Dissecting the physics of line strengths: how to use experiments to understand the strengths and limitations of atomic theory

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Collaborators

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- Erlangen/Remeis: Jakob Stierhof, Jörn Wilms
- Many others!

X-ray laboratory astrophysics serves science enabled by spectroscopy

- Most atomic data for astrophysical x-ray spectroscopy comes down to line strengths, and transition wavelengths/energies
- In many cases, the most important transition wavelengths can be measured to the needed precision
- Line strengths for all relevant lines in all relevant environments cannot be measured, so we need to rely on theory, which therefore needs to be benchmarked
- When benchmarks indicate that theory does not meet accuracy requirements, we need to do physics to diagnose the issue

What science is enabled by line strengths?

- Charge balance -> temperature distribution (or ionization parameter)
- DR line strengths -> temperature, …
- Elemental abundances
- Metastable diagnostics, e.g. density
- Optical depth effects, e.g. resonance scattering
- …

How well do we need to know line strengths?

- Of course this depends on science requirements!
- But for example if your question is “easy”, e.g. is O / Fe strongly supersolar, then the requirements are not strong
- Or if you want to diagnose high densities, lines from metastable levels are quite sensitive
- On the other hand if you want precision diagnostics rather than qualitative, you need precision data
- Resonance scattering is almost always a marginal effect in astrophysics, and really requires high-precision data (10% or better)

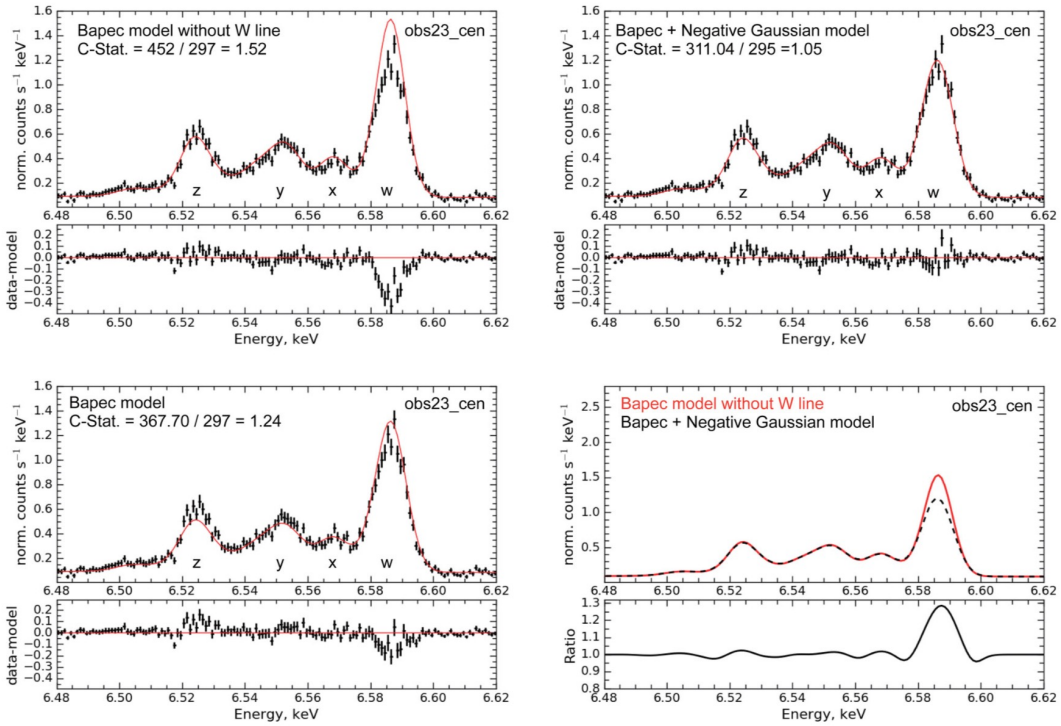
Key example: Resonance scattering

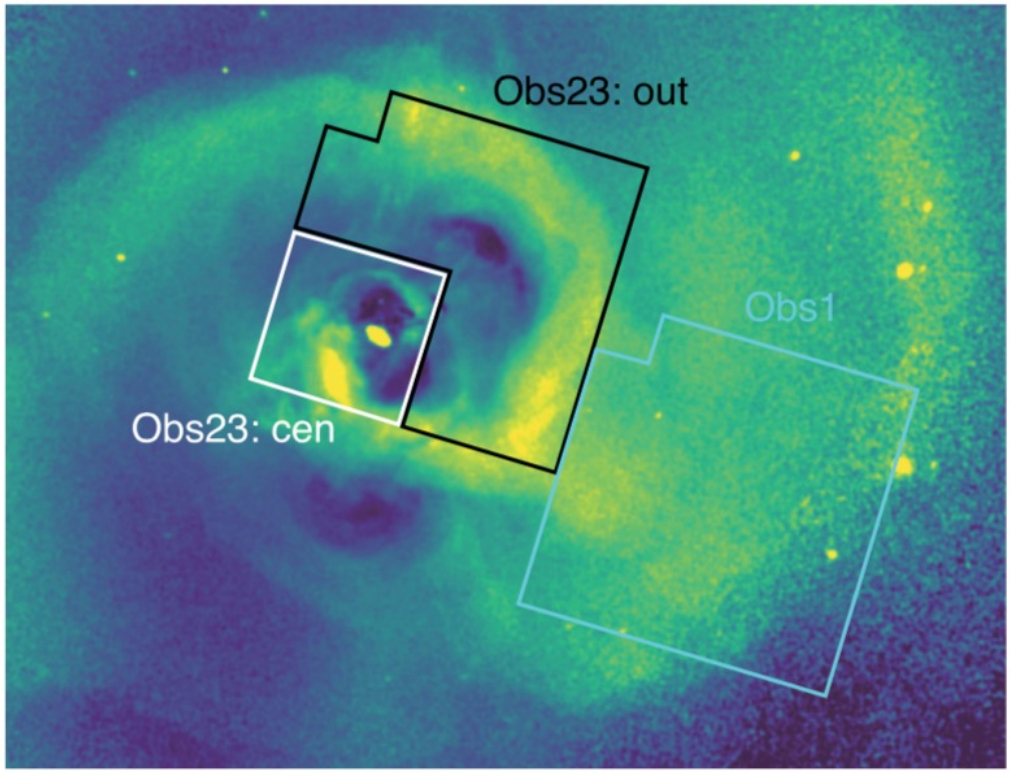
- Clusters of galaxies are mostly dark matter (by mass)
- Most of the baryonic mass is diffuse hot gas
- This gravitational potential of the dark matter is converted into thermal energy in the hot gas
- The very-low-density, highly-ionized, hot gas radiates x-rays
- The plasma is mostly optically thin to its own x-ray emission (it is very low density)
- But the volume is enormous, and perhaps in strong resonance lines of abundant elements the optical depth is no longer negligible

Key example: Resonance scattering

- Groups of galaxies are similar to clusters but smaller and therefore cooler
- Some giant elliptical galaxies are also basically similar (hot gas in the potential well of dark matter), but smaller and cooler yet
- Optical depth is linearly proportional to density, while surface brightness scales with density squared
- Optical depth (at line center) also depends on velocity dispersion
- Constraints on plasma density, size, and turbulence thus come from brightness, Doppler broadening, and resonance scattering!

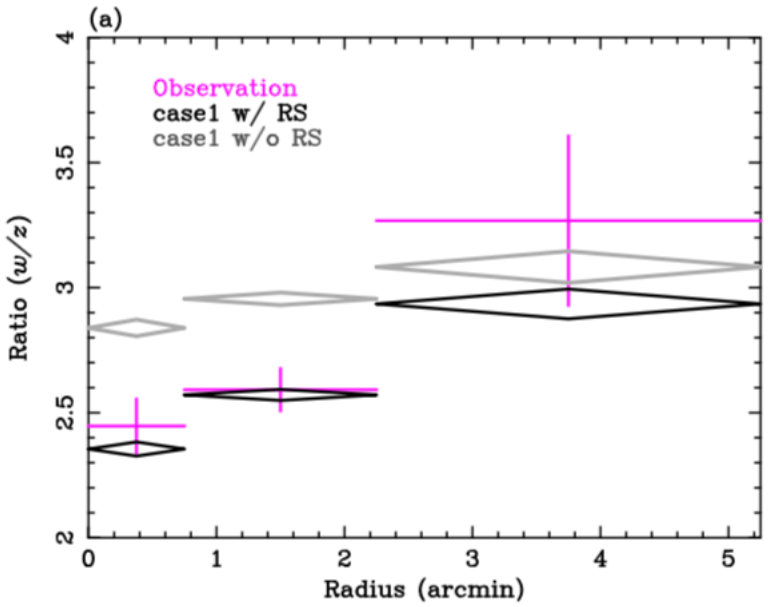
Resonance scattering in the Perseus cluster

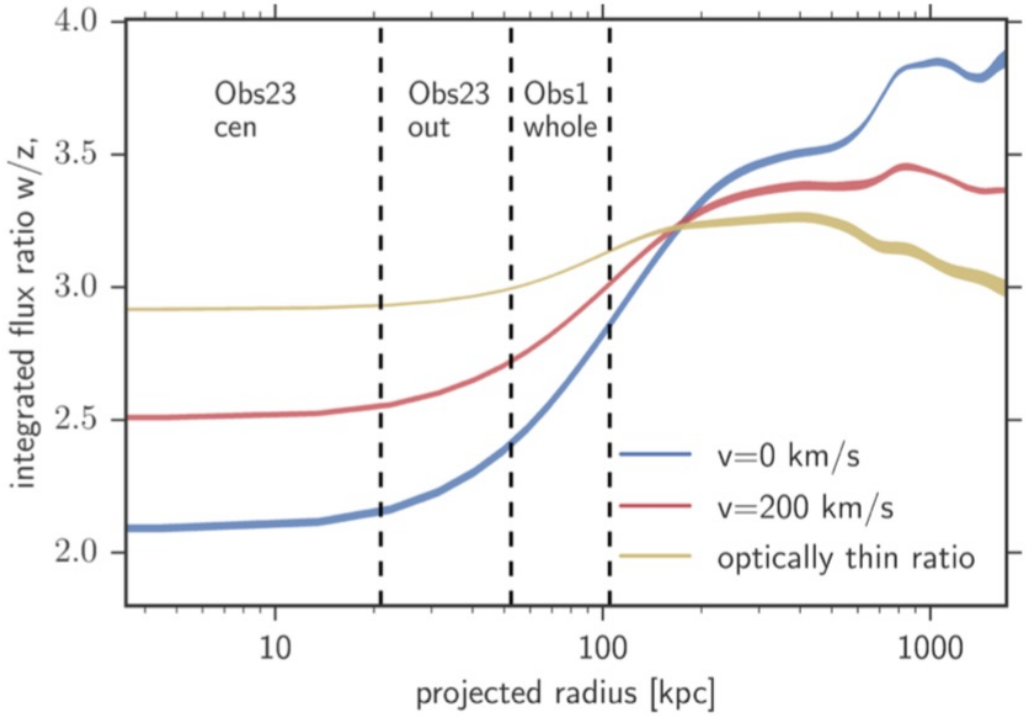




Hitomi collaboration 2018

Resonance scattering in the Perseus cluster





Uncertainties on model line strengths are on the order of 10-30%!

Hitomi collaboration 2018

Resonance scattering in giant elliptical galaxies

- Xu+2002, Werner+2009, Ogorzalek+2017, XMM RG: depressed resonance line 3C (15 Å) of Ne-like Fe XVII in cores of giant ellipticals – therefore v_{turb} is small

Mild T gradient

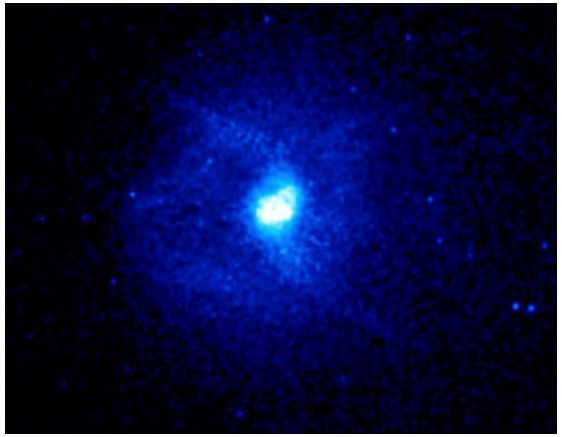
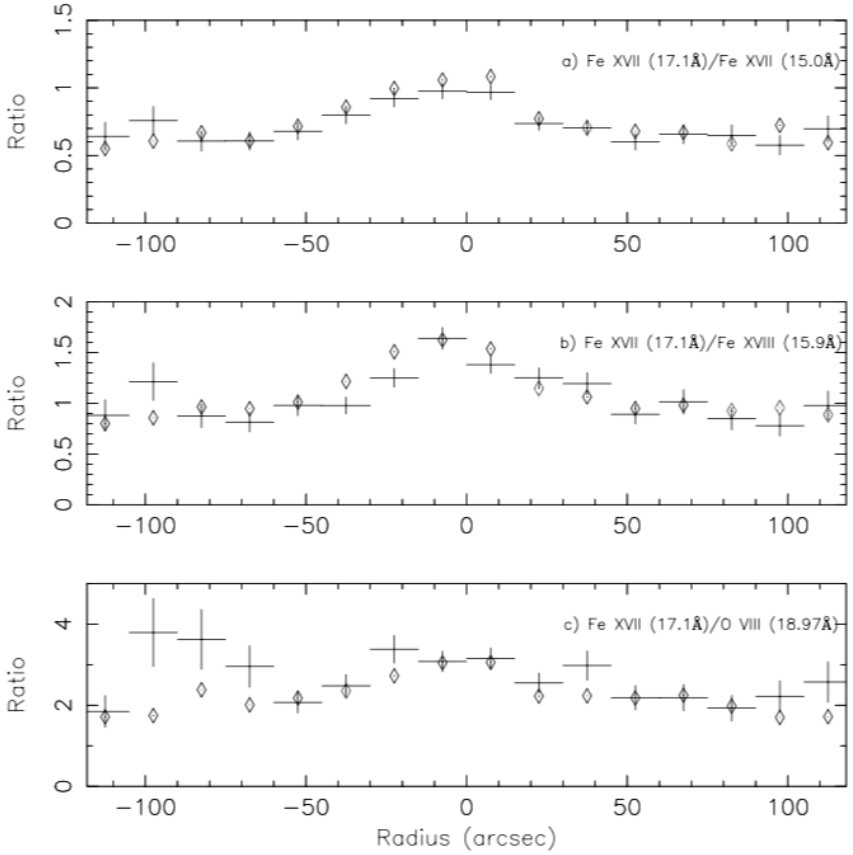


Image: NGC4636 - C. Jones+

No strong abundance gradient



Resonance Scattering

Xu+ 2002; NGC 4636

What is actually limiting the model accuracy? How can we test and improve models?

