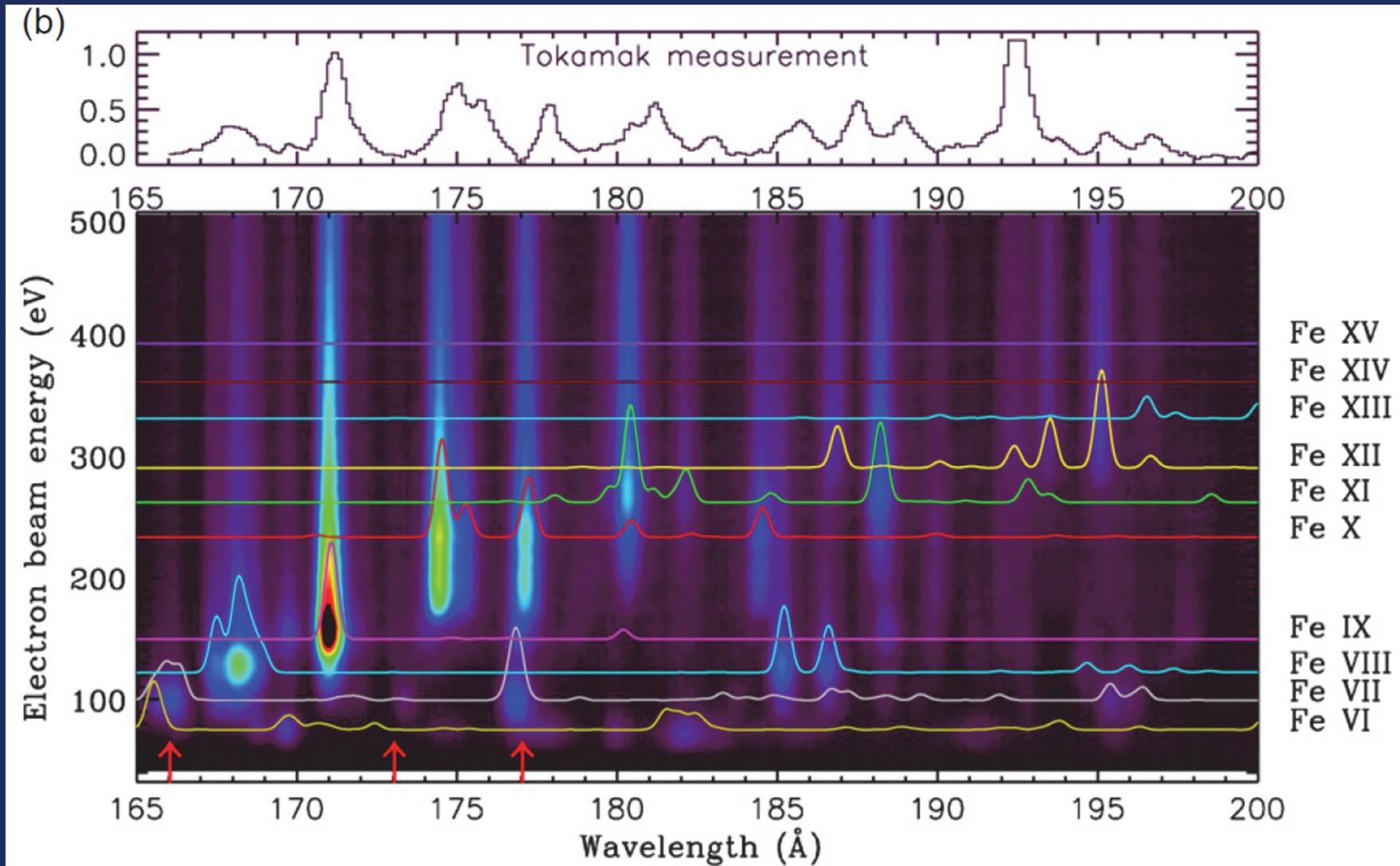
SOHO



SOHO: Solar Heliospheric Observatory



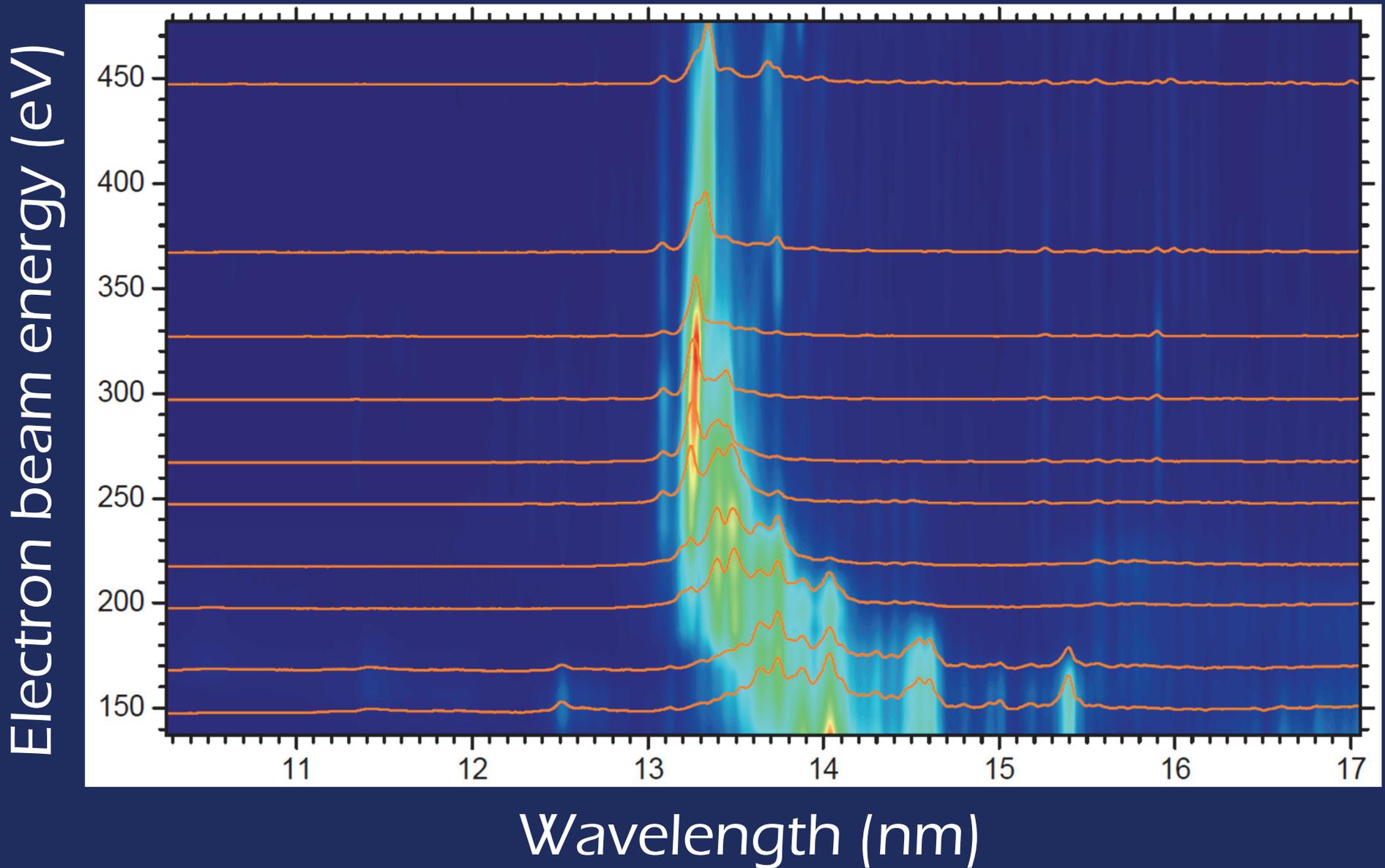
Studies of Fe H α with charge-state resolution



Gu et al., *Astrophys. J.* 696, 2275 (2009)

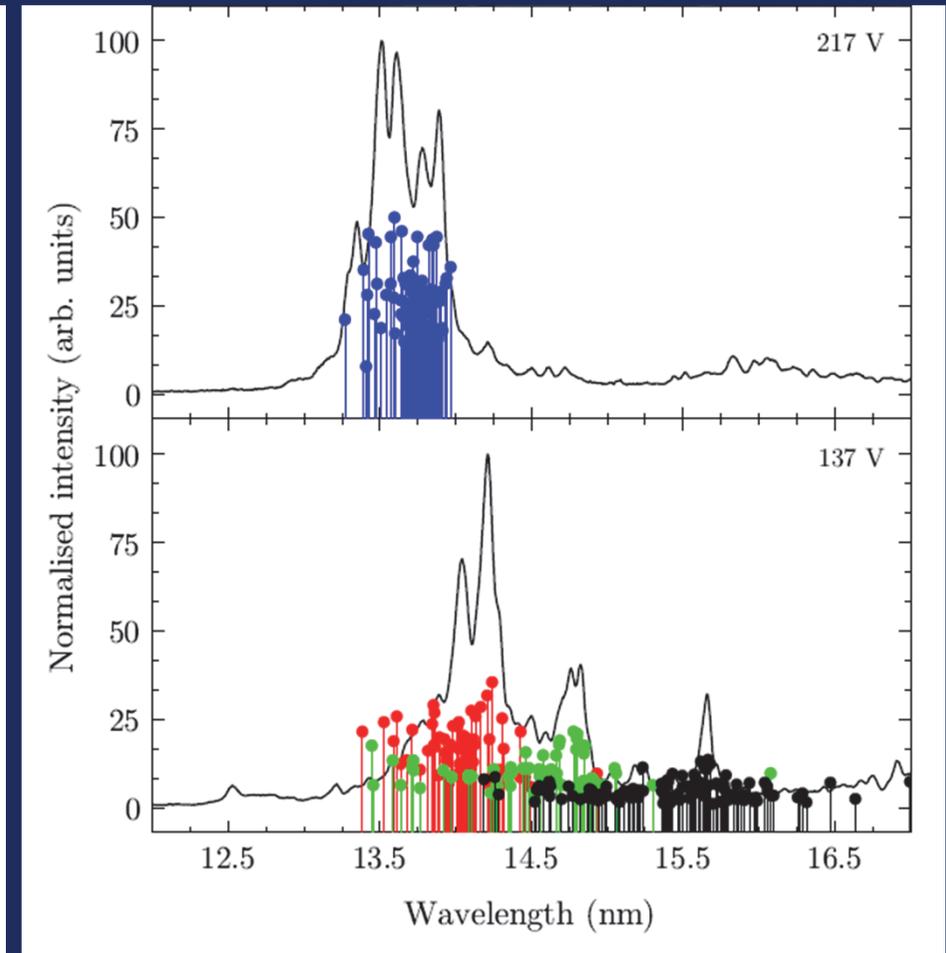
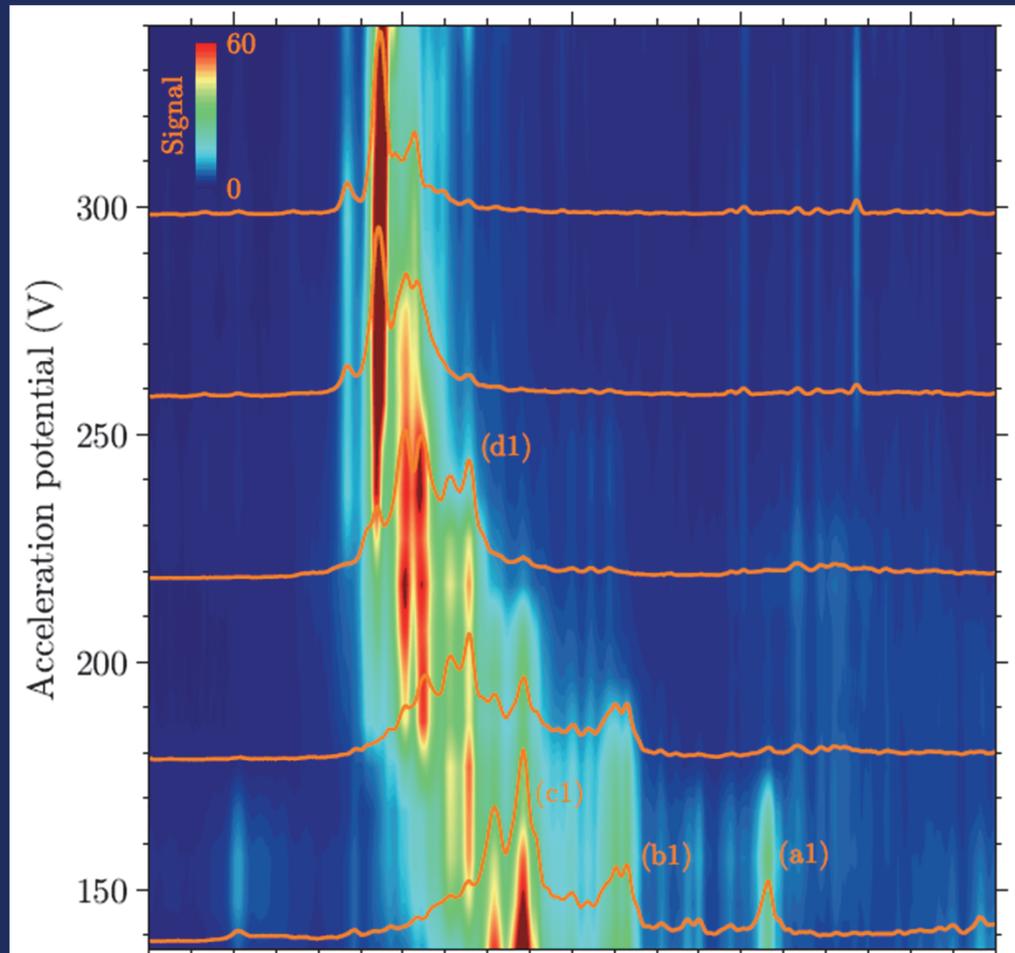
Understanding optical and EUV spectra of Sn ions