- Direct uncertainty on oscillator/collision strengths of resonance lines?
- Collision strengths of other lines that resonance lines are compared to?
  - Is method for treatment of excitations important? (i.e. treatment of collision physics – distorted wave vs. R-matrix)
  - Are all processes and levels that we need in the models? (completeness)
- Uncertainty due to blending, e.g. with DR satellite lines
- How to use lab measurements to diagnose these issues? What are the limitations of experiments?

Princeton Large Tokamak Results

Beiersdorfer+2004 3C/3D = 2.0 - 3.2

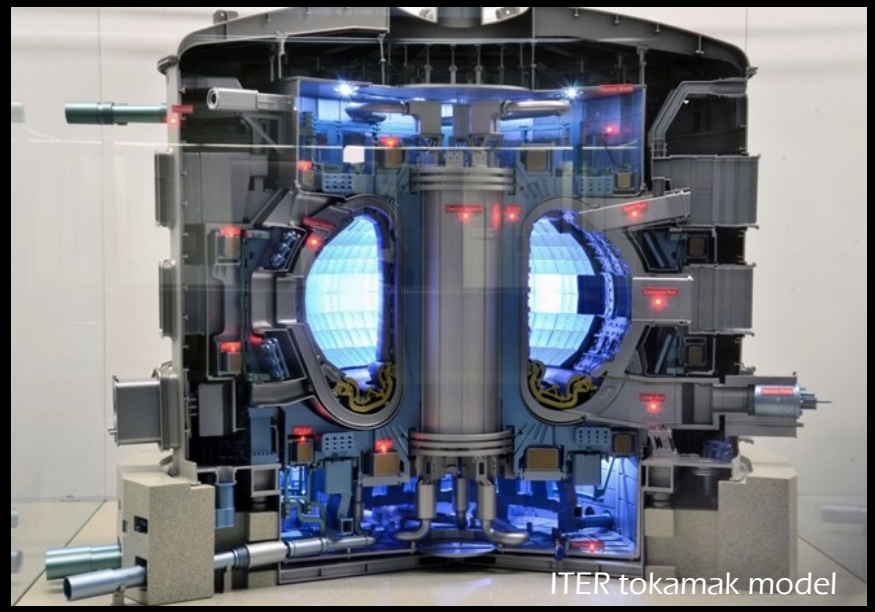
Theory exceeds TOKAMAK data

TABLE 1

RATIO OF THE INTENSITY OF THE Fe XVII $3s \rightarrow 2p$ TRANSITION $3F$ TO THAT OF THE $3d \rightarrow 2p$ TRANSITION $3C$, AS WELL AS THE RATIO OF THE SUM OF ALL $3s \rightarrow 2p$ TRANSITIONS (LINES $3F$, $3G$, AND $M2$) TO THAT OF LINE $3C$ INFERRED FROM TOKAMAK MEASUREMENTS

Source	I_{3F}/I_{3C}	$I_{3F+3G+M2}/I_{3C}$	I_{3D}/I_{3C}
PLT	0.75 ± 0.07	2.49 ± 0.22	0.44 ± 0.08
PLT	0.52 ± 0.06	2.18 ± 0.20	0.49 ± 0.10
PLT	0.72 ± 0.08	2.50 ± 0.30	0.47 ± 0.10
PLT	0.7 ± 0.1	1.88 ± 0.23	0.30 ± 0.05
DITE[a]	0.77 ± 0.08	2.15 ± 0.2	0.31 ± 0.05
JET[a]	0.7 ± 0.1	2.1 ± 0.3	0.35 ± 0.06

[a] Inferred from the spectrum presented by Phillips et al. (1997).



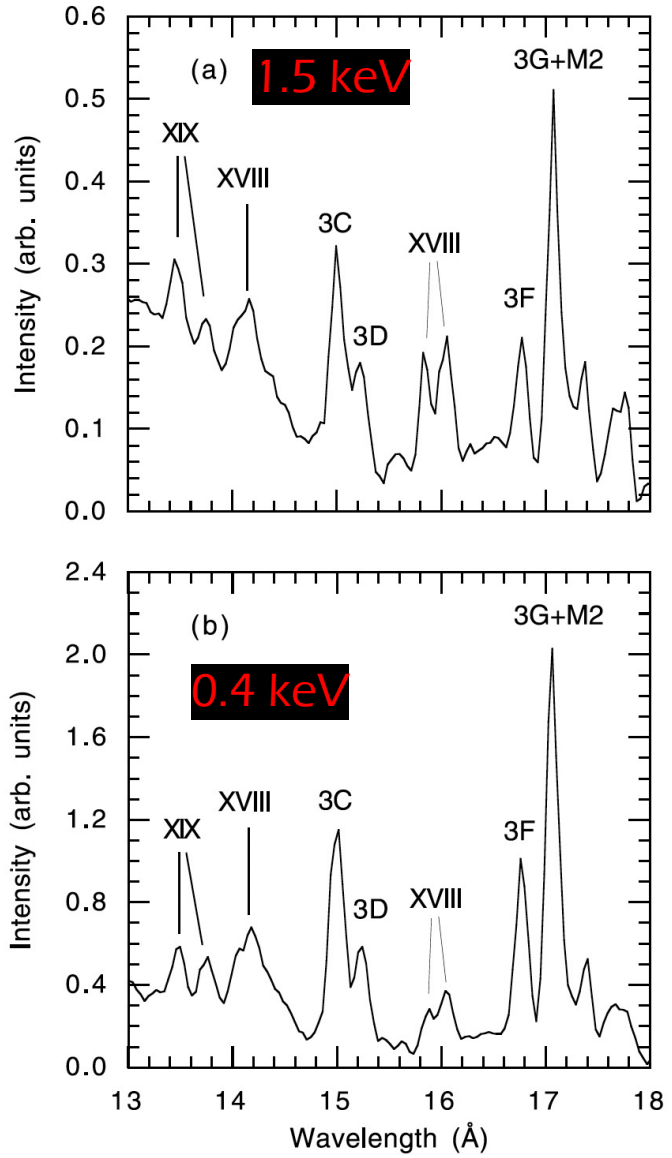


FIG. 3.—L-shell emission spectrum of Fe XVII recorded with the vacuum flat-crystal spectrometer on the PLT tokamak. The central electron temperatures are (*a*) 1500 eV and (*b*) 400 eV. The two spectra were recorded during different times in the same set of plasma discharges: (*a*) 400–520 ms and (*b*) 540–660 ms. The drop in temperature is the result of hydrogen pellet injection at 530 ms. The Fe XVII lines are labeled in standard notation, where $3C$, $3D$, $3F$, and $3G$ denote the electric dipole transitions from upper levels $2p^5_{1/2}3d_{3/2}\ ^1P_1$, $2p^5_{3/2}3d_{5/2}\ ^3D_1$, $2p^5_{1/2}3s_{1/2}\ ^1P_1$, and $2p^5_{3/2}3s_{1/2}\ ^3P_1$, respectively, to the $2p^6\ ^1S_0$ ground level. $M2$ denotes the magnetic quadrupole transition $2p^5_{3/2}3s_{1/2}\ ^3P_2 \rightarrow 2p^6\ ^1S_0$.

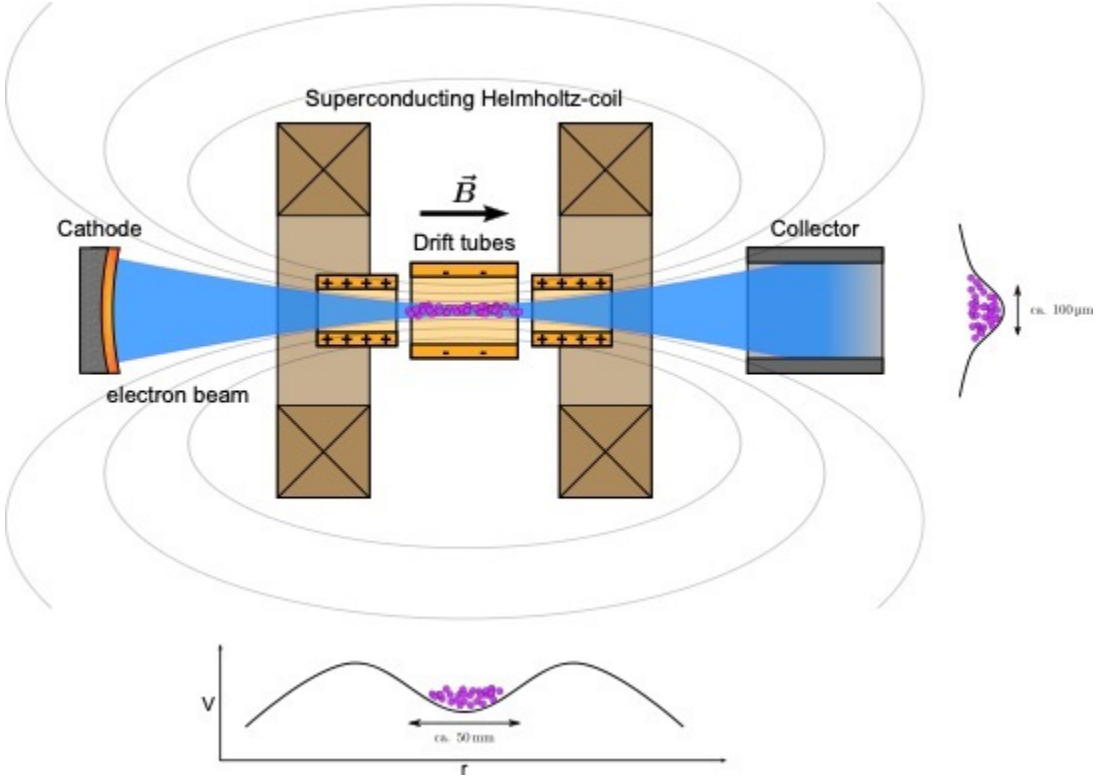
Can’t you just do Tokamak experiments?

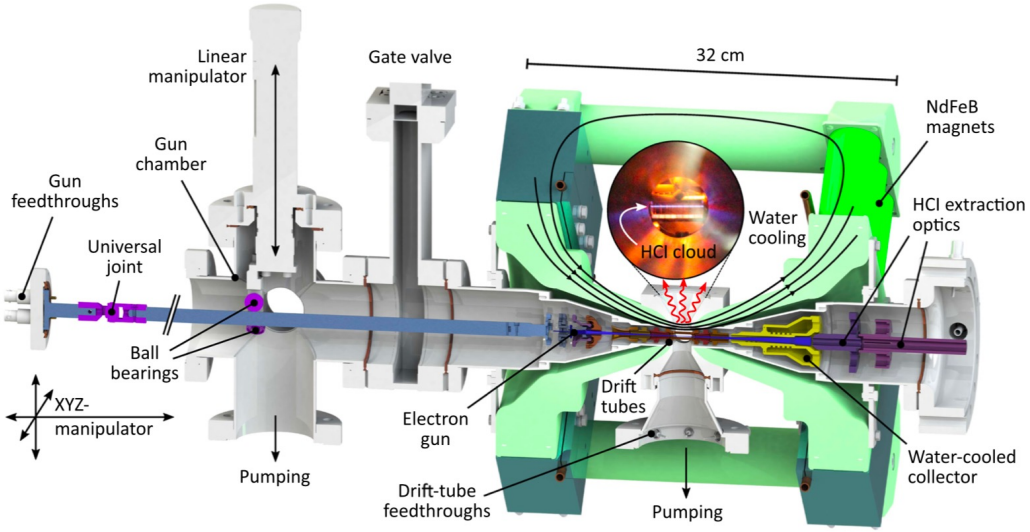
- Sure! It seems obvious that in many ways this is the closest thing to directly “simulating” APEC models (i.e. a CIE plasma, more or less)
- Actually there are a lot of limitations:
  - How uniform? Other non-ideal effects (CX, …)
  - Densities too high compared to (most) astrophysics
- Biggest limitation: if you find a discrepancy between theory and experiment, and you are sure the experiment is “correct”, how do you know which part of theory is going wrong?

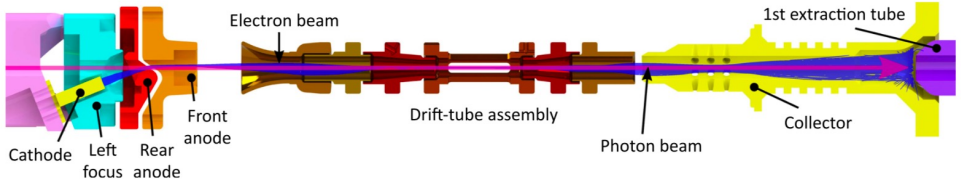
Atomic physics experiments with EBITs

- EBITs (electron beam ion traps) can be used to produce, trap, and study highly charged ions of arbitrary charge state
- The electron beam energy is quasi-monoenergetic, and is chosen to create desired charge states and probe desired physics
- Simplest experiments: attach one or more spectrometers, and study emission of ions in trap caused by electron impact
- Even better: put bright synchrotron x-rays through EBIT axis, exciting and/or ionizing trapped ions, and study fluorescence; also can exctract ions from trap to study photoionization

EBITs: produce, trap, excite, ions

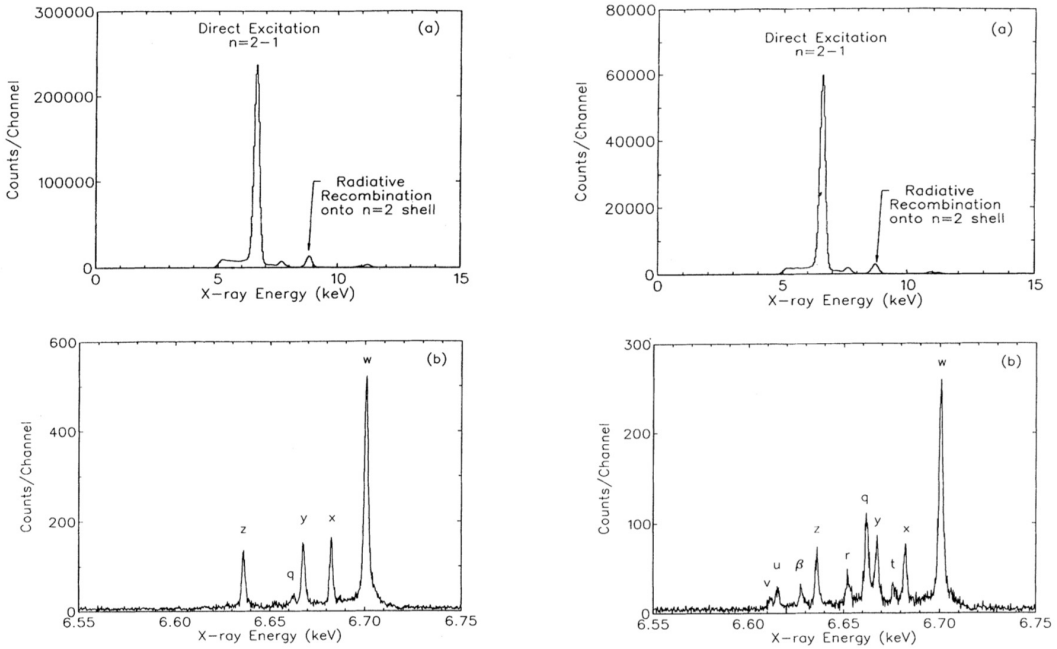






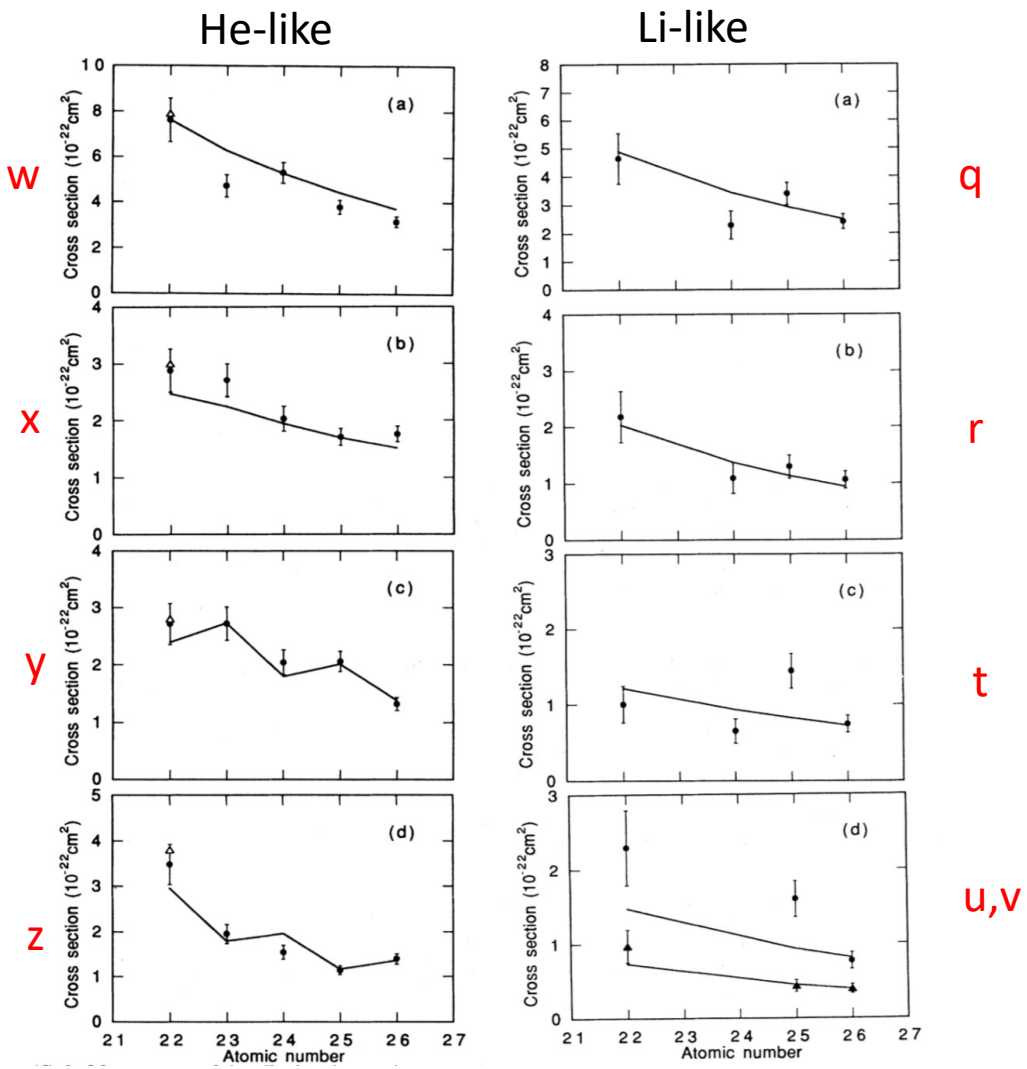
Measurement of absolute electron impact cross sections using LLNL EBIT

Top: Ge detector (low resolution)



Bottom: crystal spectrometer (high resolution)

Wong+ 1995



Theoretical polarization predictions can be benchmarked with crystal spectrometers

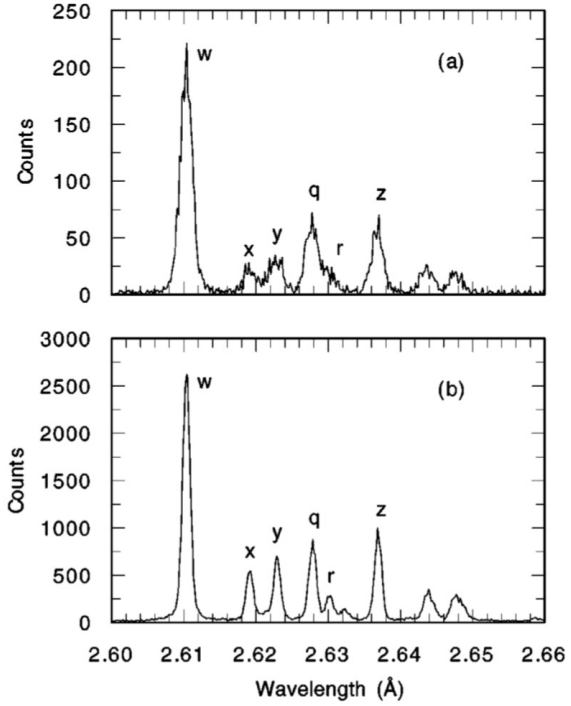
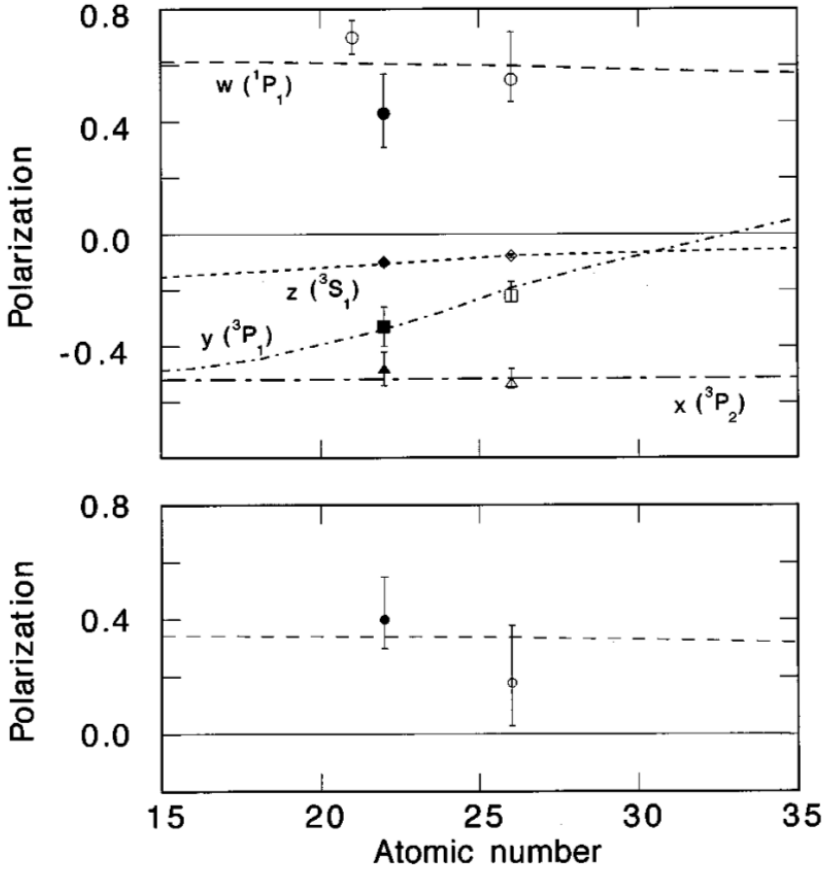
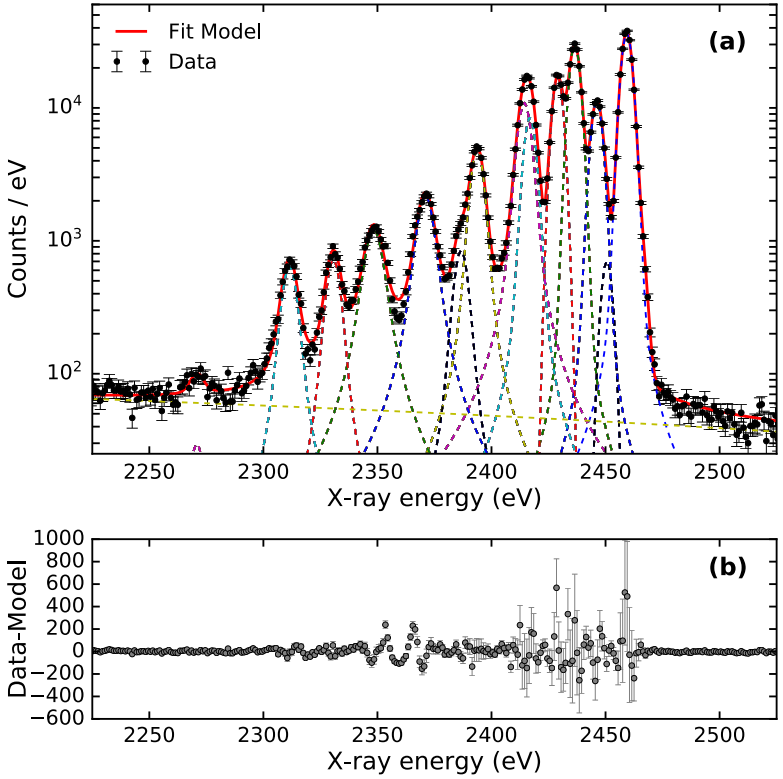


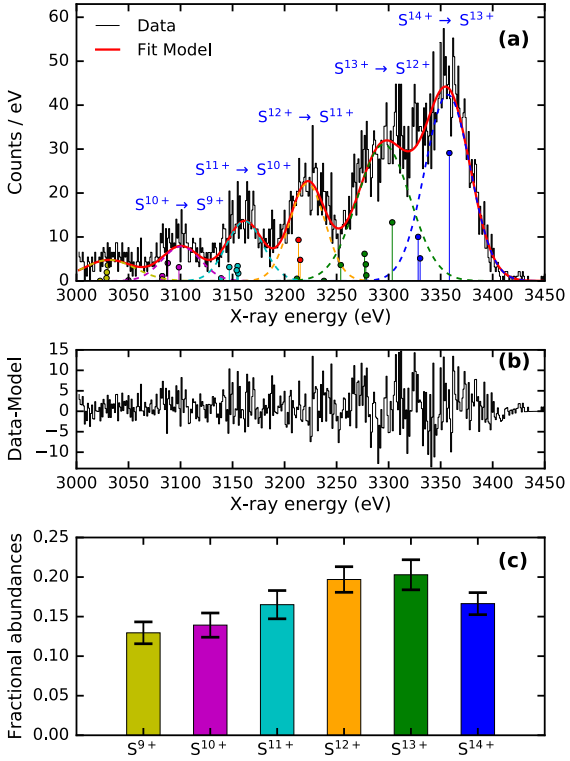
FIG. 1. Crystal-spectrometer spectra of lines w, x, y, and z in heliumlike Ti^{20+} and lines q and r in lithiumlike Ti^{19+} excited by a 4800-eV electron beam. (a) Spectrum obtained with a Si(220) crystal at a Bragg angle of 43.1°; (b) spectrum obtained with a Si(111) crystal at a Bragg angle of 24.7°. Unlabled features are inner-shell satellites from lower charge states.