Understanding Sn spectra



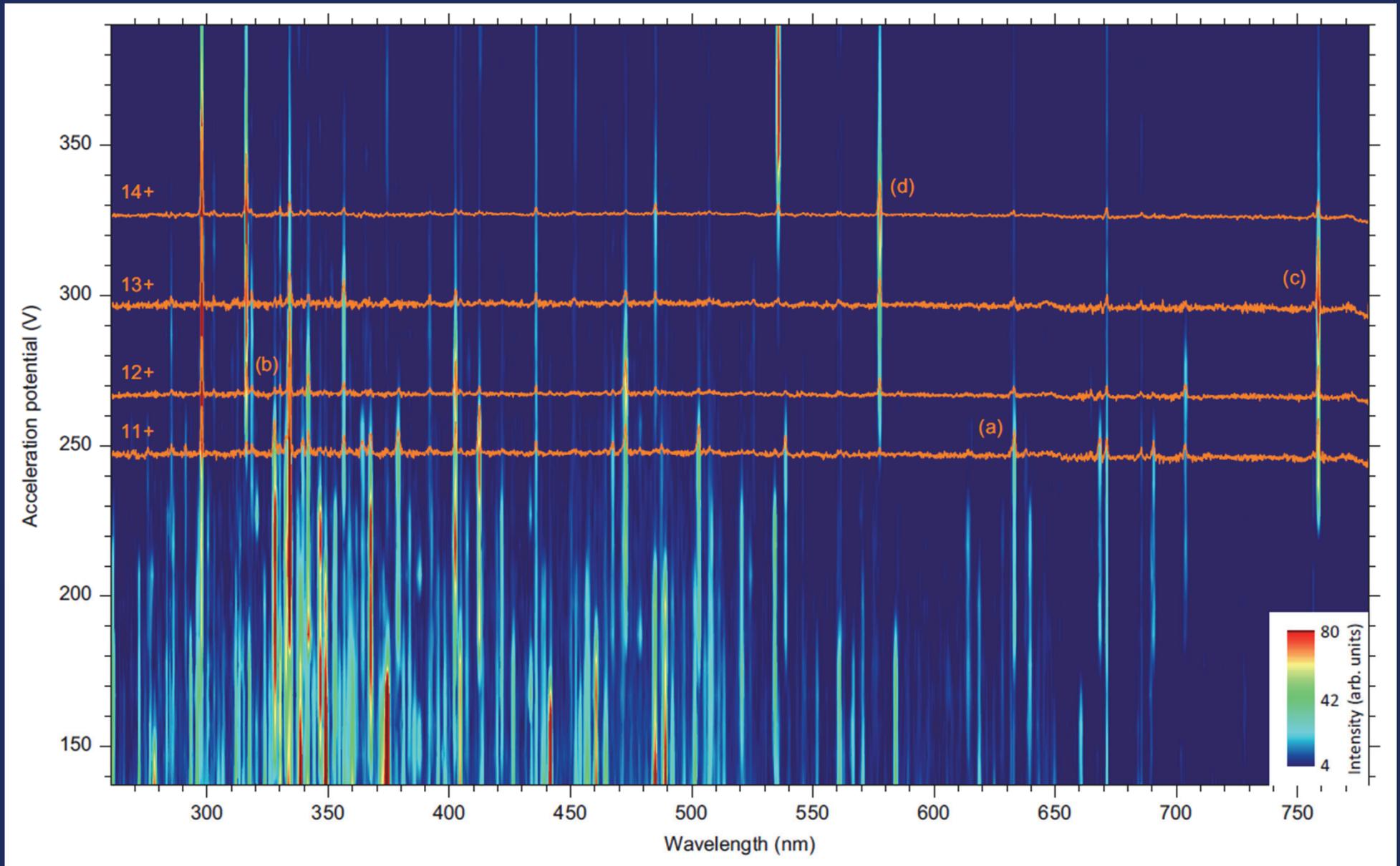
H. Bekker et al., *J. Phys. B* 48, 144018 (2015)

Understanding Sn spectra



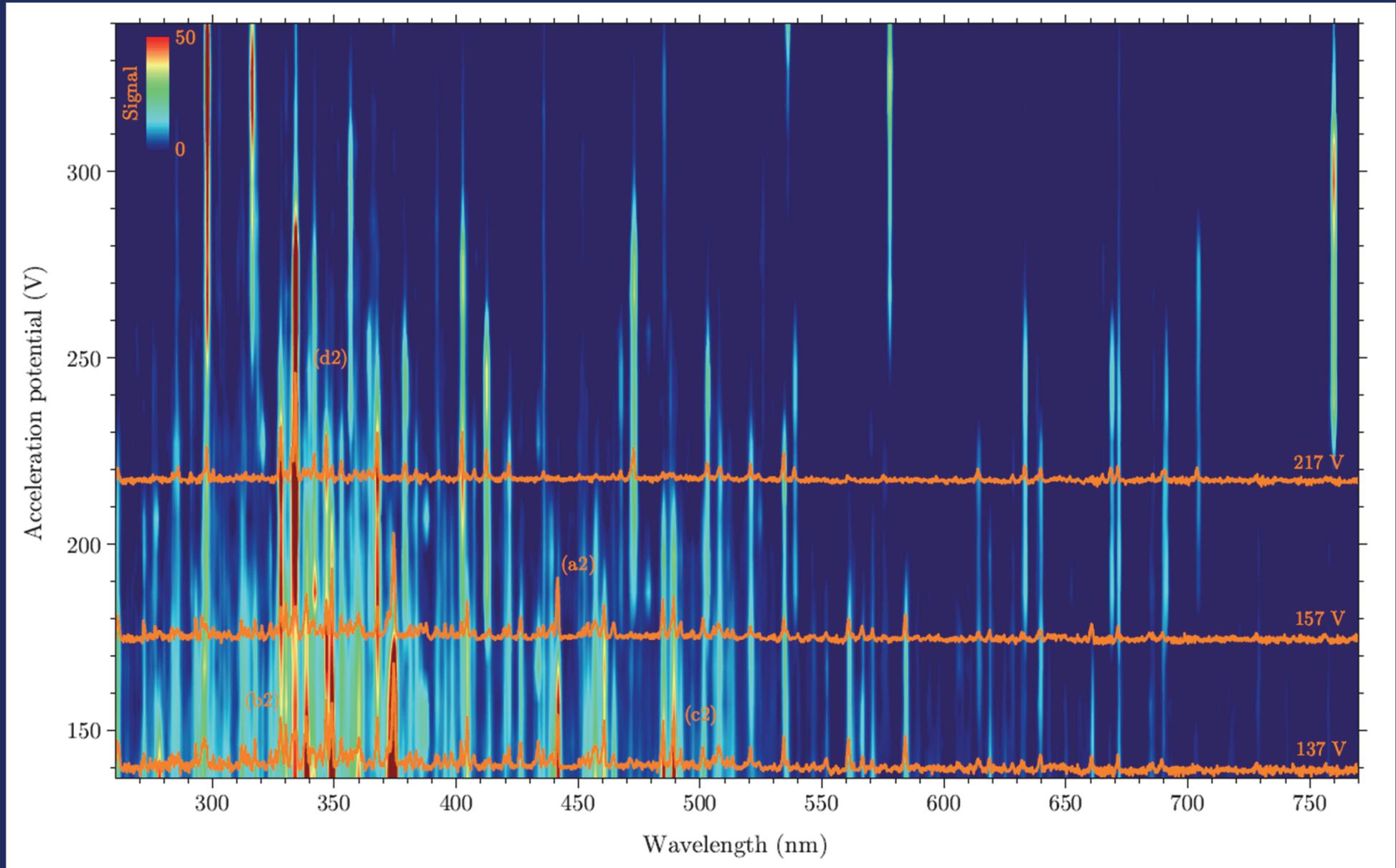
F. Torretti, ARCNL, PRA (2017)

Understanding Sn spectra



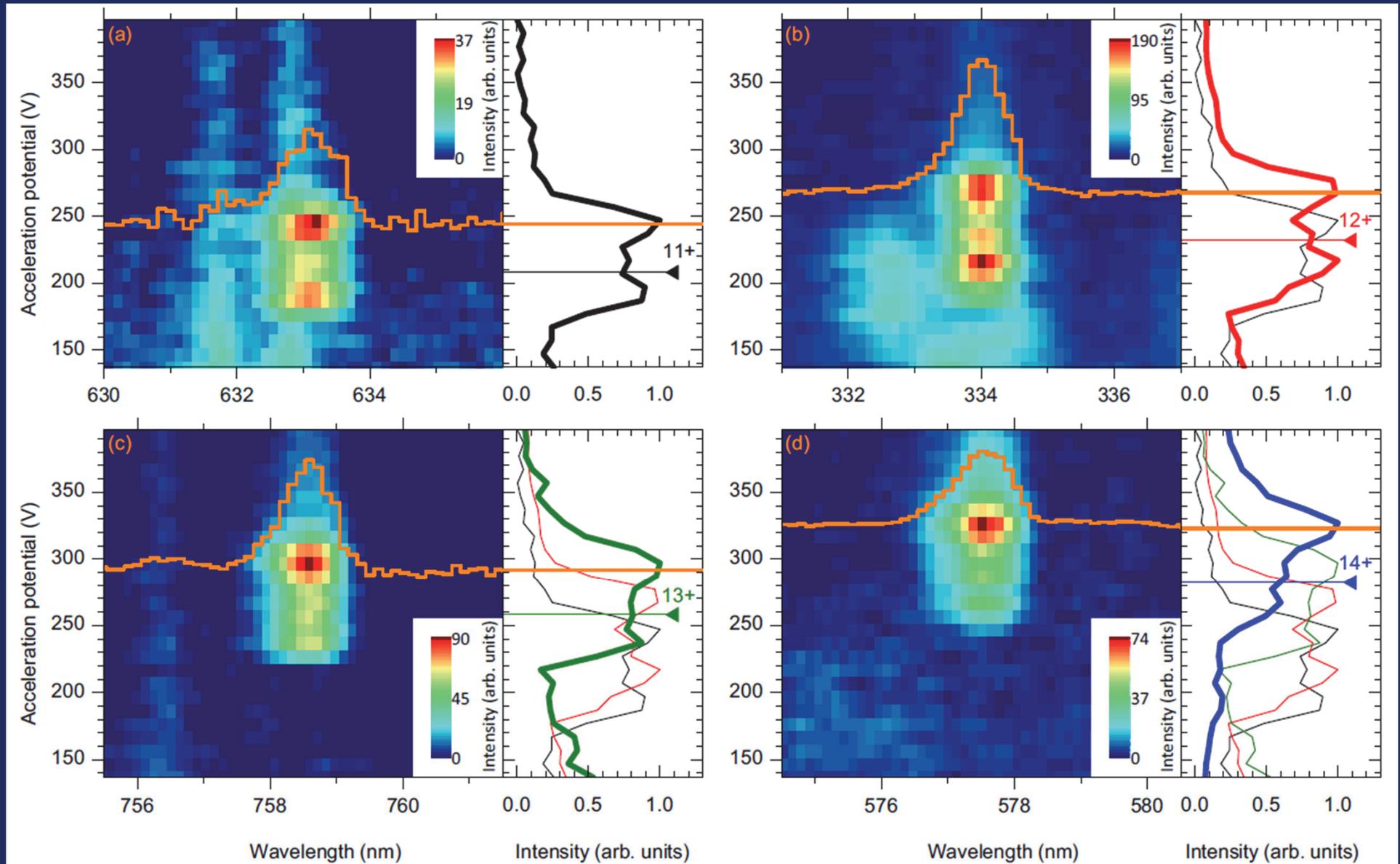
A. Windberger et al., Phys. Rev A 94, 012506 (2016)