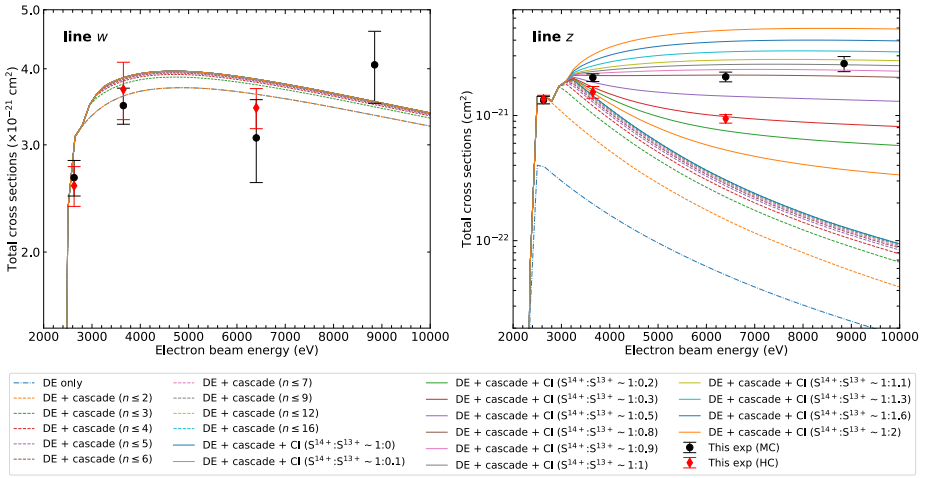


Beiersdorfer+ 1999

Improved measurement of cross sections using an x-ray calorimeter

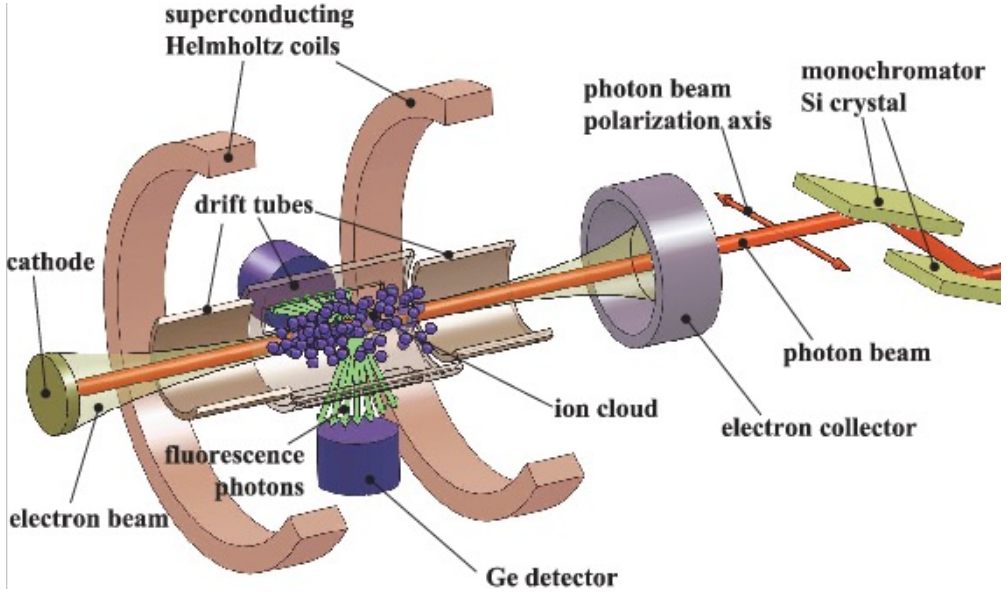


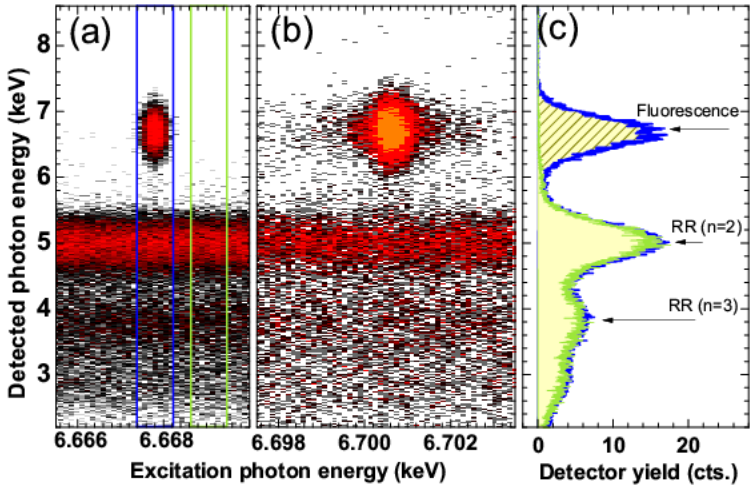


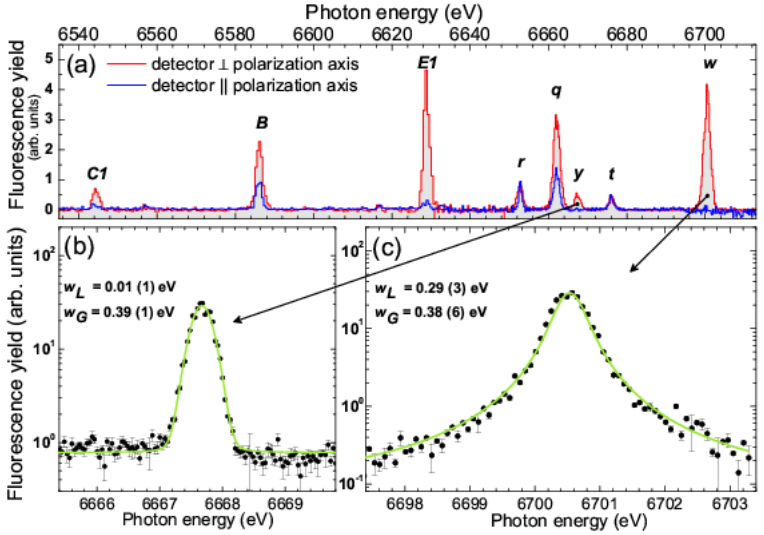


Shah+ 2021

Measurement of Fe XXV linewidth at Petra III (DESY/Hamburg)







Agrees with theory to within error bars (few %)!

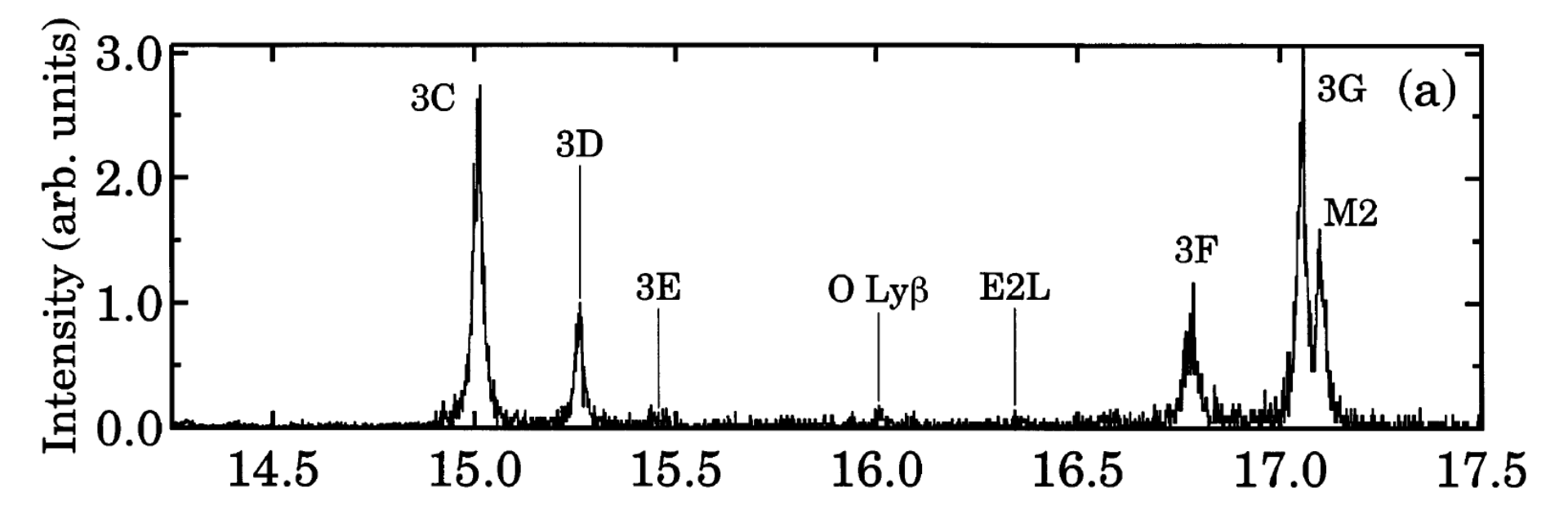
Rudolph+ 2013

What about Fe XVII?

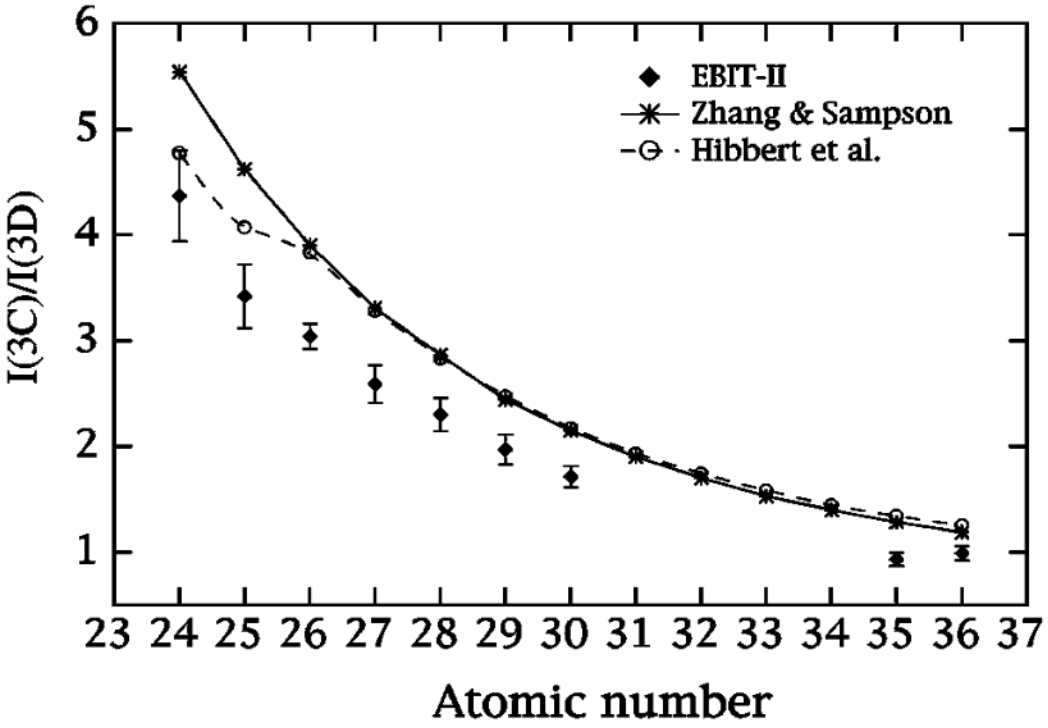
- Long history of measurements in MCF plasmas, sun, astrophysics and EBITs
- Plenty of disagreement, but perhaps some of this is expected, e.g. due to real astrophysical effects like optical depth?
- But there were disagreements between different EBIT experiments, and also between different theoretical approaches

Livermore EBIT measurements

Brown+1998 : 3C/3D ~ 3.0



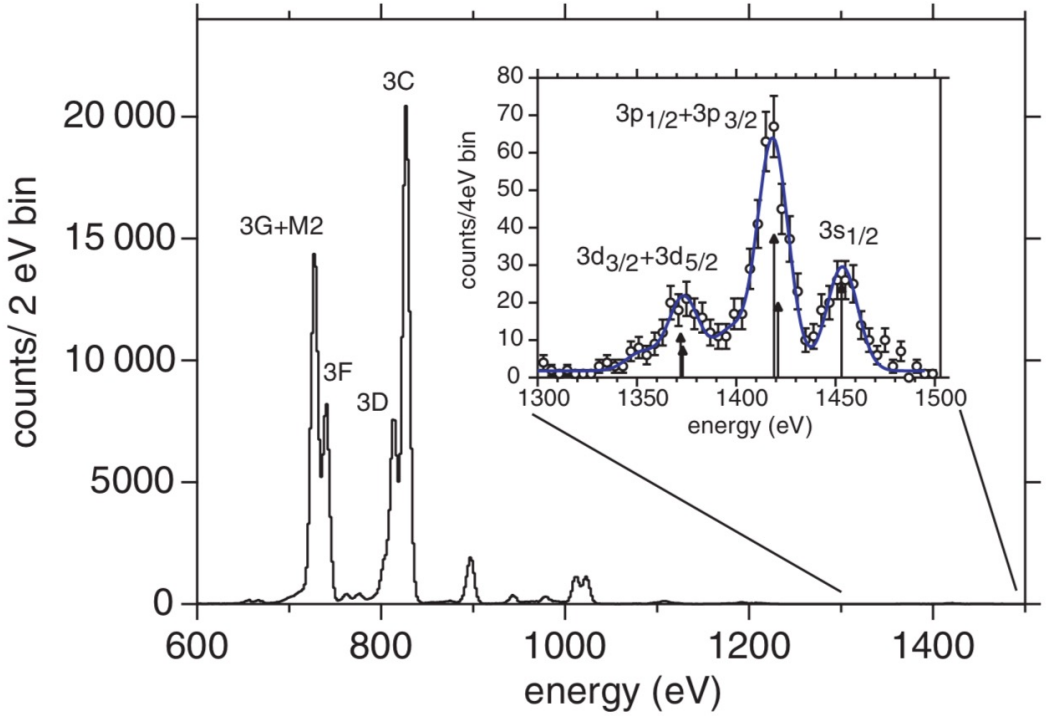
Ne-like ion 3C/3D ratios



- Brown+2001 measured 3C/3D as a function of Z
- Systematic offset between theory and experiment

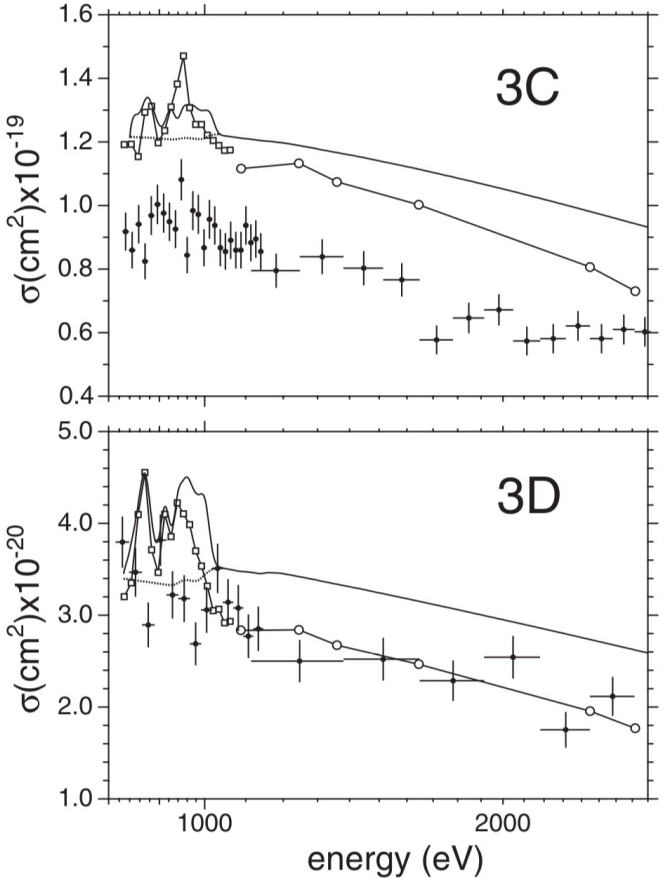
Fe XVII absolute cross sections

- Measure strong lines of Fe XVII simultaneously with weak radiative recombination features
- RR lines are thought to have better understood cross sections so can be used to normalize to absolute scale



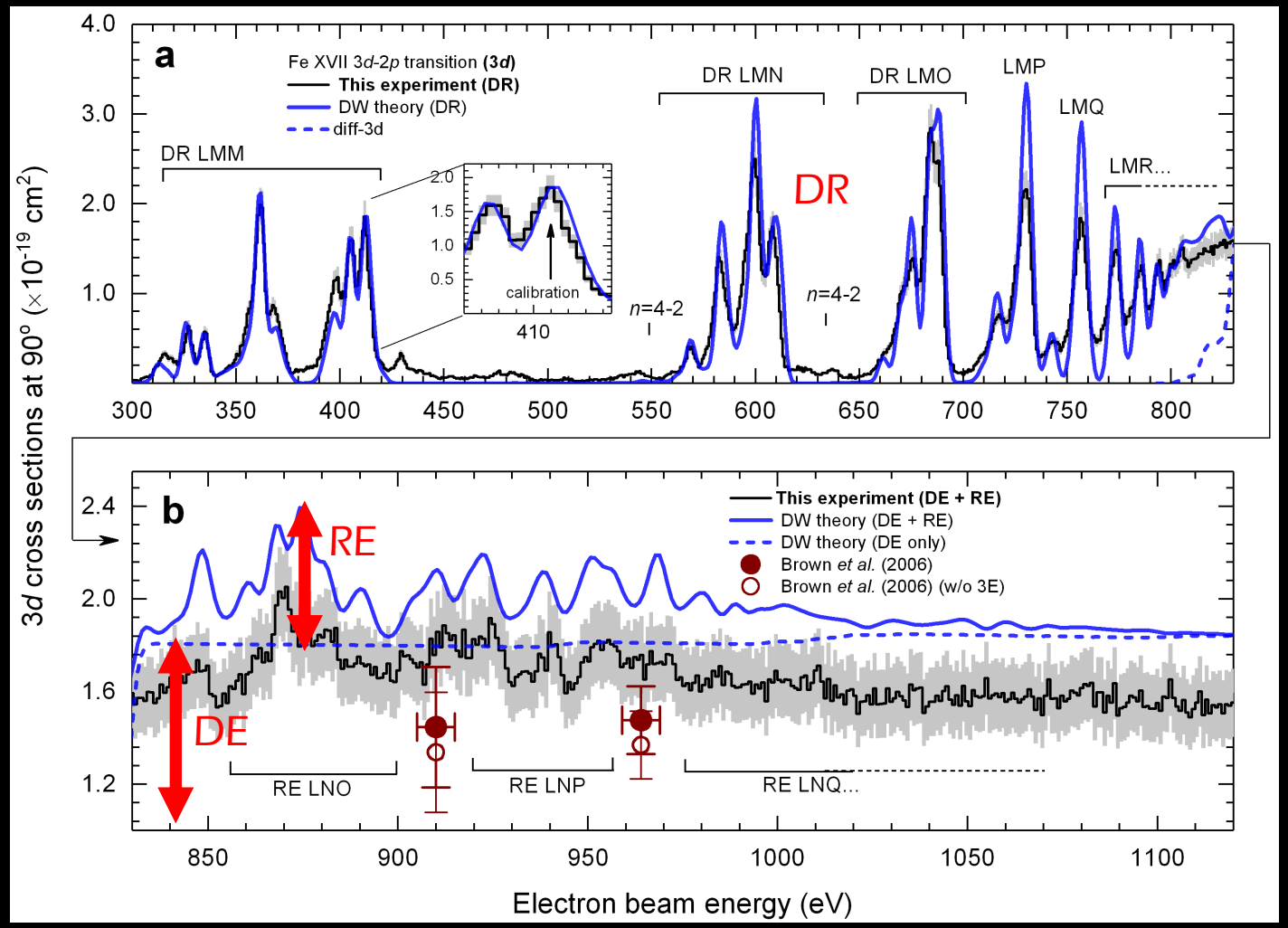
Fe XVII absolute cross sections

- Results: resonance line 3C is overpredicted by theory; intercombination line 3D is better matched
- The problem seems to be in the continuum!
- This implies fundamental issues with atomic structure - previous theoretical efforts focused on other effects



Dielectronic Recombination and Resonance Exc.

3d (3C + 3D + 3E)

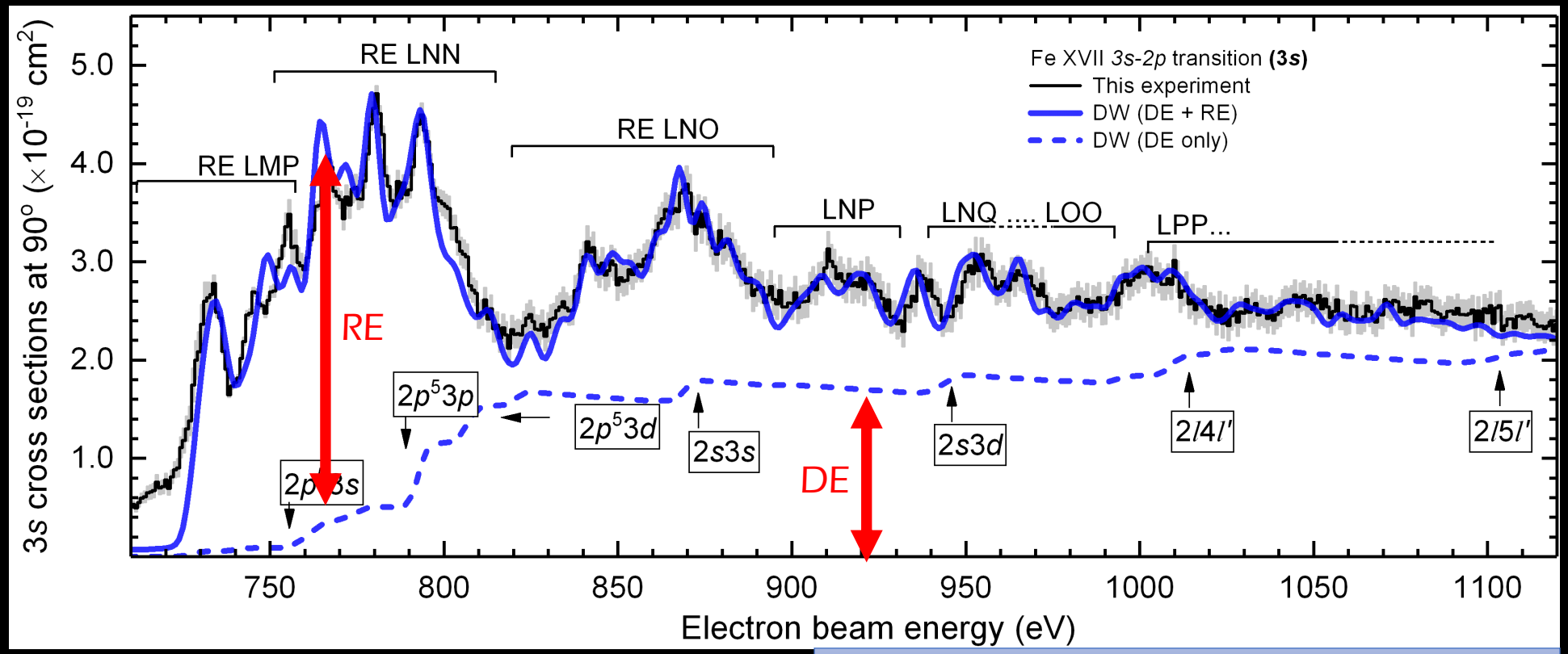


3d DW theory overpredicts
- high-n DR,
- RE,
- CE cross sections by approx. ~20%

Resonance Excitation and Cascades

3s (3G + 3F + M2) DW theory looks fine ...

The 3s emission is fully dominated by Resonance Excitation and Cascades

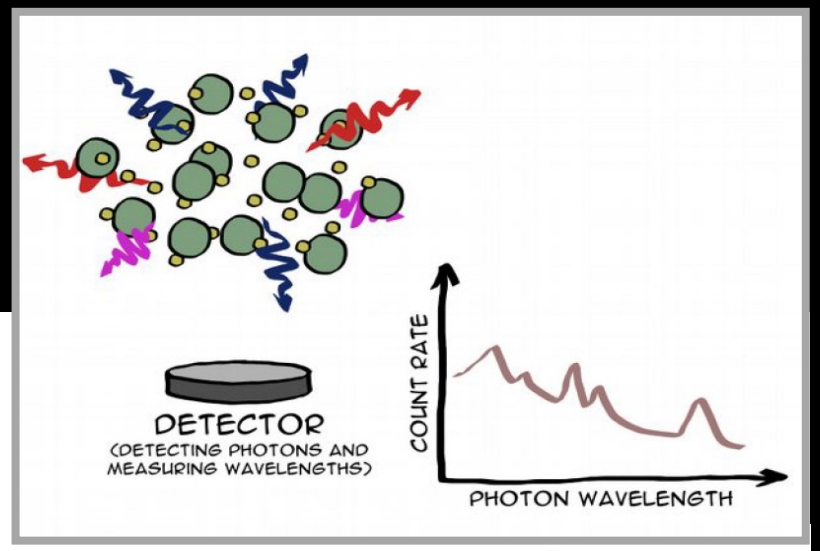


C. Shah et al., ApJ (2019); Gu+Shah et al., A&A (2020)

Classical Spectroscopy using EBITs

Electron beam drives ionization, excitation, and recombination,

same as coronal plasmas
$n_{electron} \sim 10^{9\text{-}13}$ /cm^3
$n_{ion} \sim 10^{6\text{-}8}$ /cm^3



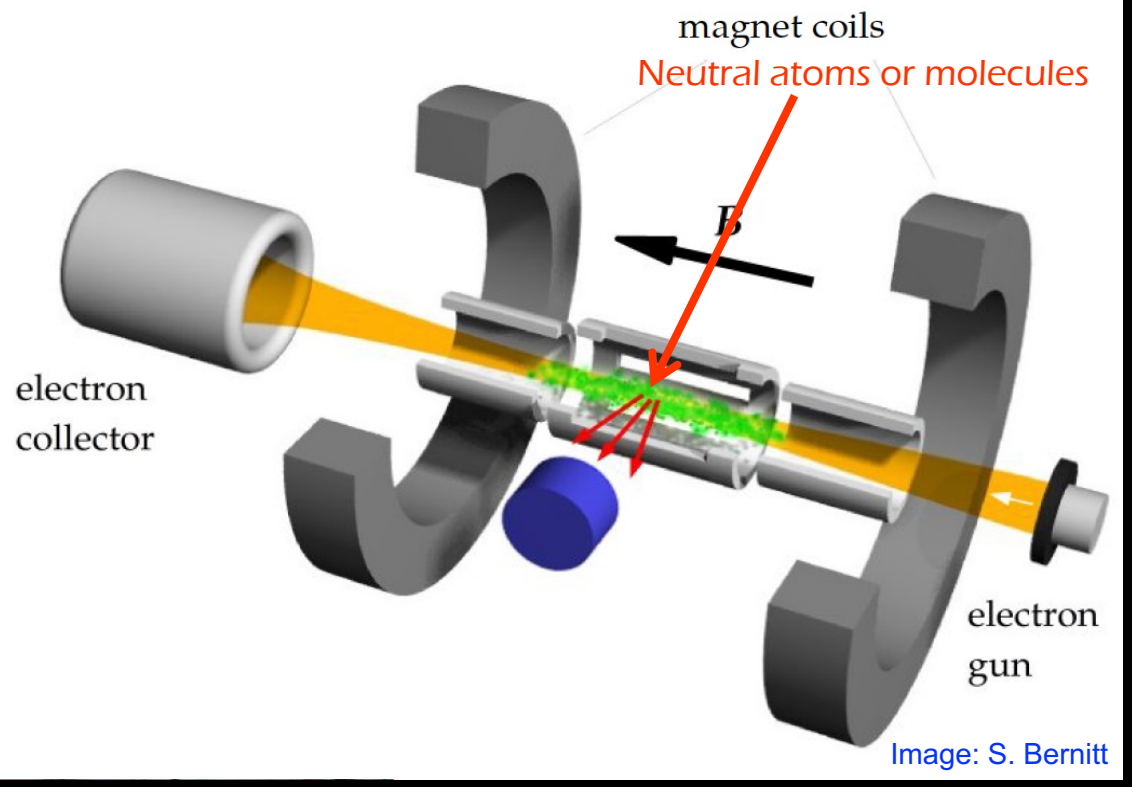
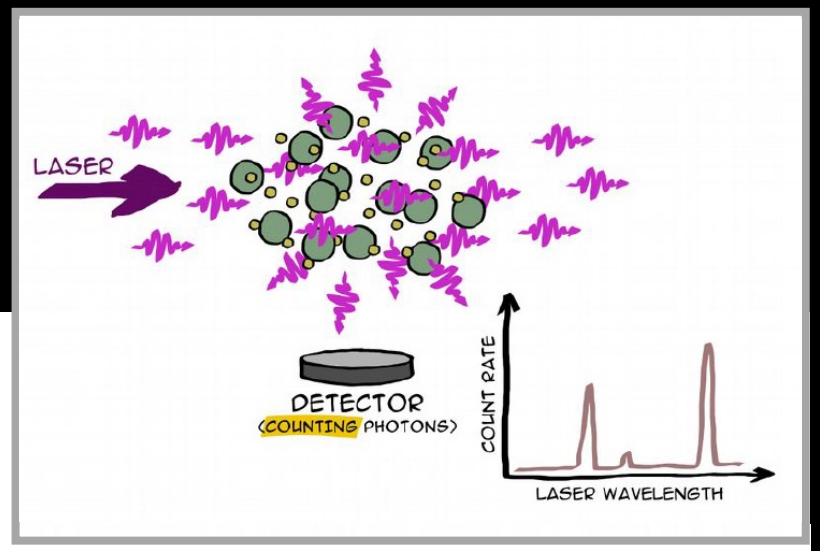


Image: S. Bernitt

Laser Spectroscopy using EBITs

EBIT: production and trapping of ions
X-ray laser: photo-excited trapped ions



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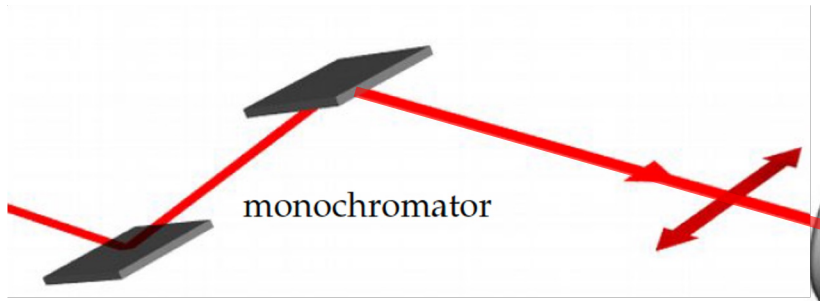


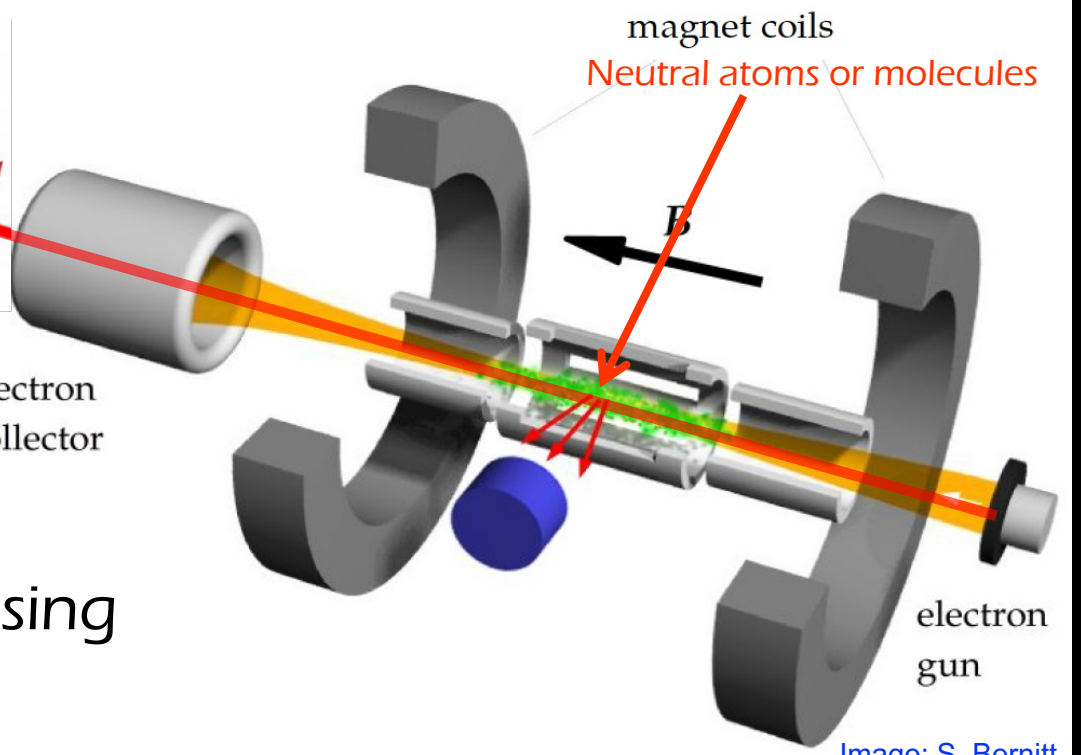


Image: S. Bernitt

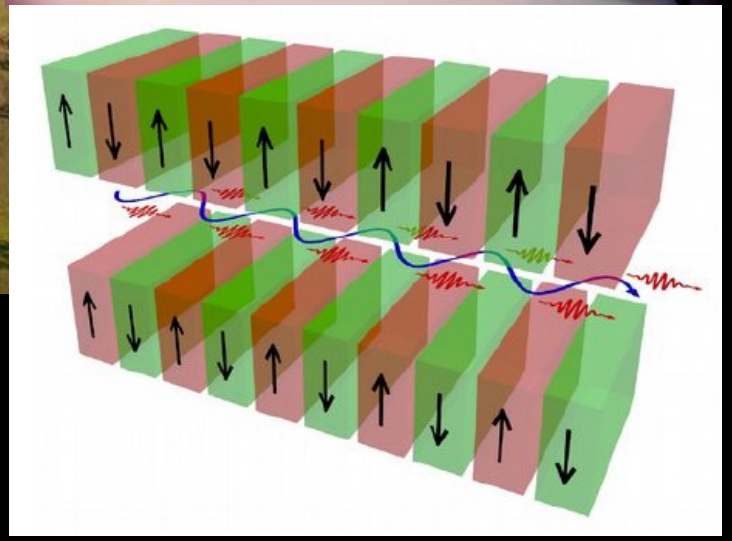
Key advantage :

purely photonic excitation suppresses uncertainties arising from collisional excitation