Understanding Sn spectra



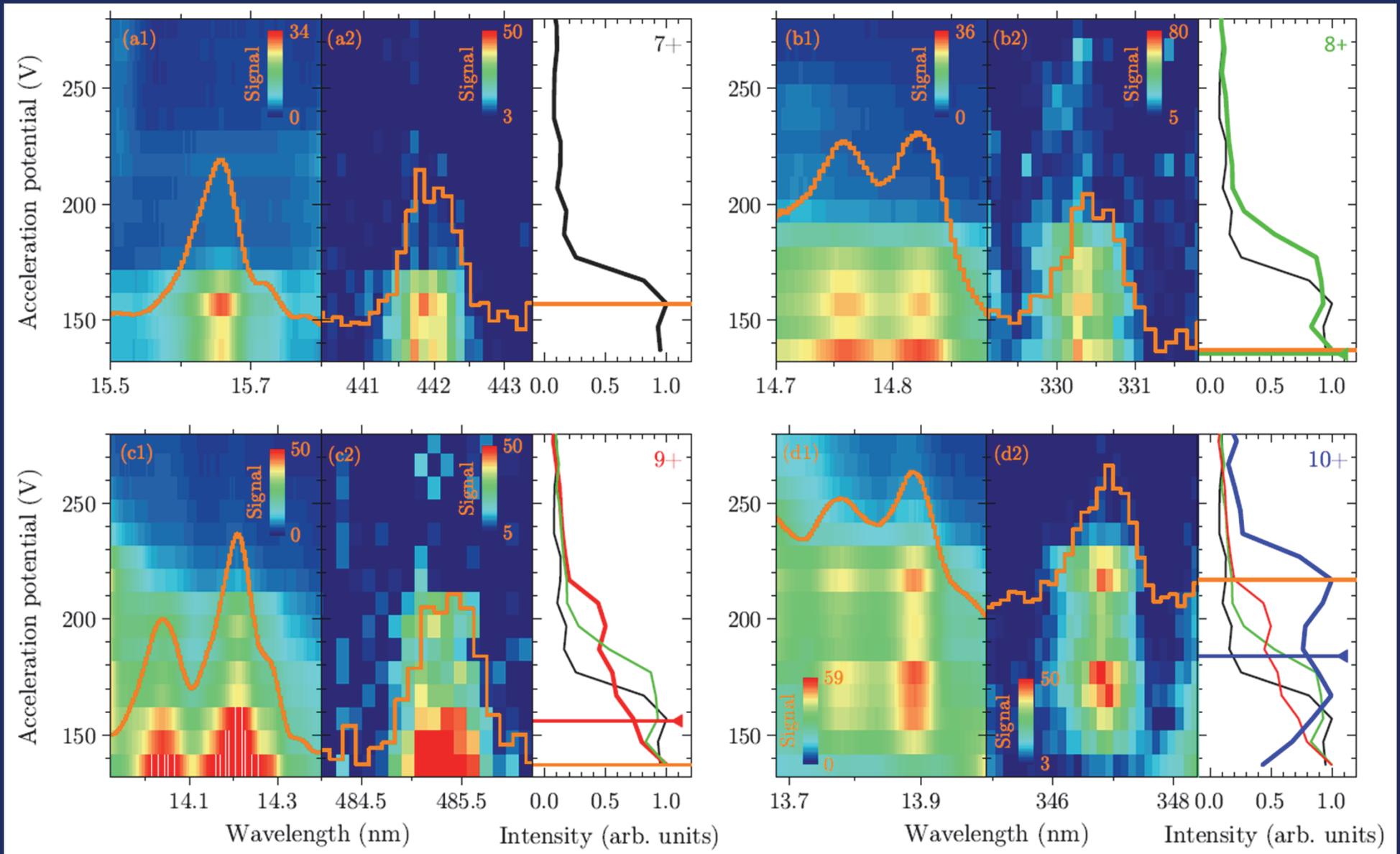
F. Torretti, ARCNL, PRA (2017)

Understanding Sn spectra



A. Windberger et al., Phys. Rev A 94, 012506 (2016)

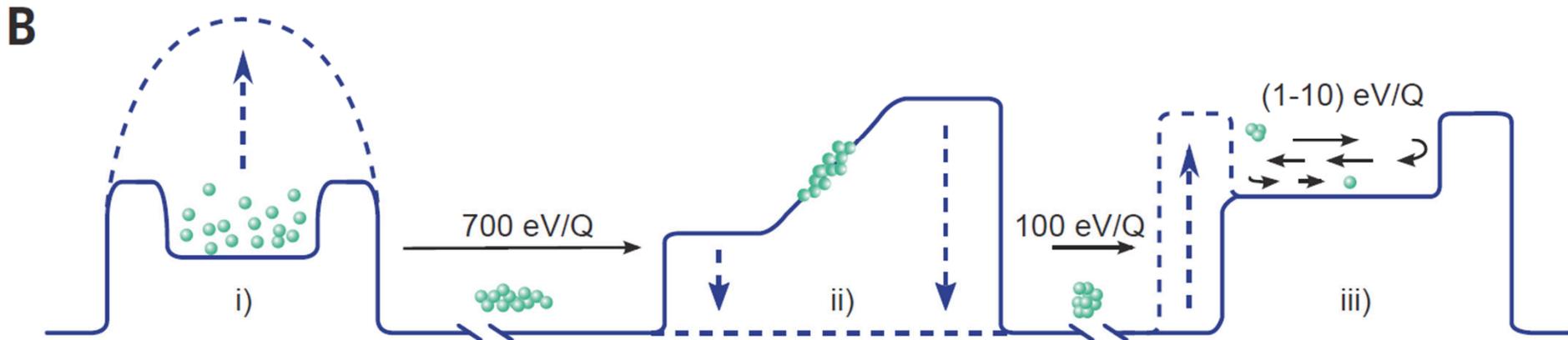
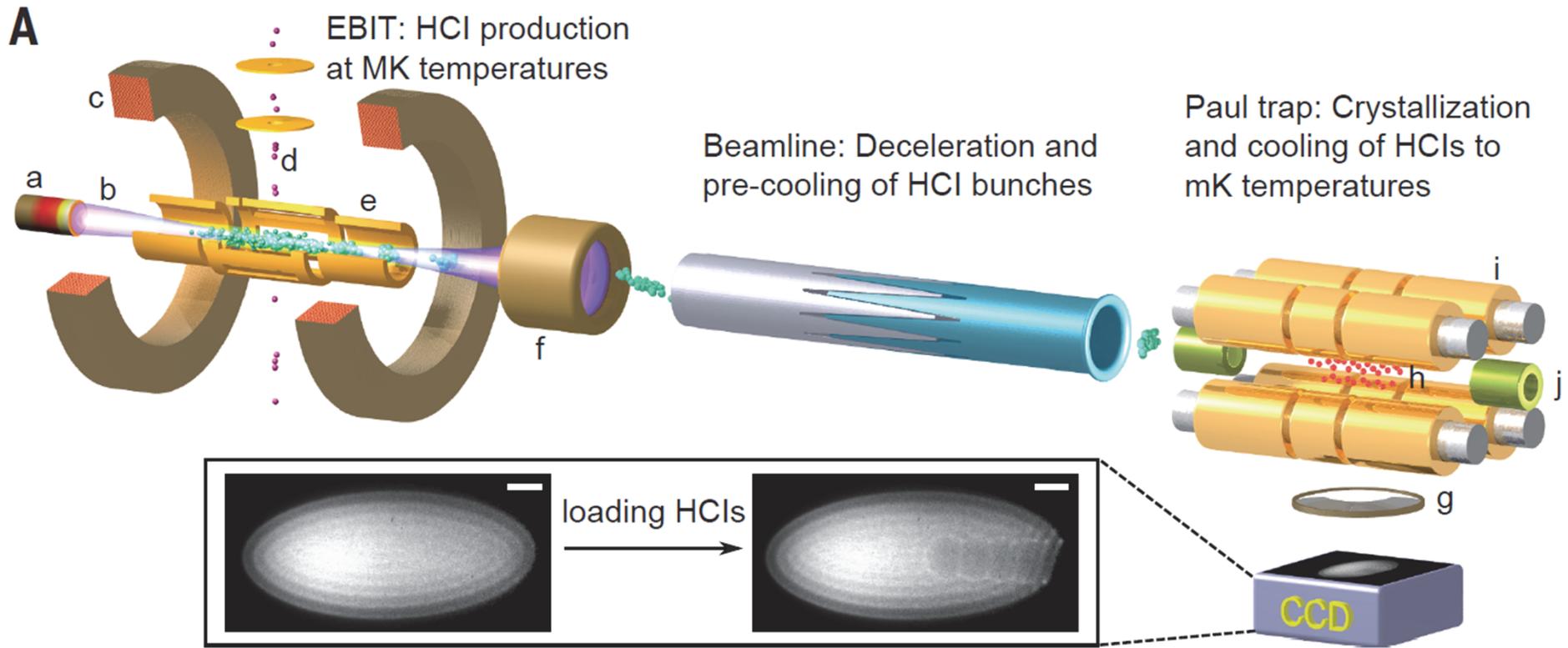
Understanding Sn spectra



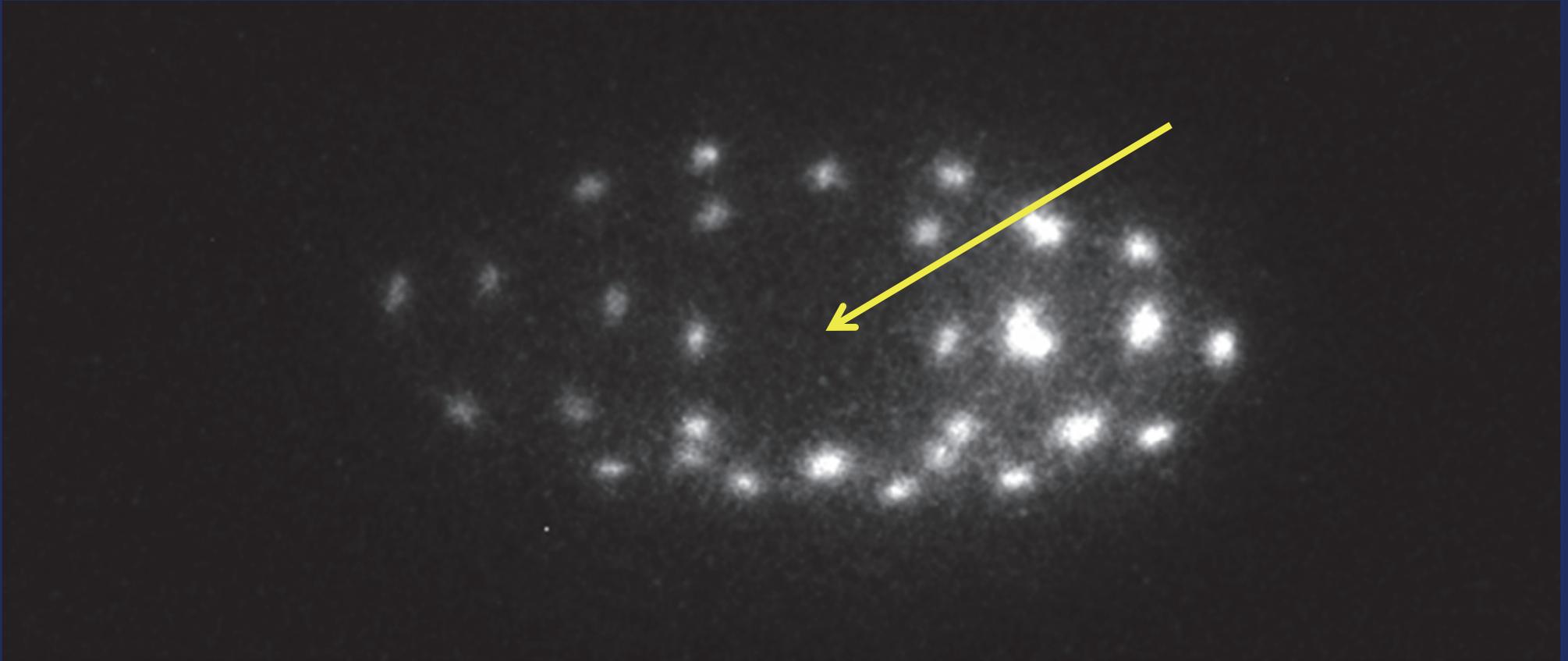
F. Torretti, ARCNL, PRA (2017)

Optical frequency metrology with HCl stabilization

Production, deceleration, implantation of HCI



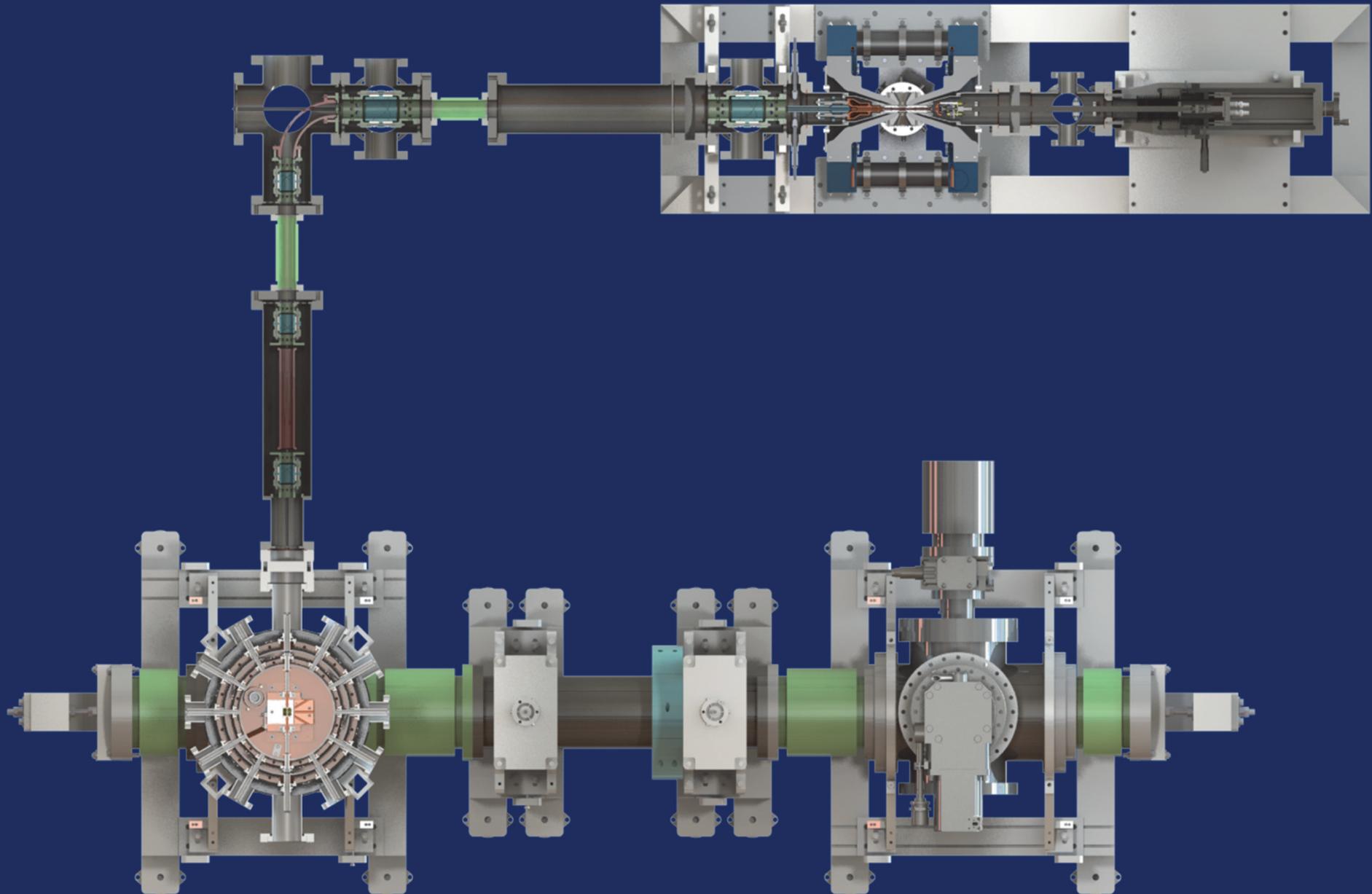
HCI identification by image analysis



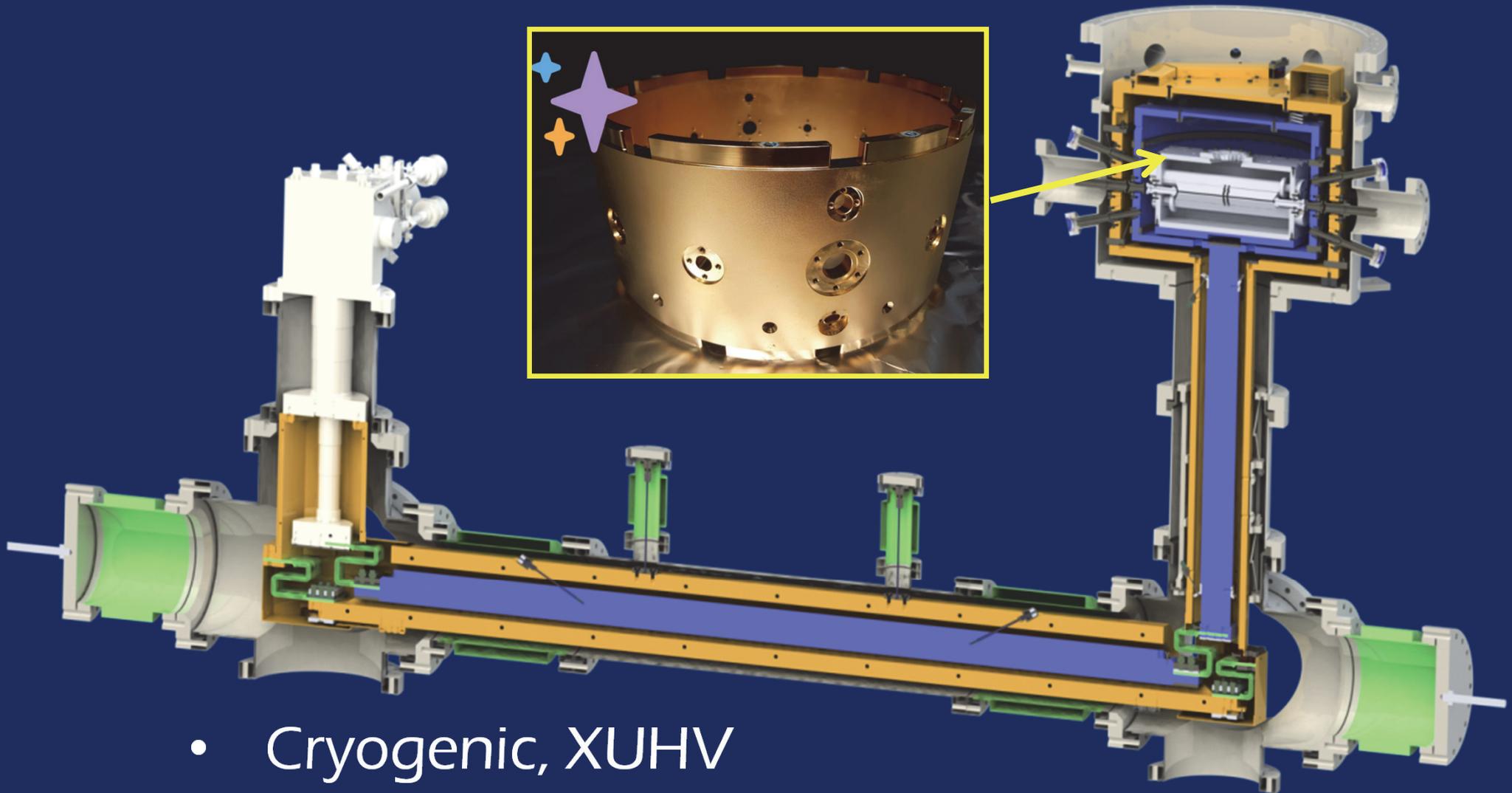
- The single HCI (here Ar^{13+}) repels Be^+ ions and produces a hole in the Coulomb crystal
- Addressing a single ion in the trap with a focused beam is possible due to large separation.

Lisa Schmöger et al., *Science* 347, 1233 (2015)

Setup at PTB

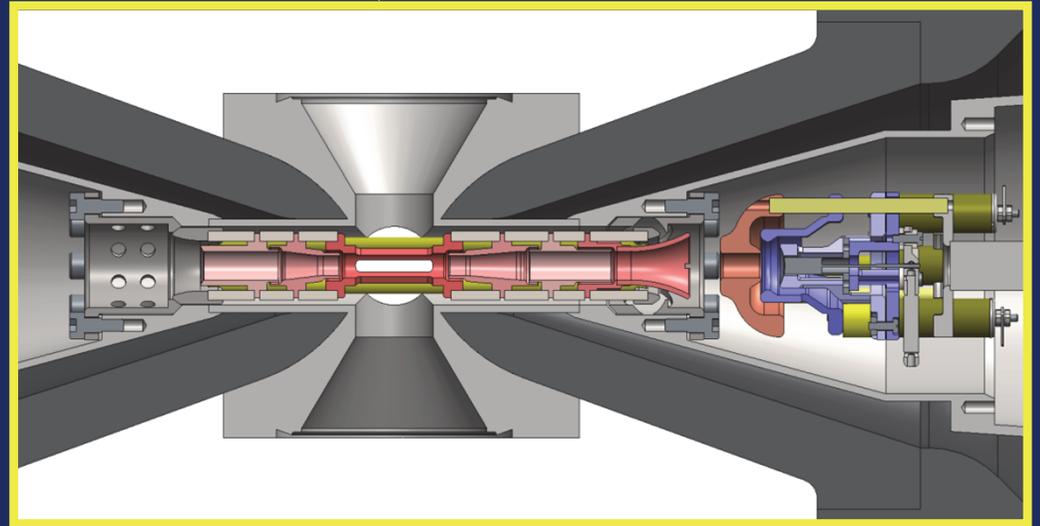
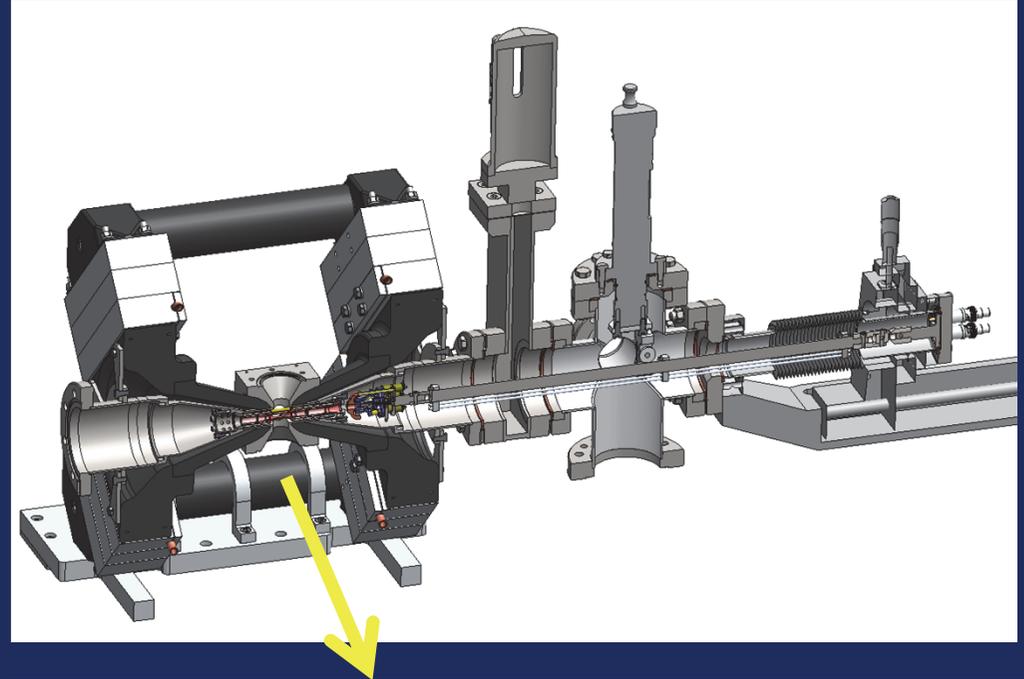
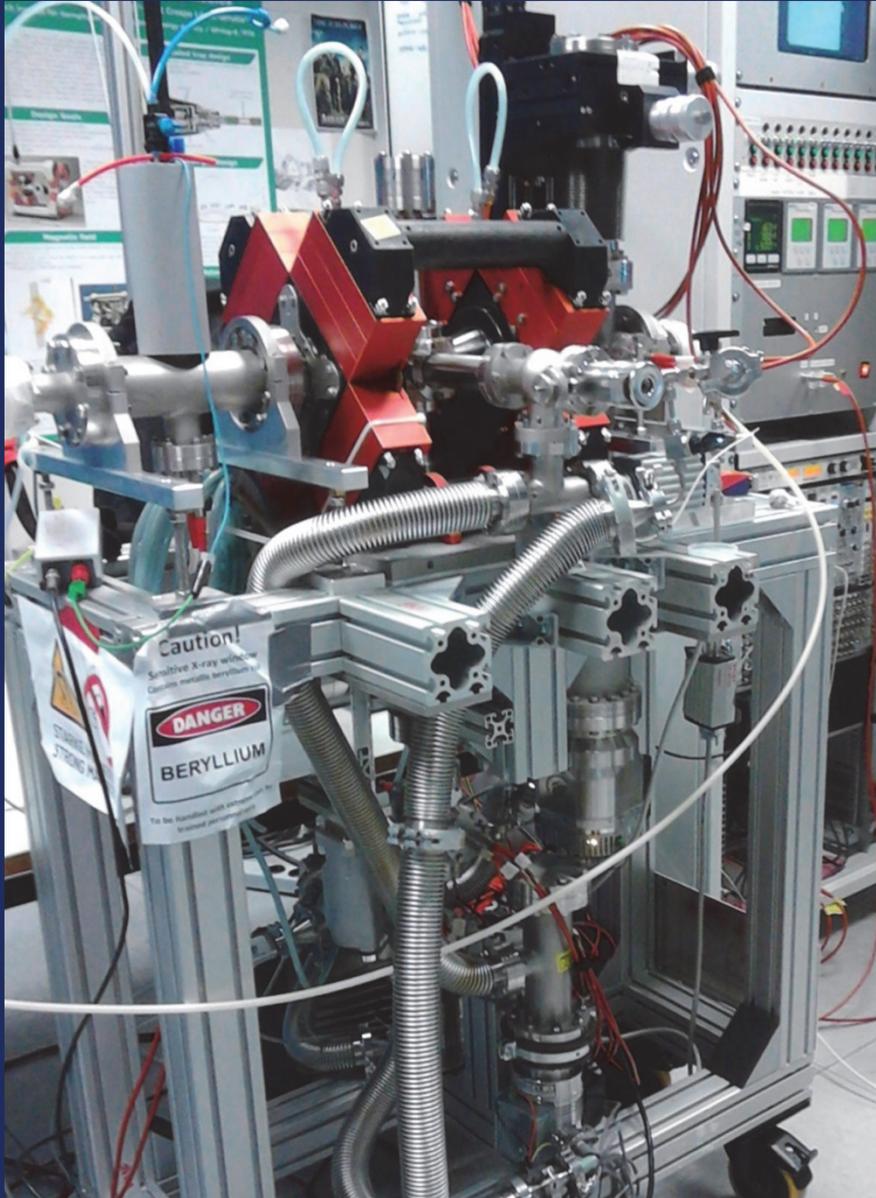