LCLS Stanford campaign (2012)

(World's first and most powerful FEL Free Electron Laser)

LCLS undulator hall



EBIT at SXR

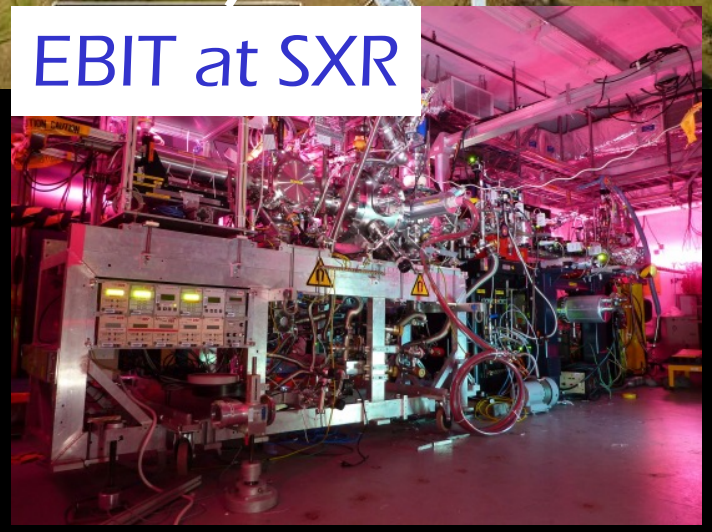


Image: J. Crespo

FLASH-EBIT at soft X-ray beamline (LCLS)

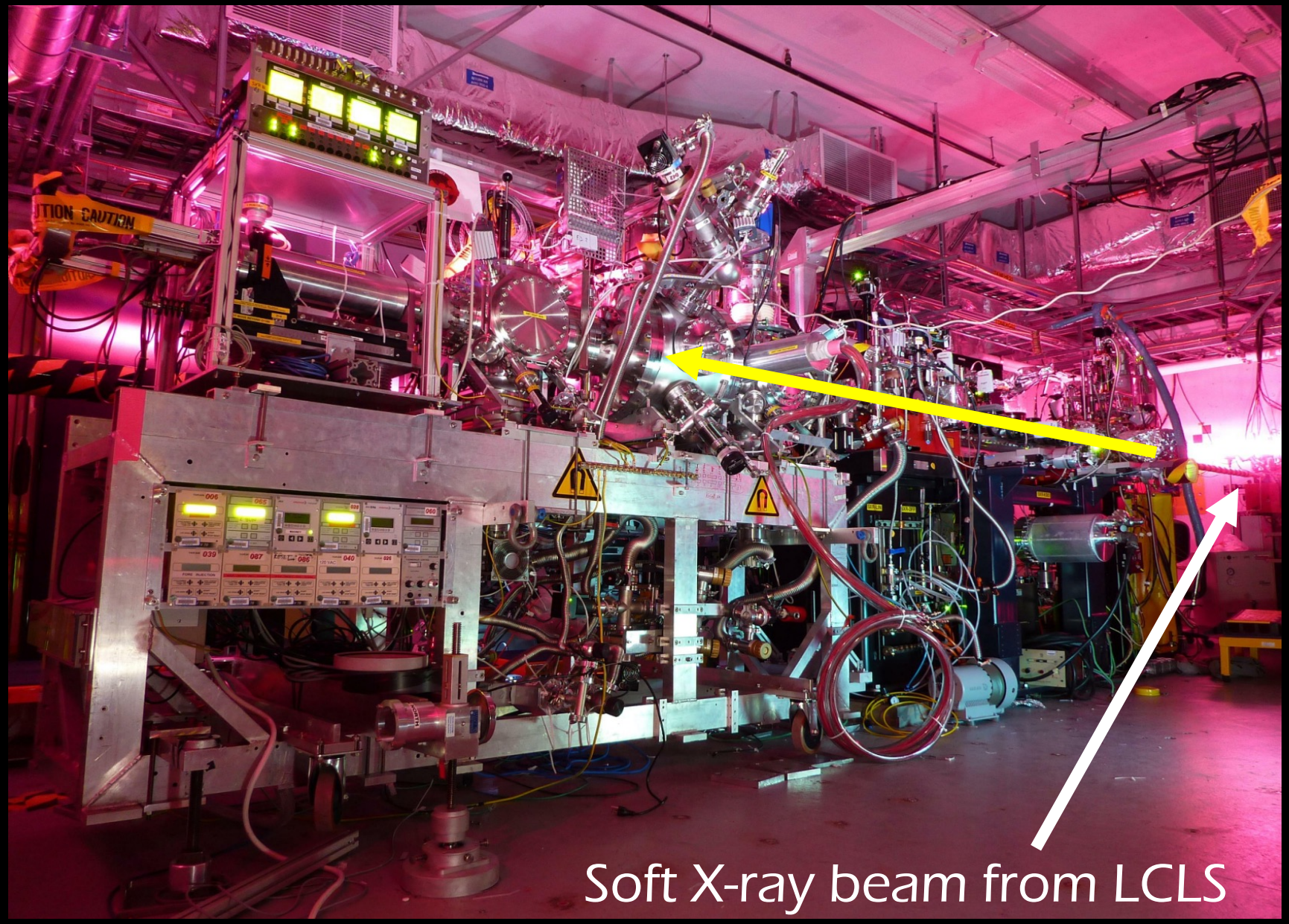
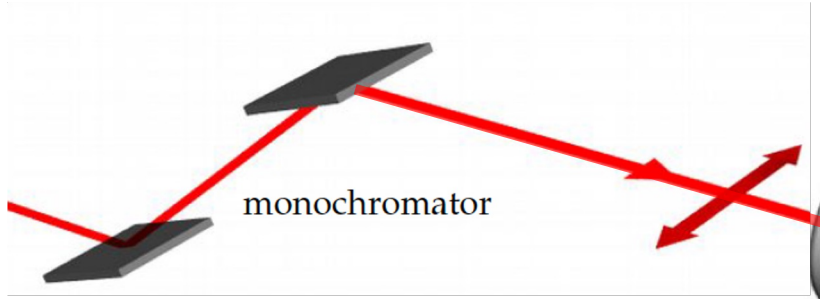
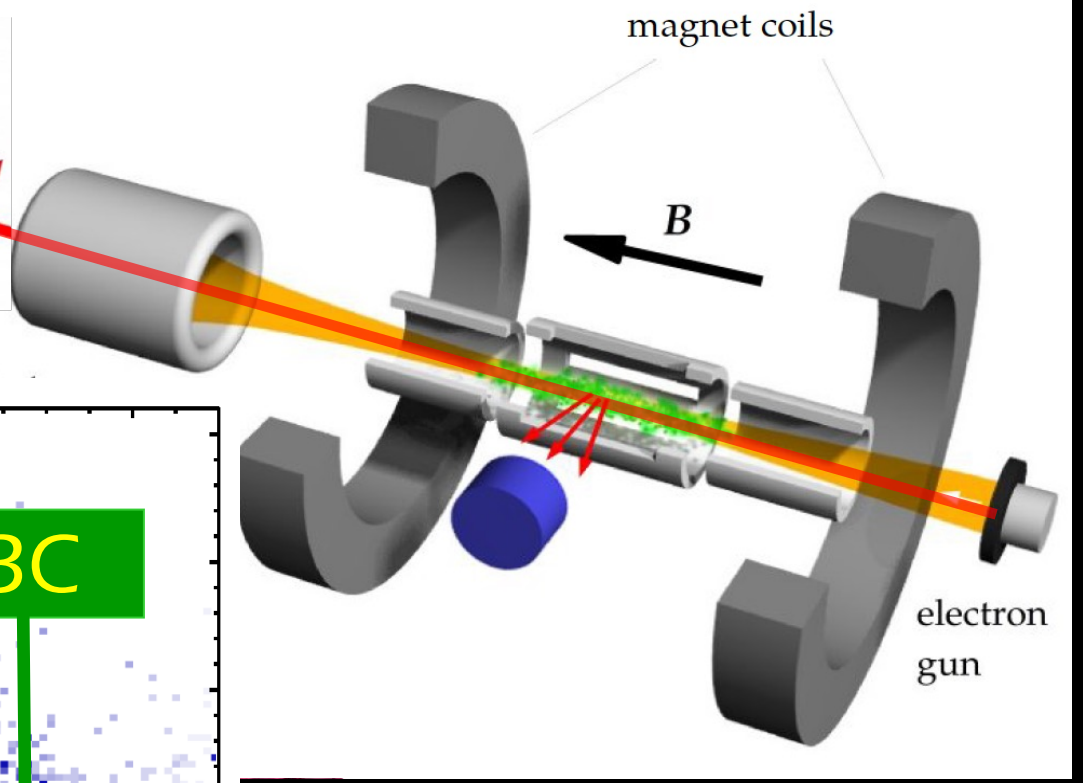


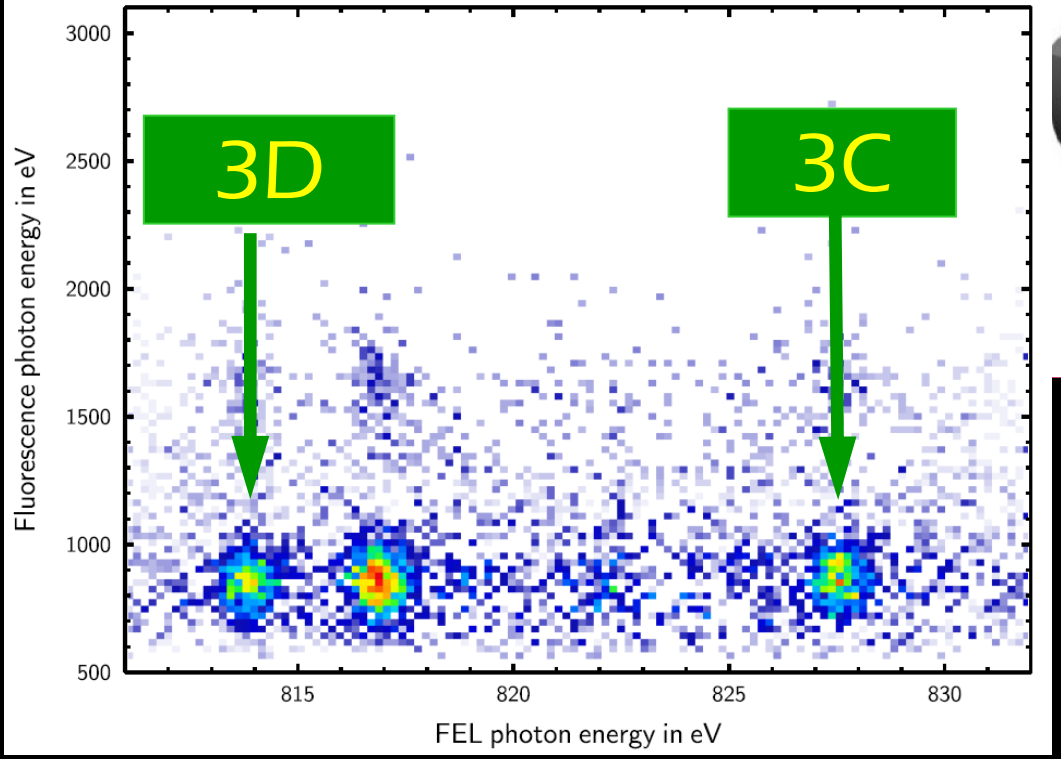
Image: J. Crespo

Measurement Technique

EBIT: production and trapping of highly charged ions
X-ray laser: photo-excited trapped highly charged ions







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

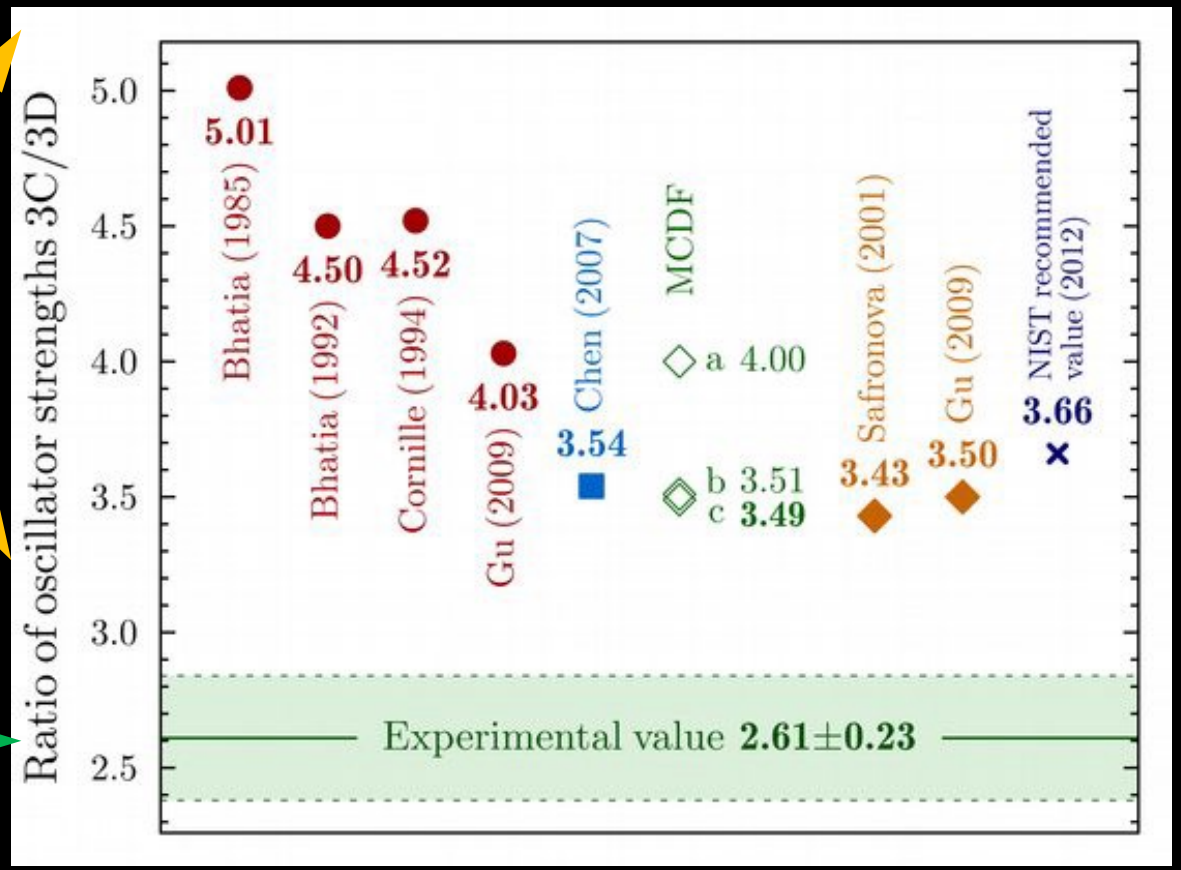
Experiment solves (serious) old problem

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

Theoretical oscillator strength ratios 3C/3D

Experimental oscillator strength ratio 3C/3D

3σ away from best theory



Conclusion:

Inaccurately predicted oscillator strengths for 3C and 3D are the root cause of the long-standing discrepancy between models/theory and astro. observation/experiments

Experiment solves (serious) old problem (May be?)