Next generation cryogenic trap



- Cryogenic, XUHV
- Ultra-low vibration
- Superconducting high-Q RF resonator

Table-top EBITs for PTB, Petra-III, Blaum division



Peter Micke et al., RSI (2018)

Possibilities through frequency metrology

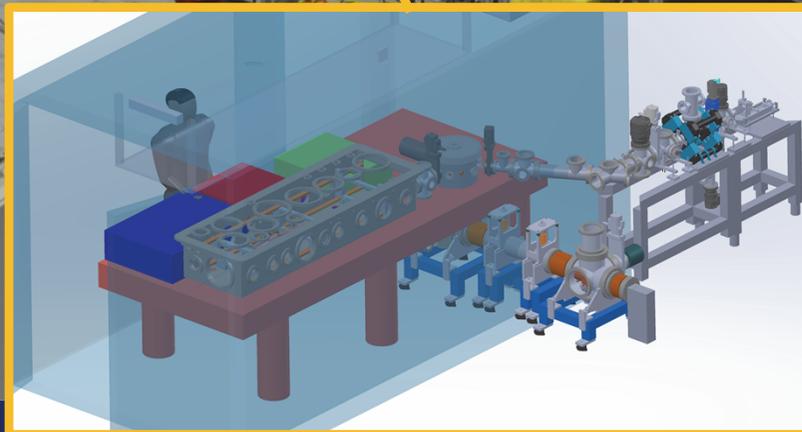
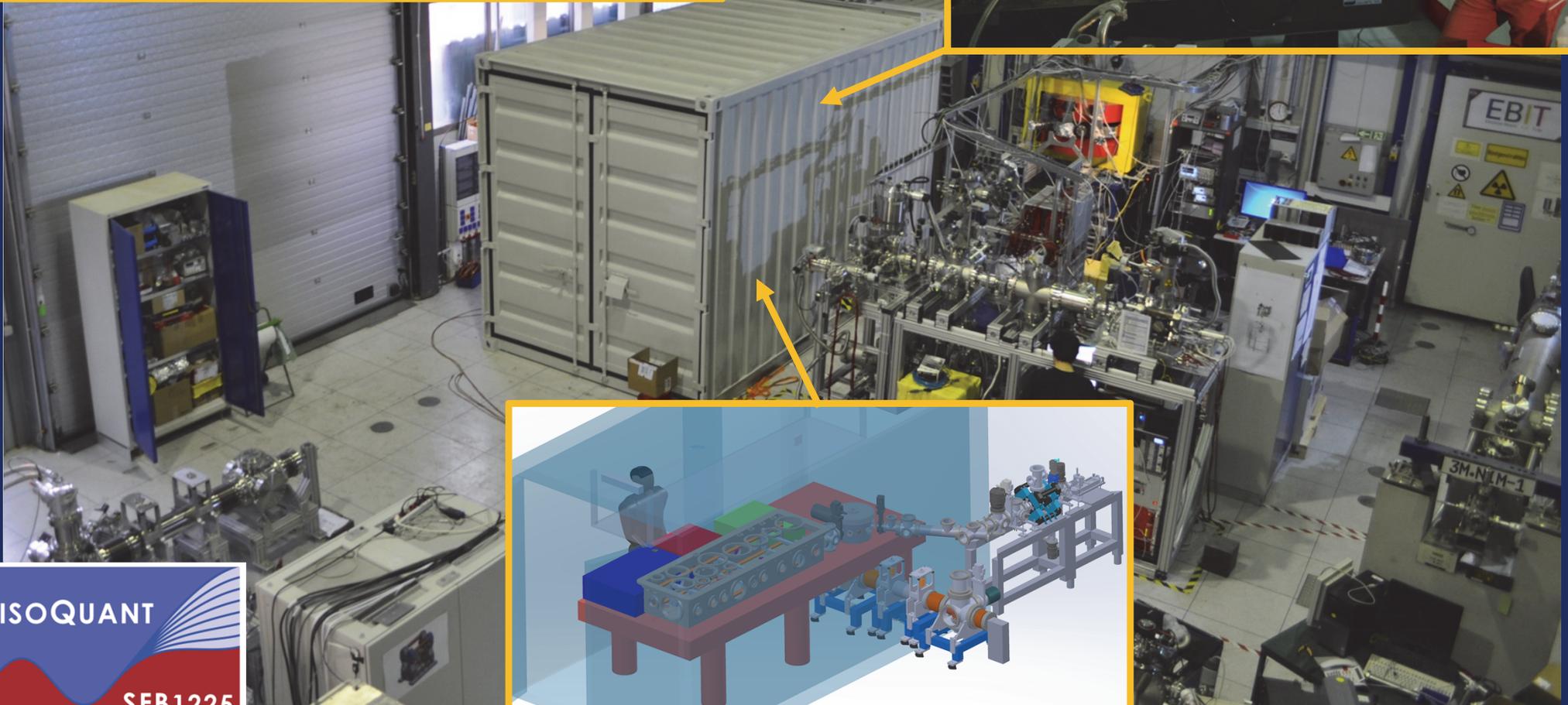
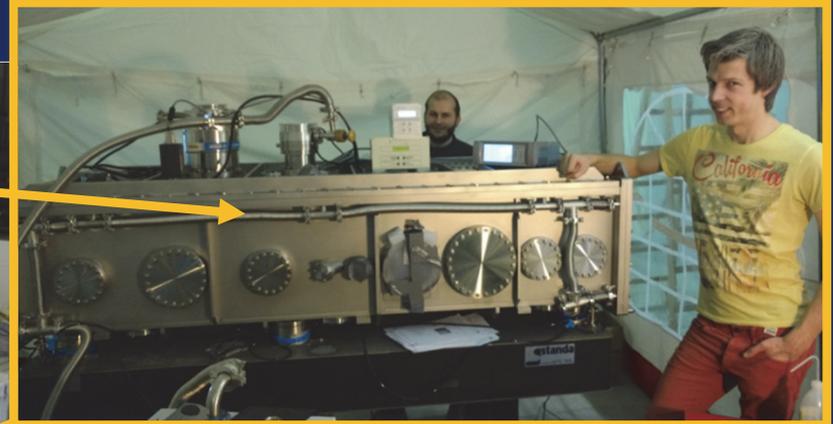
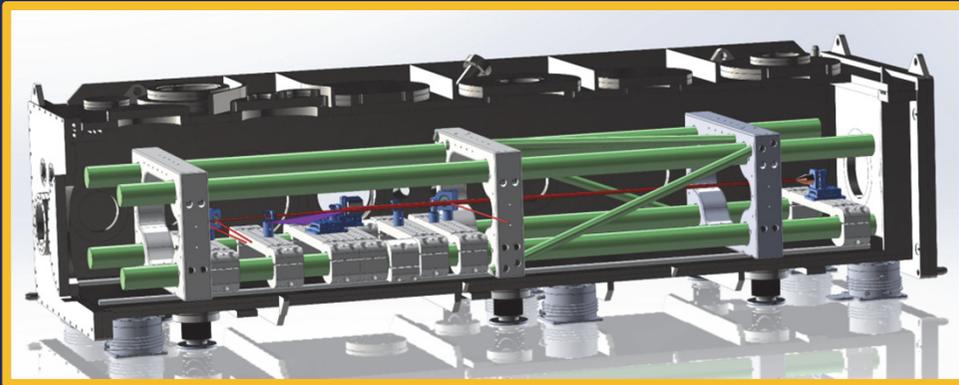
- **Whole new class** of laser-accessible targets, with **Z** and **ionic charge** as parameters
- **Great variety of optical and EUV lines** from fine and hyperfine transitions up to the highest charge states
- **Stable up to X-ray region**
- **Forbidden transitions** suitable as frequency standards
- **Low sensitivity** to DC, AC Stark, Zeeman and blackbody shifts
- **Highest sensitivity to** fine-structure constant α in atomic systems

A laser high harmonic frequency comb in the VUV



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Temperature-controlled container for HHG-frequency comb



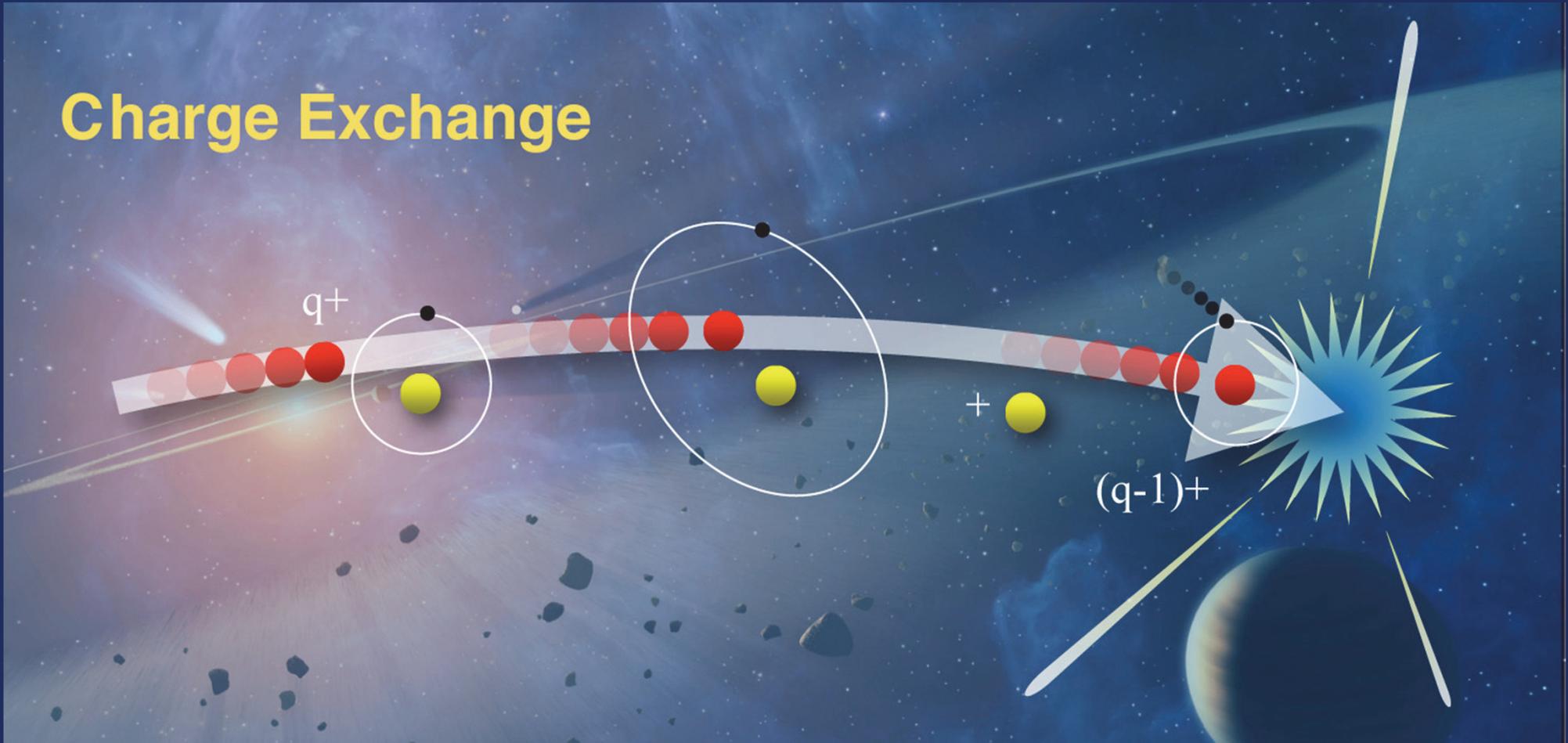
ISOQUANT

SFB1225

Charge exchange studies with photon emission

Charge exchange from neutrals to HCl

Charge Exchange



Solar wind:

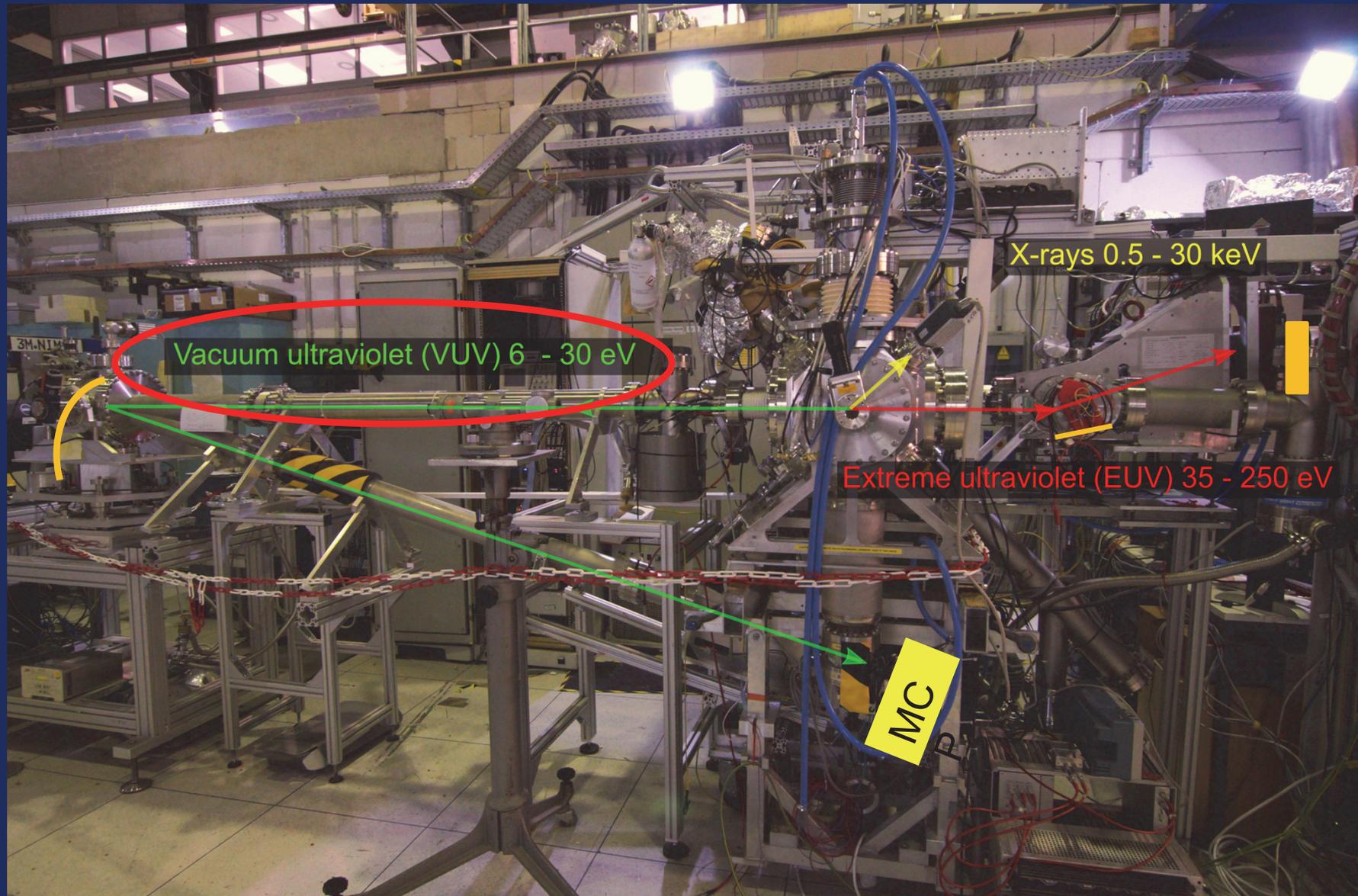
Beiersdorfer, P., Boyce, K. R., Brown, G. V., et al. 2003, *Science*, **300**, 1558 (2003)

Beiersdorfer, P., Schweikhard, L., Liebisch, P., & Brown, G. V., *ApJ*, **672**, 726 (2008)

Galaxy Clusters:

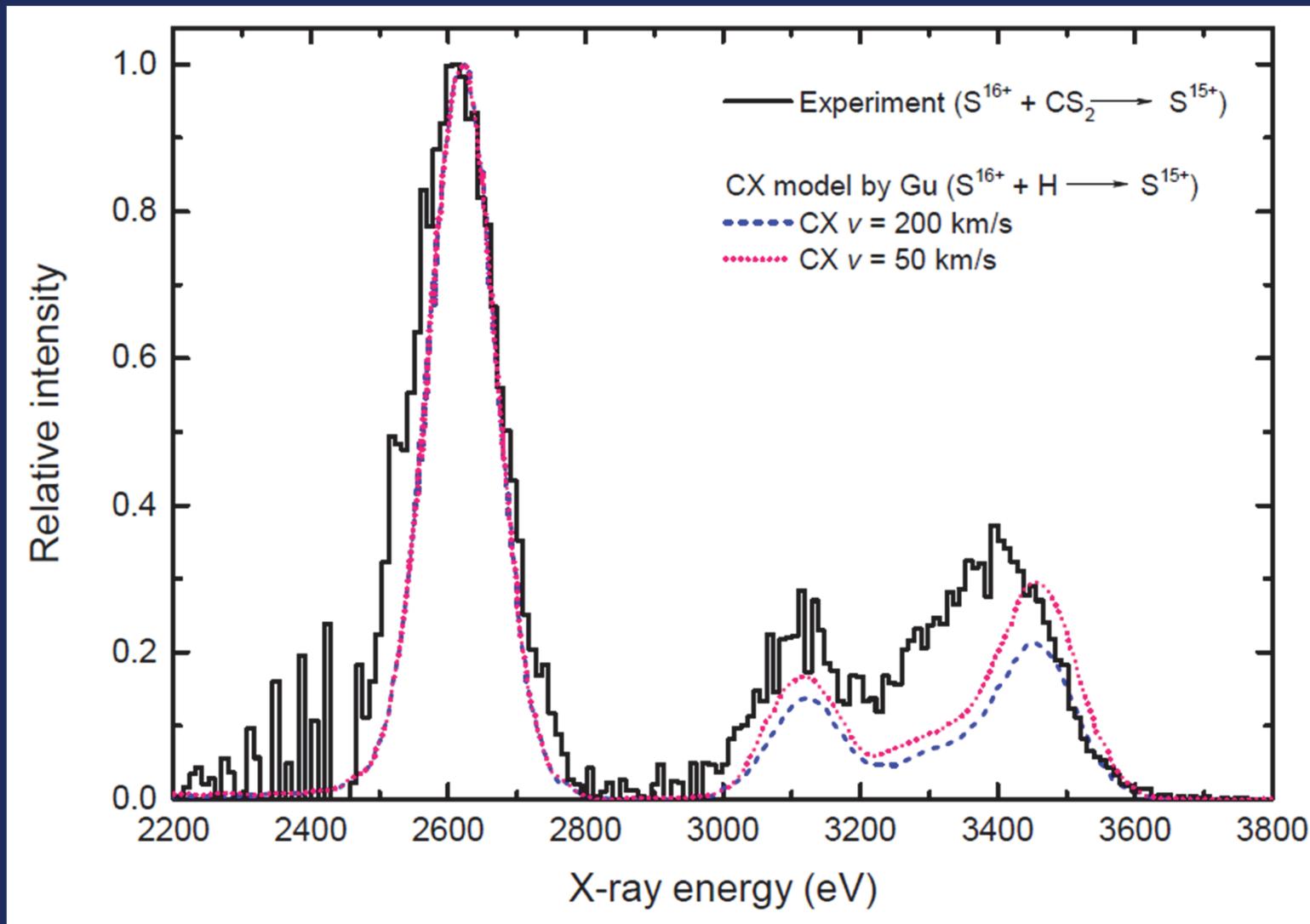
L. Gu, ... C. Shah, ... et al, *A&A* **611**, A26 (2018)

Charge exchange in the laboratory



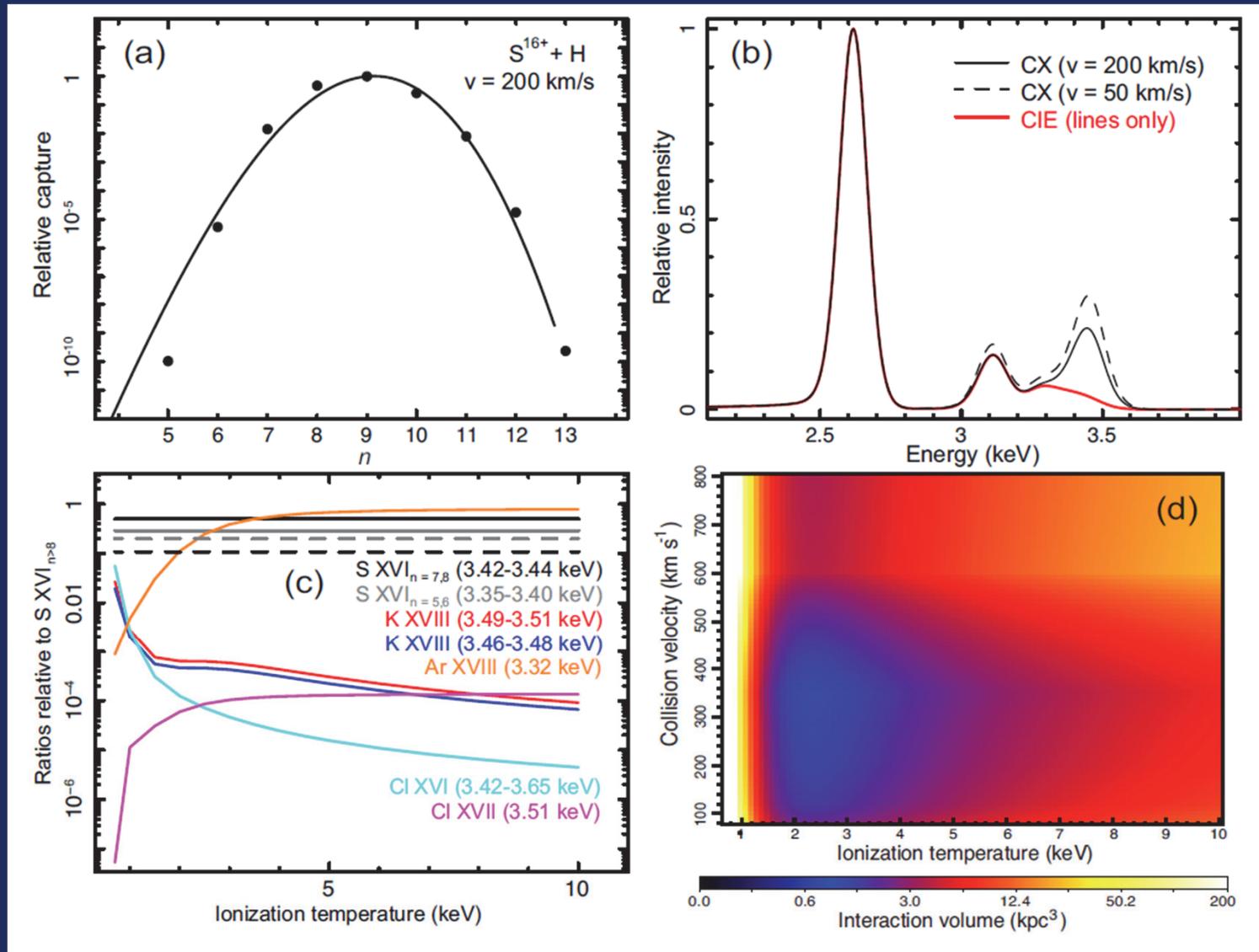
Shah, C., Dobrodey, S., Bernitt, S., JRCLU et al., *ApJ* 833, 52 (2016)