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Astrophysical Line Diagnosis Requires Nonlinear Dynamical Atomic Modeling

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NON-EQUILIBRIUM MODELING OF THE FE XVII 3C/3D LINE RATIO IN AN INTENSE X-RAY FREE-ELECTRON LASER EXCITED PLASMA

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Non-equilibrium modeling of the Fe XVII 3C/3D ratio for an intense X-ray free electron laser[1]

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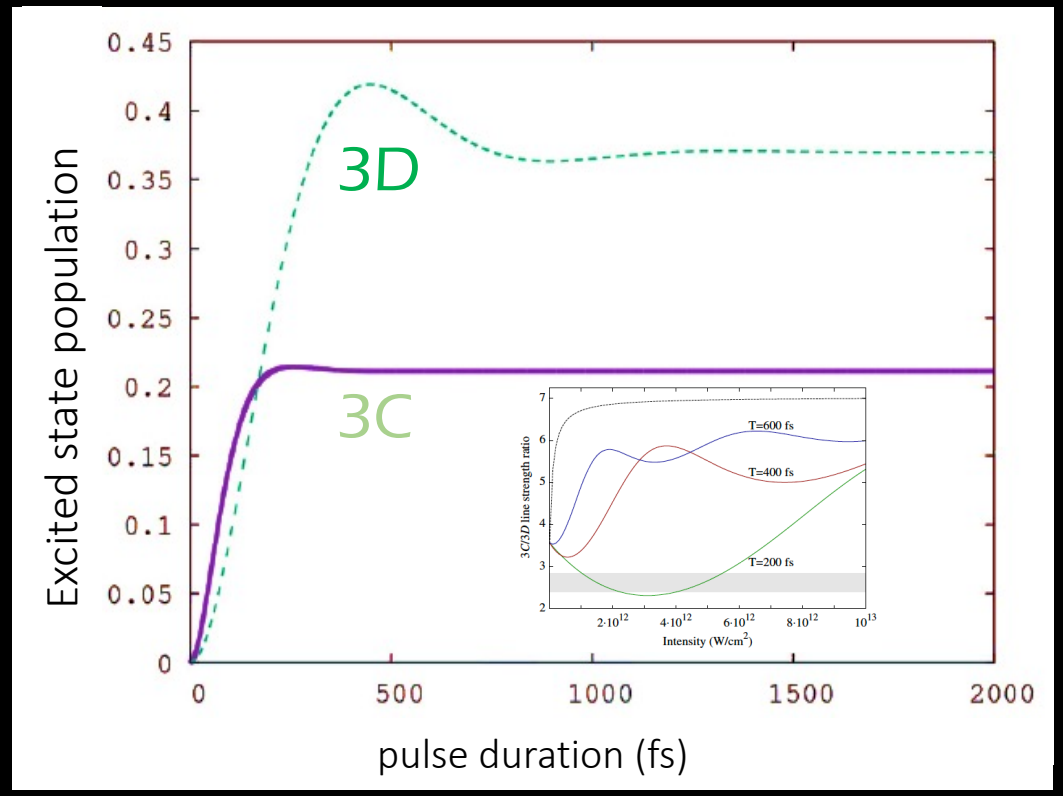


Problem 1: Non-linear Dynamics?

Femtosecond X-ray laser with intensities above ~10^{12} W/cm^2,

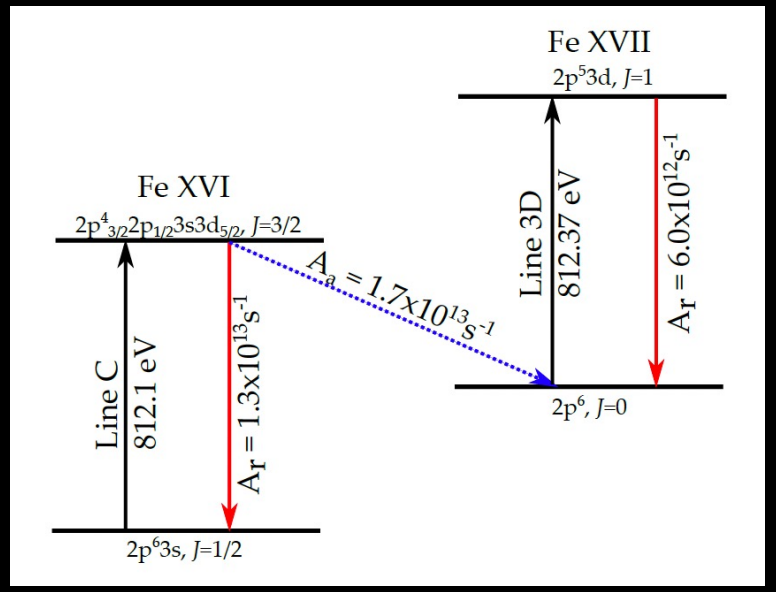
then upper state population of (3C and 3D) states cannot reach equilibrium...

Exact values of LCLS laser pulse width, duration, and intensities are hard to estimate...

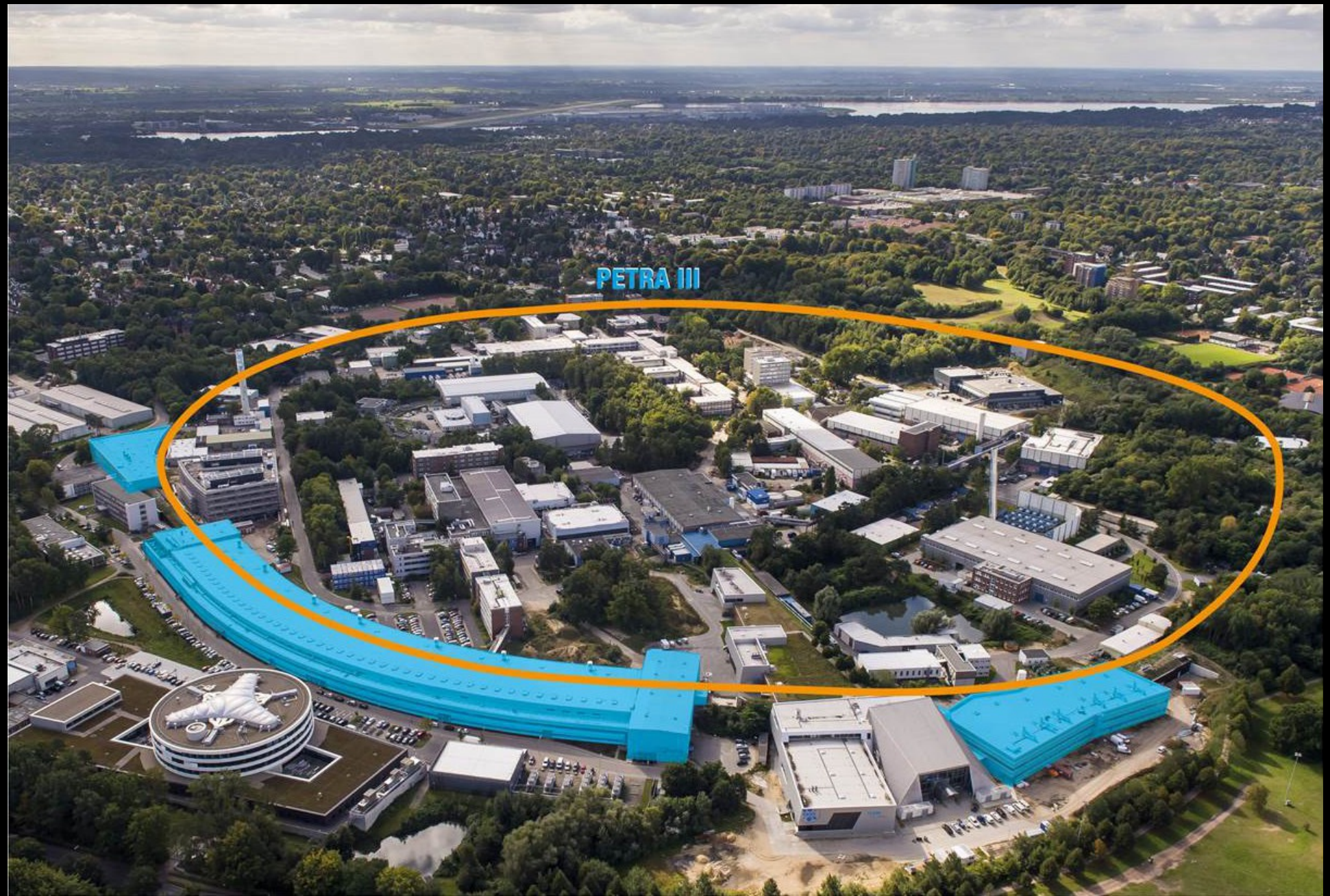
Problem 2:

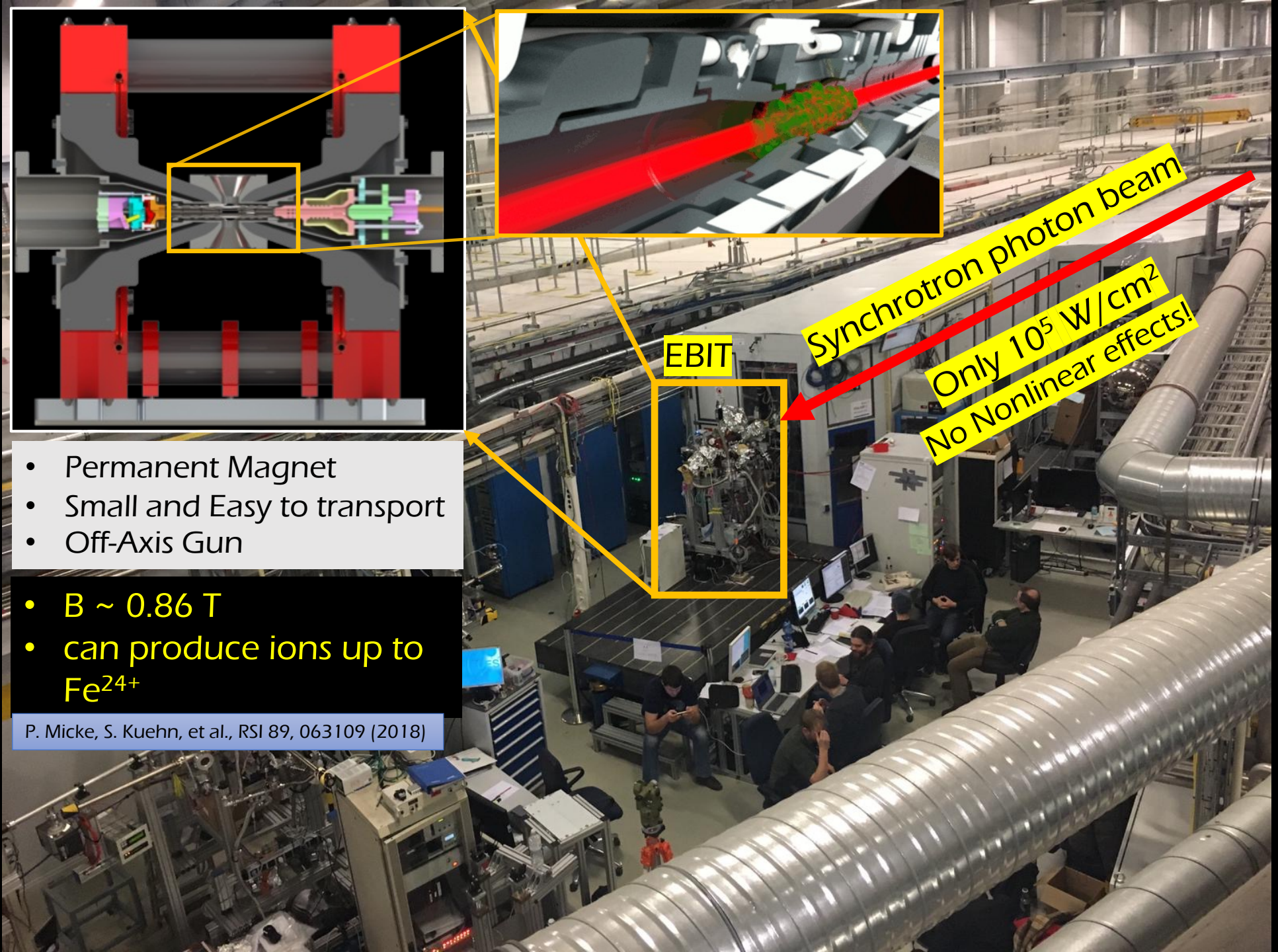
Population transfer?

between Fe15+ and Fe16+ due to strong autoionization channel of Fe15+ C-line, blended with 3D, feeding ground state of Fe16+