3.5 keV line (a.k.a. Dark Matter annihilation signal) is produced in the laboratory with recombining S^{16+} ions



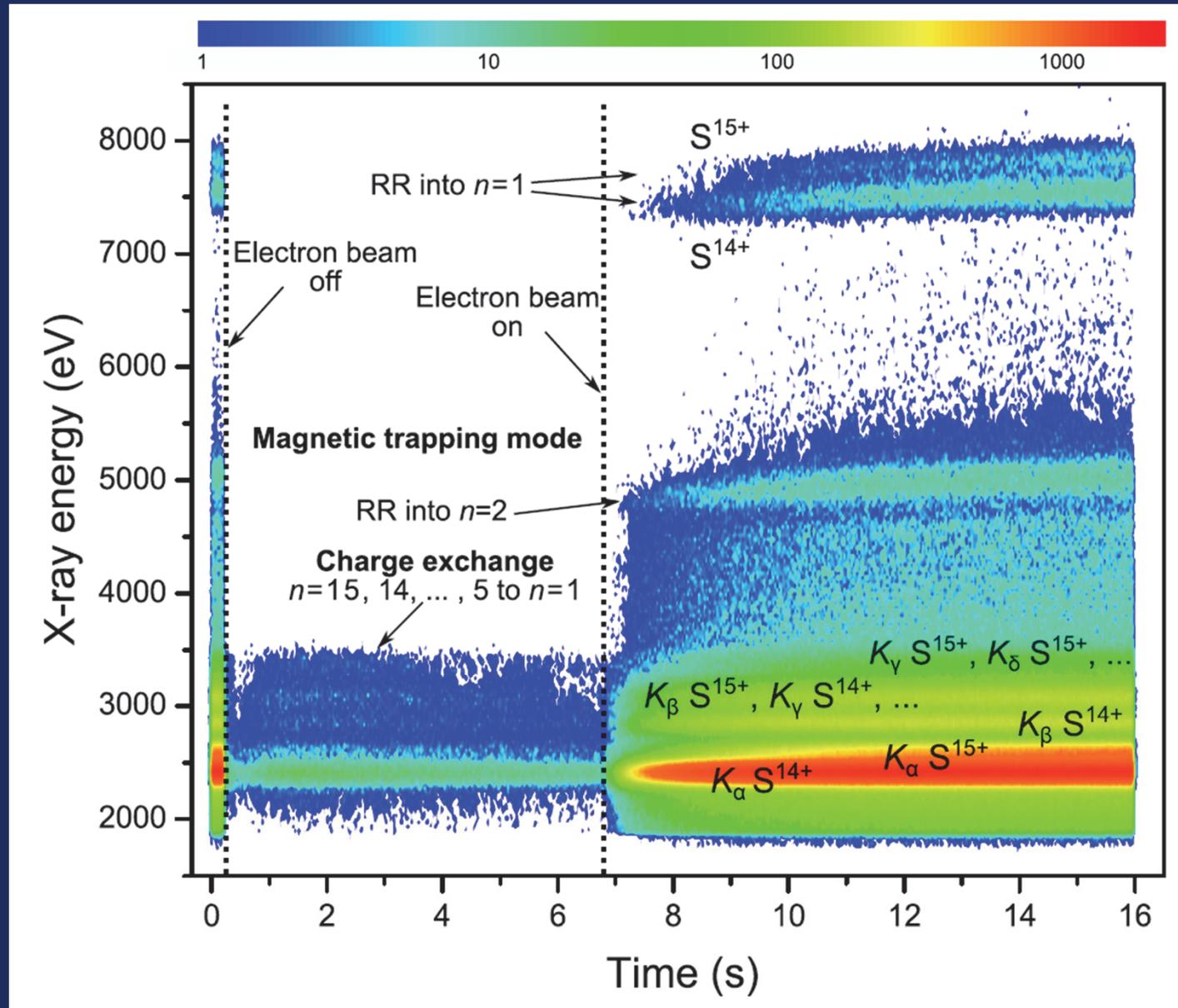
Shah, C., Dobrodey, S., Bernitt, S., JRCLU et al., *ApJ* 833, 52 (2016)

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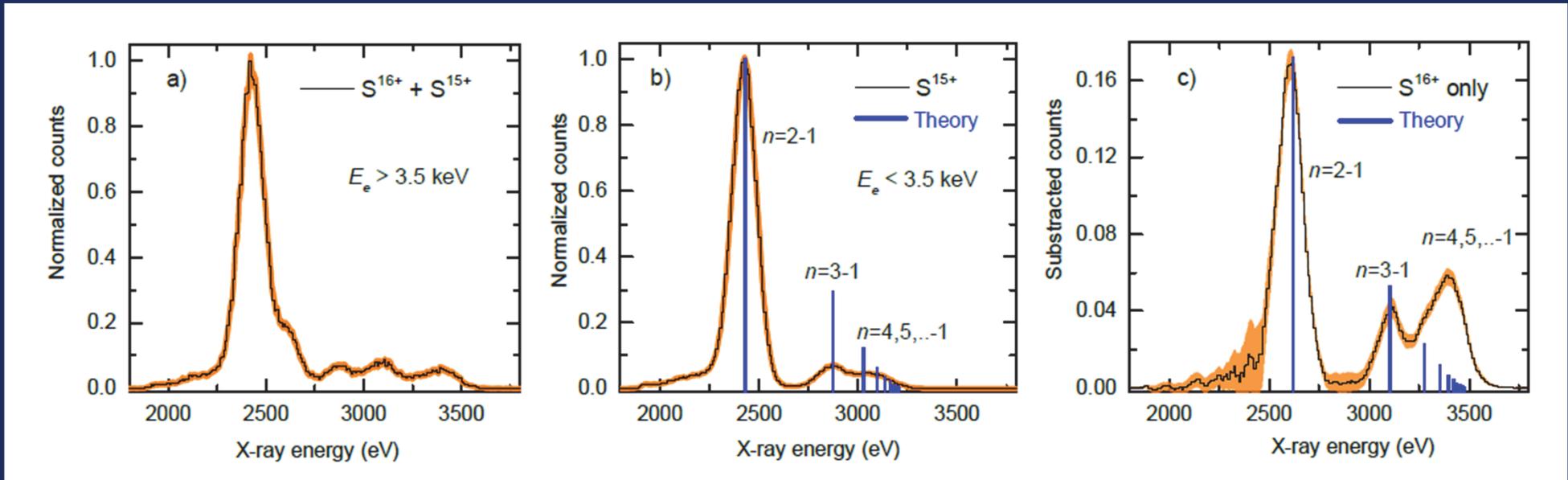
Shah, C., Dobrodey, S., Bernitt, S., JRCLU et al., ApJ 833, 52 (2016)

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Shah, C., Dobrodey, S., Bernitt, S., JRCLU et al., ApJ 833, 52 (2016)

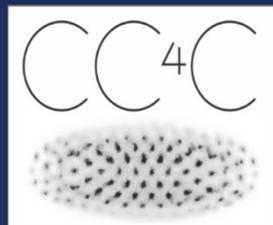
L. Gu, ... C. Shah, ... et al, A&A 611, A26 (2018)

Summary

- X-ray Lyman- α and He-like studies with ppm accuracy
- EUV, VUV studies with ppm accuracy
- Photoionization studies from N^{3+} to Fe^{23+}
- X-ray laser spectroscopy demonstrated:
 - $Fe^{15+...17+}$ resonance transitions at ~ 800 eV
 - Ly-series lines of F^{8+} and O^{7+} at ~ 800 eV
 - Fe $K\alpha$ in $Fe^{21+...24+}$ ions excited at 6.7 keV
 - Kr^{34+} , Br^{33+} high-resolution studies up to 14 keV
 - Soft x-ray calibrations with $\Delta E \approx 20$ meV
- Oscillator strengths, line widths, cross sections determinations
- Charge exchange with photon emission
- VUV frequency comb in preparation
- Optical clock tests at PTB already running in collaboration

MPIK current and former team members

T. M. Baumann, C. Beilmann, H. Bekker, S. Bernitt,
M. Blessenohl, S. Bogen, A. Borodin, G. Brenner,
S. Dobrodey, S. Epp, K. Fujii, K. Kubicek, S. Kühn,
V. Mäckel, P. Micke, J. Nauta, J.-H. Oelmann, L. Schmöger,
K. Schnorr, M. Schwarz, C. Shah, M. C. Simon, J. Stark,
R. Steinbrügge, O. O. Versolato, A. Windberger,
C. Warnecke, JRCLU, T. Pfeifer



Collaborations

UNL

P. Amaro

ARCNL

F. Torretti, R. Hoekstra,
W. Ubachs, J. Scheers,
O. O. Versolato

Petra III

H.-Ch. Wille, K. Schlage

LCLS

J. Turner, W. F. Schlotter

BESSY II

O. Schwarzkopf, R. Follath

FLASH

N. Guerassimova, R. Treusch
G. Brenner

Heidelberg University

S. Tashenov

Hamburg University

L. Mercadier, N. Rohringer

Groningen University

A. Borschevsky

TRIUMF

J. Dilling, L. Graham

EBIT LCLS Collaboration

G. V. Brown, P. Beiersdorfer, LLNL

E. Behar, Technion

E. Träbert, Bochum University

A. Graf, A. Rasmussen, SLAC

M. Leutenegger, NASA Goddard

A. Müller, S. Schippers, Gießen University

Aarhus University

M. Drewsen, A. K. Hansen

PTB

T. Leopold, S. King, P. O. Schmidt

UNSW

J. Berengut

University of Delaware

M. Safronova

UNIST

S.-N. Park, M. Chung

SRON

L. Gu, J. Kaastra

University Jena

S. Bernitt, T. Stöhlker

University Erlangen

J. Wilms, N. Hell

MPIK team



Some related MPIK references

X-ray resonant photoexcitation: Linewidths and energies of K α transitions in highly charged Fe ions, Rudolph, J.K., Bernitt, S., Epp, S.W., Steinbrügge, R., Beilmann, C., Brown, G.V., Eberle, S., Graf, A., Harman, Z., Hell, N., Leutenegger, M., Müller, A., Schlage, K., Wille, H.-C., Yavaş, H., Ullrich, J., Crespo López-Urrutia, J. R., Phys. Rev. Lett. **111** (2013) 103002

An unexpectedly low oscillator strength as the origin of the Fe XVII emission problem, Bernitt, S., Brown, G.V., Rudolph, J.K., Steinbrügge, R., Graf, A., Leutenegger, M., Epp, S.W., Eberle, S., Kubiček, K., Mäckel, V., Simon, M.C., Träbert, E., Magee, E.W., Beilmann, C., Hell, N., Schippers, S., Müller, A., Kahn, S.M., Surzhykov, A., Harman, Z., Keitel, C.H., Clementson, J., Porter, F.S., Schlotter, W., Turner, J.J., Ullrich, J., Beiersdorfer, P. & Crespo López-Urrutia, J. R., Nature **492** (2012) 225

Resonant and near-threshold photoionization cross sections of Fe¹⁴⁺, Simon, M.C., Crespo López-Urrutia, J. R., Beilmann, C., Schwarz, M., Harman, Z., Epp, S.W., Schmitt, B.L., Baumann, T.M., Behar, E., Bernitt, S., Follath, R., Ginzler, R., Keitel, C.H., Klawitter, R., Kubiček, K., Mäckel, V., Mokler, P.H., Reichardt, G., Schwarzkopf, O. & Ullrich, J. Phys. Rev. Lett. **105** (2010) 183001

Strongly enhanced recombination via two-center electronic correlations, Müller, C., Voitkiv, A.B., López-Urrutia, J.R.C. & Harman, Z., Phys. Rev. Lett. **104** (2010) 233002

Prominent higher-order contributions to electronic recombination, Beilmann, C., Mokler, P.H., Bernitt, S., Keitel, C.H., Ullrich, J., López-Urrutia, J.R.C. & Harman, Z., Phys. Rev. Lett. **107** (2011) 143201

State-selective quantum interference observed in the recombination of highly charged Hg^{75+...78+} mercury ions in an electron beam ion trap, A. J. González Martínez, J. R. Crespo López-Urrutia, J. Braun, G. Brenner, H. Bruhns, A. Lapierre, V. Mironov, R. Soria Orts, H. Tawara, M. Trinczek, J. Ullrich, J. H. Scofield, Phys. Rev. Lett. **94** (2005) 203201

Optical spectroscopy of complex open-4d-shell ions Sn⁷⁺-Sn¹⁰⁺, F. Torretti, A. Windberger, A. Ryabtsev, S. Dobrodey, H. Bekker, W. Ubachs, R. Hoekstra, E. V. Kahl, J. C. Berengut, J. R. Crespo López-Urrutia, O. O. Versolato, Physical Review A - Atomic, Molecular, and Optical Physics **95**, 042503 (2017)

State-selective influence of the Breit interaction on the angular distribution of emitted photons following dielectronic recombination P. Amaro, C. Shah, R. Steinbrügge, C. Beilmann, S. Bernitt, J. R. Crespo López-Urrutia, S. Tashenov, Physical Review A - Atomic, Molecular, and Optical Physics, **95**, 022712 (2017)

Identifications of 5s_{1/2}-5p_{3/2} and 5s²-5s5p EUV transitions of promethium-like Pt, Ir, Os and Re, Bekker, H., Versolato, O.O., Windberger, A., Oreshkina, N.S., Schupp, R., Baumann, T.M., Harman, Z., Keitel, C.H., Schmidt, P.O., Ullrich, J., Crespo López-Urrutia, J.R., Journal of Physics B: Atomic, Molecular and Optical Physics, **48**, 144018, (2015)

Some related MPIK references

Laboratory measurements compellingly support a charge-exchange mechanism for the “Dark Matter” ~3.5 keV X-ray line, C. Shah, S. Dobrodey, S. Bernitt, R. Steinbrugge, J. R. Crespo López-Urrutia, L. Y. Gu, J. Kaastra, *Astrophys. J.* **833**, 52 (2016)

Polarization measurement of dielectronic recombination transitions in highly charged krypton ions, C. Shah, H. Jörg, S. Bernitt, S. Dobrodey, R. Steinbrugge, C. Beilmann, P. Amaro, Z. M. Hu, S. Weber, S. Fritzsche, A. Surzhykov, J. R. Crespo López-Urrutia, S. Tashenov, *Physical Review A - Atomic, Molecular, and Optical Physics*, 2016, **94**, 029905

Analysis of the fine structure of Sn^{11+} - Sn^{14+} ions by optical spectroscopy in an electron-beam ion trap, A. Windberger, F. Torretti, A. Borschevsky, A. Ryabtsev, S. Dobrodey, H. Bekker, E. Eliav, U. Kaldor, W. Ubachs, R. Hoekstra, J. R. Crespo López-Urrutia, O. O. Versolato, *Physical Review A - Atomic, Molecular, and Optical Physics*, 2016, **94**, 012506

Strong higher-order resonant contributions to x-ray line polarization in hot plasmas, C. Shah, P. Amaro, R. Steinbrugge, C. Beilmann, S. Bernitt, S. Fritzsche, A. Surzhykov, J. R. Crespo López-Urrutia, S. Tashenov, *Physical Review E* 2016, **93**, 061201

Measurement of the radiative decay rate and energy of the metastable $(1s^2 2p_{1/2} 5s_{1/2})(J=0)$ level in Fe XVII, Beiersdorfer, P., Crespo López-Urrutia, J.R., Träbert, E., *Astrophysical Journal* **817**, 67 (2016)

Polarization measurement of dielectronic recombination transitions in highly charged krypton ions, Shah, C., Jörg, H., Bernitt, S., Dobrodey, S., Steinbrügge, R., Beilmann, C., Amaro, P., Hu, Z., Weber, S., Fritzsche, S., Surzhykov, A., Crespo López-Urrutia, J.R., Tashenov, S., *Physical Review A - Atomic, Molecular, and Optical Physics*, **92**, 042702 (2015)

Deceleration, precooling, and multi-pass stopping of highly charged ions in Be⁺ Coulomb crystals, Schmöger, L., Schwarz, M., Baumann, T.M., Versolato, O.O., Piest, B., Pfeifer, T., Ullrich, J., Schmidt, P.O., Crespo López-Urrutia, J.R., *Review of Scientific Instruments* **86**, 103111 (2015)

Absolute radiative and Auger transition rates of K-shell excited few-electron iron ions, Steinbrügge, R., Bernitt, S., Rudolph, J.K., Crespo López-Urrutia, J.R., *Journal of Physics: Conference Series* **635**, 092146 (2015)

Single-photon excitation of $K\alpha$ in heliumlike Kr^{34+} : Results supporting quantum electrodynamics predictions, Epp, S.W., Steinbrügge, R., Bernitt, S., Rudolph, J.K., Beilmann, C., Bekker, H., Müller, A., Versolato, O.O., Wille, H.-C., Yavaş, H., Ullrich, J., Crespo López-Urrutia, J.R., *Physical Review A - Atomic, Molecular, and Optical Physics* **92**, 020502 (2015)



Some related MPIK references

Absolute measurement of radiative and Auger rates of K-shell-vacancy states in highly charged Fe ions, Steinbrügge, R., Bernitt, S., Epp, S.W., Rudolph, J.K., Beilmann, C., Bekker, H., Eberle, S., Müller, A., Versolato, O.O., Wille, H.-C., Yavaş, H., Ullrich, J., Crespo López-Urrutia, J.R., *Physical Review A - Atomic, Molecular, and Optical Physics* **91**, 032502 (2015)

Complete measurements of anisotropic x-ray emission following recombination of highly charged ions, Shah, C., Amaro, P., Steinbrügge, R., Beilmann, C., Bernitt, S., Fritzsche, S., Surzhykov, A., López-Urrutia, J.R.C., Tashenov, S., *Journal of Physics: Conference Series*, **635**, 052093 (2015)

Coulomb crystallization of highly charged ions, Schmöger, L., Versolato, O.O., Schwarz, M., Kohnen, M., Windberger, A., Piest, B., Feuchtenbeiner, S., Pedregosa, J., Leopold, T., Micke, P., Hansen, A.K., Baumann, T.M., Drewsen, M., Ullrich, J., Schmidt, P.O., Crespo López-Urrutia, J.R., *Journal of Physics: Conference Series*, **635**, 022059 (2015)

Linear polarization of x rays due to dielectronic recombination into highly charged ions, Shah, C., Jörg, H., Hu, Z., Bernitt, S., Bekker, H., Blessenohl, M.A., Hollain, D., Weber, S., Dobrodey, S., Fritzsche, S., Surzhykov, A., López-Urrutia, J.R.C., Tashenov, S., *Journal of Physics: Conference Series* **635**, 052091 (2015)

Kinematically complete study of electron transfer and rearrangement processes in slow Ar¹⁶⁺-Ne collisions, Xue, Y., Ginzler, R., Krauß, A., Bernitt, S., Schöffler, M., Kühnel, K.U., Crespo López-Urrutia, J.R., Moshhammer, R., Cai, X., Ullrich, J., Fischer, D., *Physical Review A - Atomic, Molecular, and Optical Physics* **90**, 052720 (2014)

Contributions of dielectronic, trielectronic, and metastable channels to the resonant intershell recombination of highly charged silicon ions, Baumann, T.M., Harman, Z., Stark, J., Beilmann, C., Liang, G., Mokler, P.H., Ullrich, J., Crespo López-Urrutia, J.R., *Physical Review A - Atomic, Molecular, and Optical Physics* **90**, 052704 (2014)

Transition energy measurements in hydrogenlike and heliumlike ions strongly supporting bound-state QED calculations, Kubiček, K., Mokler, P.H., Mäckel, V., Ullrich, J., Crespo López-Urrutia, J.R., *Physical Review A - Atomic, Molecular, and Optical Physics* **90**, 032508 (2014)

An unexpectedly low oscillator strength as the origin of the Fexvii emission problem, Bernitt, S., Brown, G.V., Rudolph, J.K., Steinbrügge, R., Graf, A., Leutenegger, M., Epp, S.W., Eberle, S., Kubiček, K., Mäckel, V., Simon, M.C., Träbert, E., Magee, E.W., Beilmann, C., Hell, N., Schippers, S., Müller, A., Kahn, S.M., Surzhykov, A., Harman, Z., Keitel, C.H., Clementson, J., Porter, F.S., Schlotter, W., Turner, J.J., Ullrich, J., Beiersdorfer, P., Crespo López-Urrutia, J. R., *Nature* **492** (2012) 225

Electron recombination in dense photonic, electronic and atomic environments, Müller, C., Hu, H., Najjari, B., Crespo López-Urrutia, J. R., Harman, Z., Voitkiv, A.B., *J. Phys.: Conf. Series* **388** (2012) 012003



Some related MPIK references

Prominent higher-order contributions to electronic recombination, Beilmann, C., Mokler, P.H., Bernitt, S., Keitel, C.H., Ullrich, J., López-Urrutia, J.R.C., Harman, Z., Phys. Rev. Lett. **107** (2011) 143201

Laser spectroscopy on forbidden transitions in trapped highly charged Ar¹³⁺ ions, Mäckel, V., Klawitter, R., Brenner, G., Crespo López-Urrutia, J. R., Ullrich, J., Phys. Rev. Lett. **107** (2011) 143002

Higher-order resonant inter-shell electronic recombination for heavy highly charged ions, Beilmann, C., Mokler, P.H., Bernitt, S., Harman, Z., Keitel, C.H., Postavaru, O., Ullrich, J., Crespo López-Urrutia, J. R., Physica Scripta T, **T144** (2011) 014014

Resonant and Near-Threshold Photoionization Cross Sections of Fe¹⁴⁺, Simon, M.C., Crespo López-Urrutia, J.R., Beilmann, C., Schwarz, M., Harman, Z., Epp, S.W., Schmitt, B.L., Baumann, T.M., Behar, E., Bernitt, S., Follath, R., Ginzler, R., Keitel, C.H., Klawitter, R., Kubiček, K., Mäckel, V., Mokler, P.H., Reichardt, G., Schwarzkopf, O., Ullrich, J., Phys. Rev. Lett. **105** (2010) 183001

Measurement of the radiative decay rate of the metastable 2s²2p_{3/2}⁵3s_{1/2}(J=2) level in Fe XVII, Crespo López-Urrutia J. R., Beiersdorfer P, Astrophys. J. **721**, 576 (2010)

X-ray laser spectroscopy of highly charged ions at FLASH, Epp, S.W., López-Urrutia, J.R.C., Simon, M.C., Baumann, T., Brenner, G., Ginzler, R., Guerassimova, N., Mäckel, V., Mokler, P.H., Schmitt, B.L., Tawara, H., Ullrich, J., J. Phys. B-At. Mol. Opt. Phys. **43**, Special Issue, (2010) 194008

Strongly Enhanced Recombination via Two-Center Electronic Correlations, Müller, C, Voitkiv, A.B., Crespo López-Urrutia, J. R., Harman, Z., Phys. Rev. Lett. **104** (2010) 233202

Photoionization of N³⁺ and Ar⁸⁺ in an electron beam ion trap by synchrotron radiation, Simon, M.C., Schwarz, M., Epp, S.W., Beilmann, C., Schmitt, B.L., Harman, Z., Baumann, T.M., Mokler, P.H., Bernitt, S., Ginzler, R., Higgins, S.G., Keitel, C.H., Klawitter, R., Kubiček, K., Mäckel, V., Ullrich, J., Crespo López-Urrutia, J. R., J. Phys. B-At. Mol. Opt. Phys. **43** (2010) 065003

Intershell trielectronic recombination with K-shell excitation in Kr³⁰⁺, C. Beilmann, O. Postavaru, L. H. Arntzen, R. Ginzler, C. H. Keitel, V. Mäckel, P. H. Mokler, M. C. Simon, H. Tawara, I. I. Tupitsyn, J. Ullrich, J. R. Crespo López-Urrutia, and Z. Harman, Phys. Rev. A **80** (2009) 050702(R)

Measurement of the radiative decay rate of the metastable (2s²2p_{3/2}⁵3s_{1/2})(J=2) level in Fe XVII, Crespo López-Urrutia, J.R., Beiersdorfer, P., Astrophys. J. Lett. **721** (2010) 576

On the transition rate of the Fe X red coronal line, G. Brenner, J. R. Crespo López-Urrutia, S. Bernitt, D. Fischer, R. Ginzler, K. Kubicek, V. Mackel, P. H. Mokler, M. C. Simon, and J. Ullrich, Astrophys. J. **703** (2009) 68