PETRA III Synchrotron at DESY, Hamburg



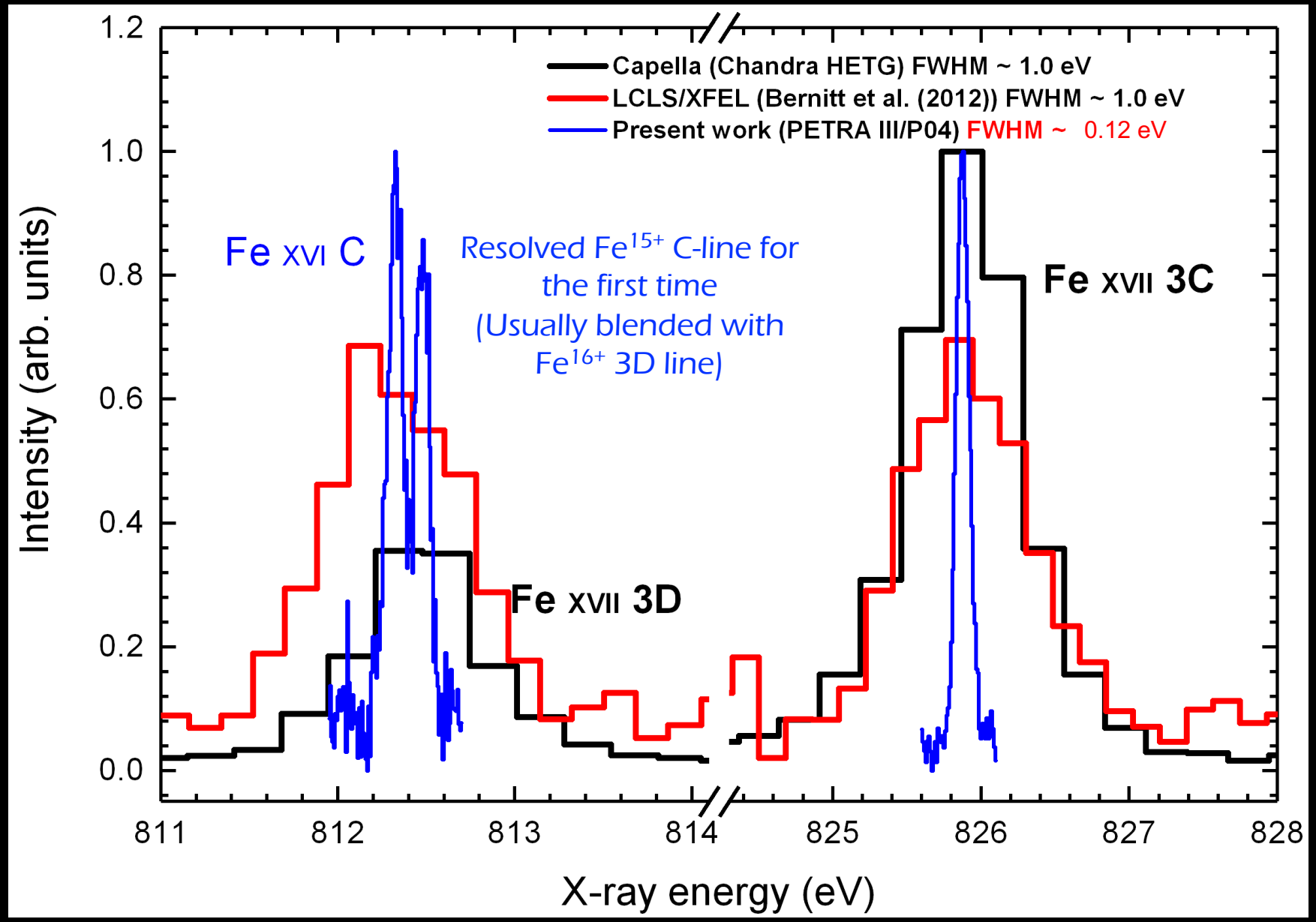


- Permanent Magnet
- Small and Easy to transport
- Off-Axis Gun

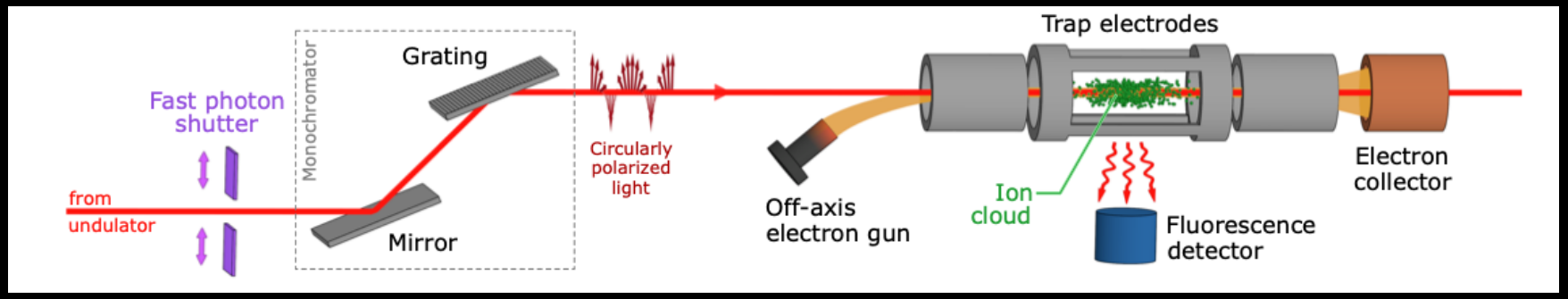
- B ~ 0.86 T
- can produce ions up to Fe^{24+}

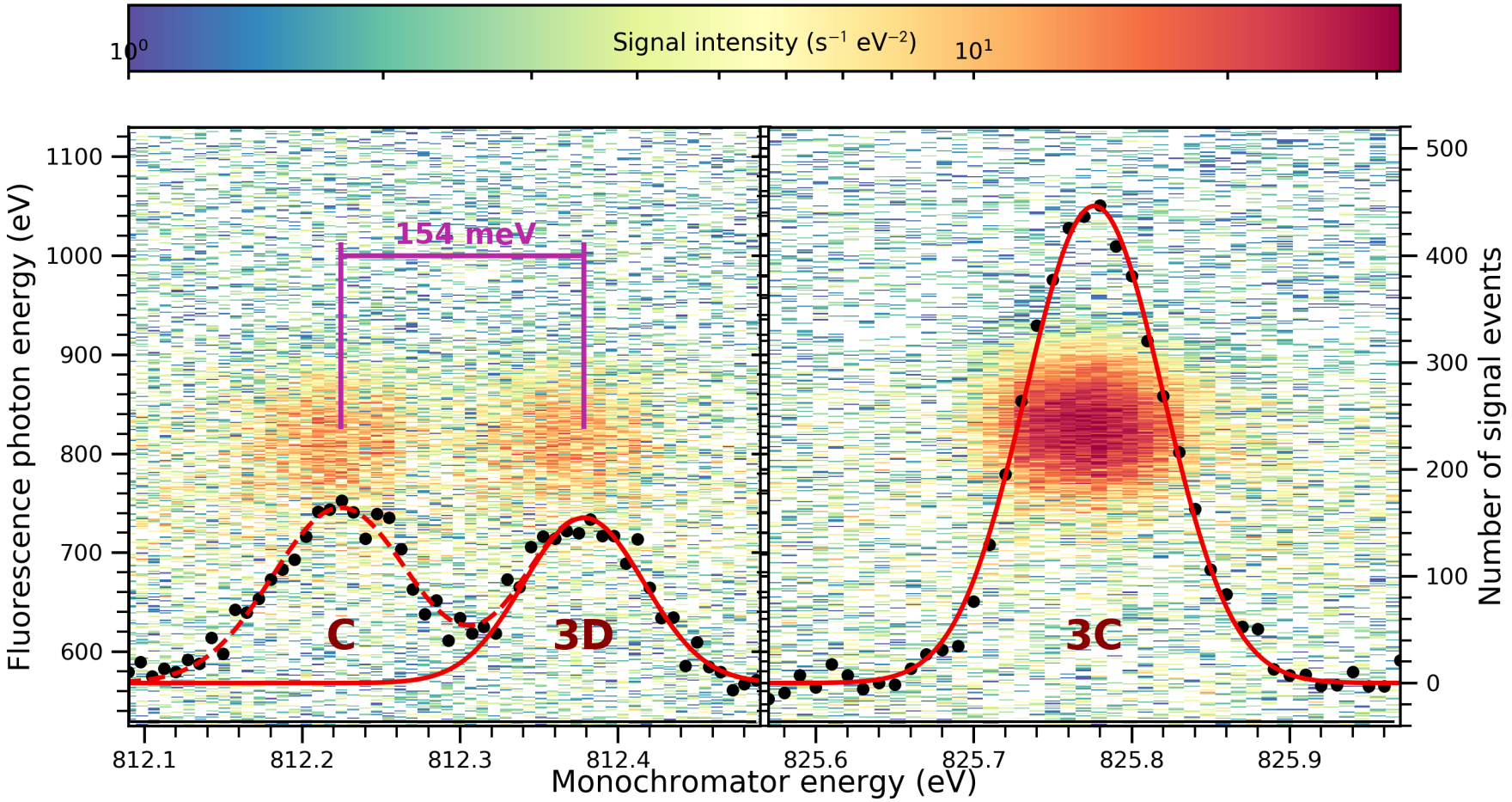
P. Micke, S. Kuehn, et al., RSI 89, 063109 (2018)

Improvement in Resolution: 8x better than Chandra

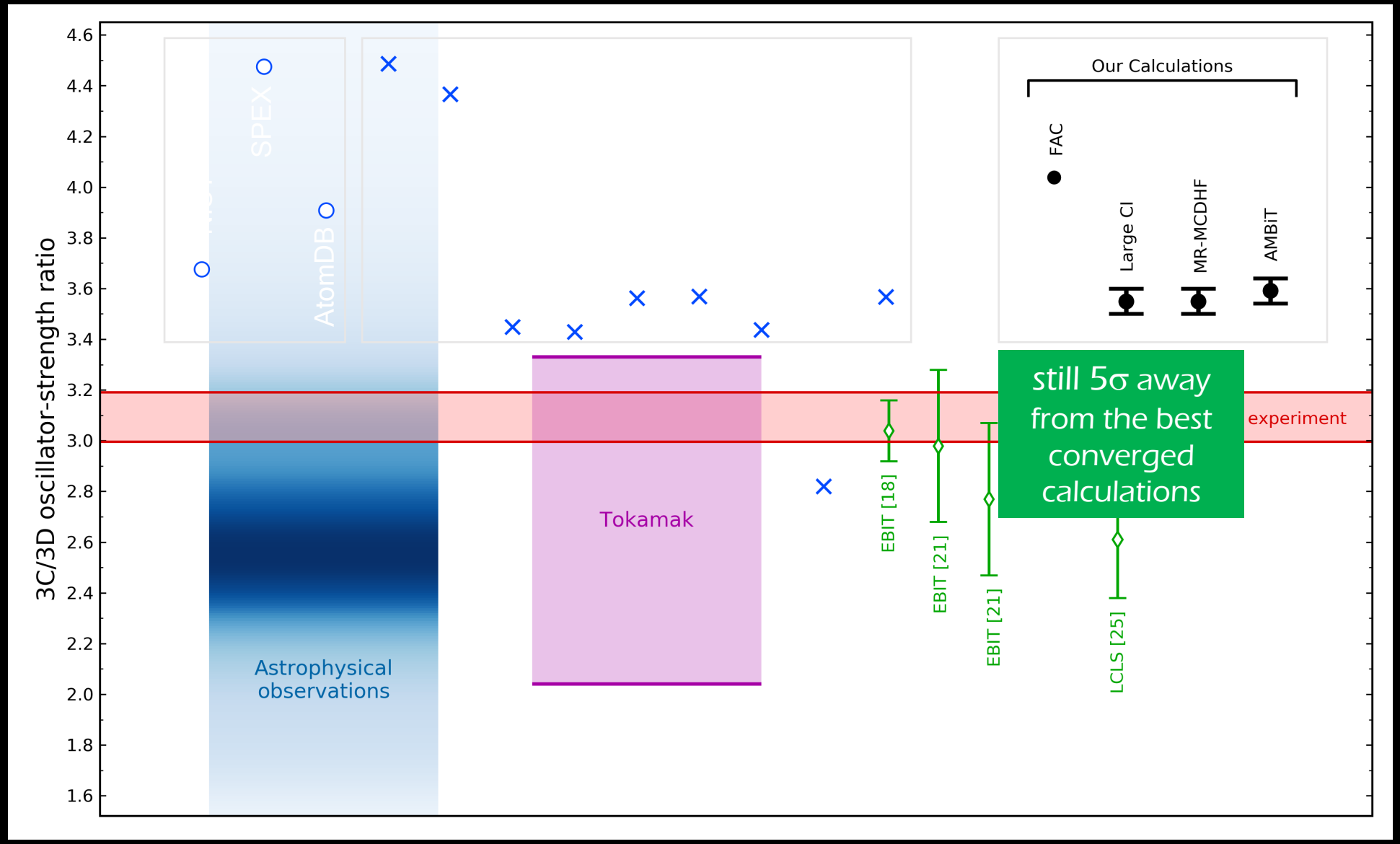


Measurement technique





Final result vs. Exp. vs. Obs. vs. Models and Theories

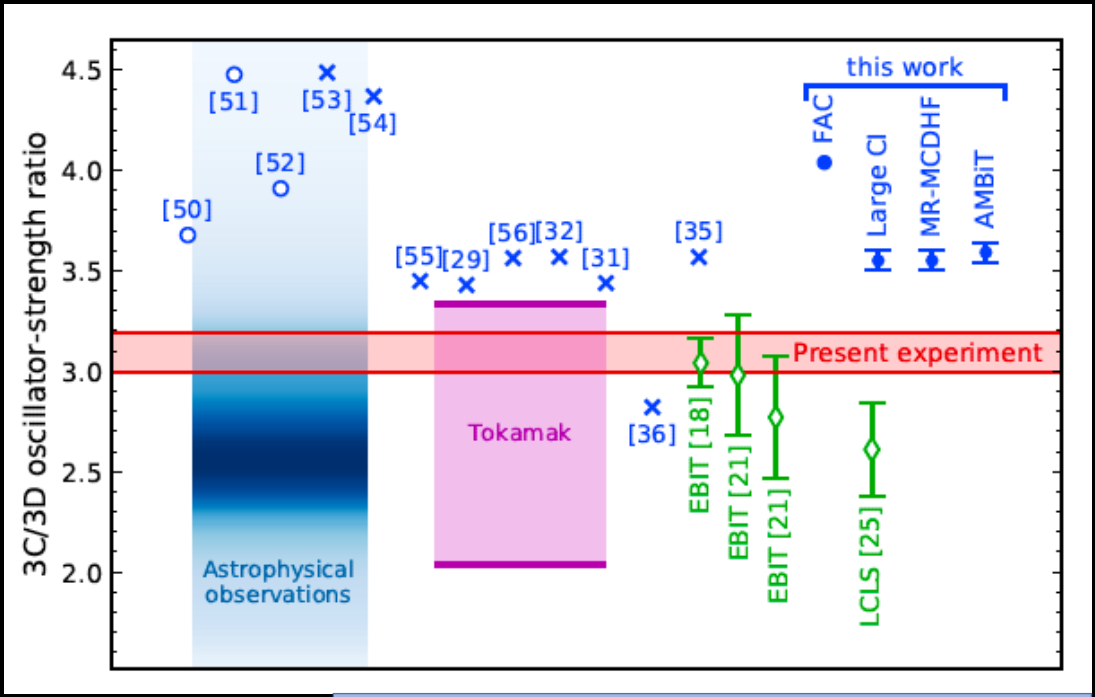


$f(3C) / f(3D) = 3.09(8)(6)$

Results on the Fe XVII problem (2018 campaign)

5 sigma discrepancy 3 % uncertainty

- ✓ Low oscillator strengths are still a root cause of this problem (as our previous experiment found).



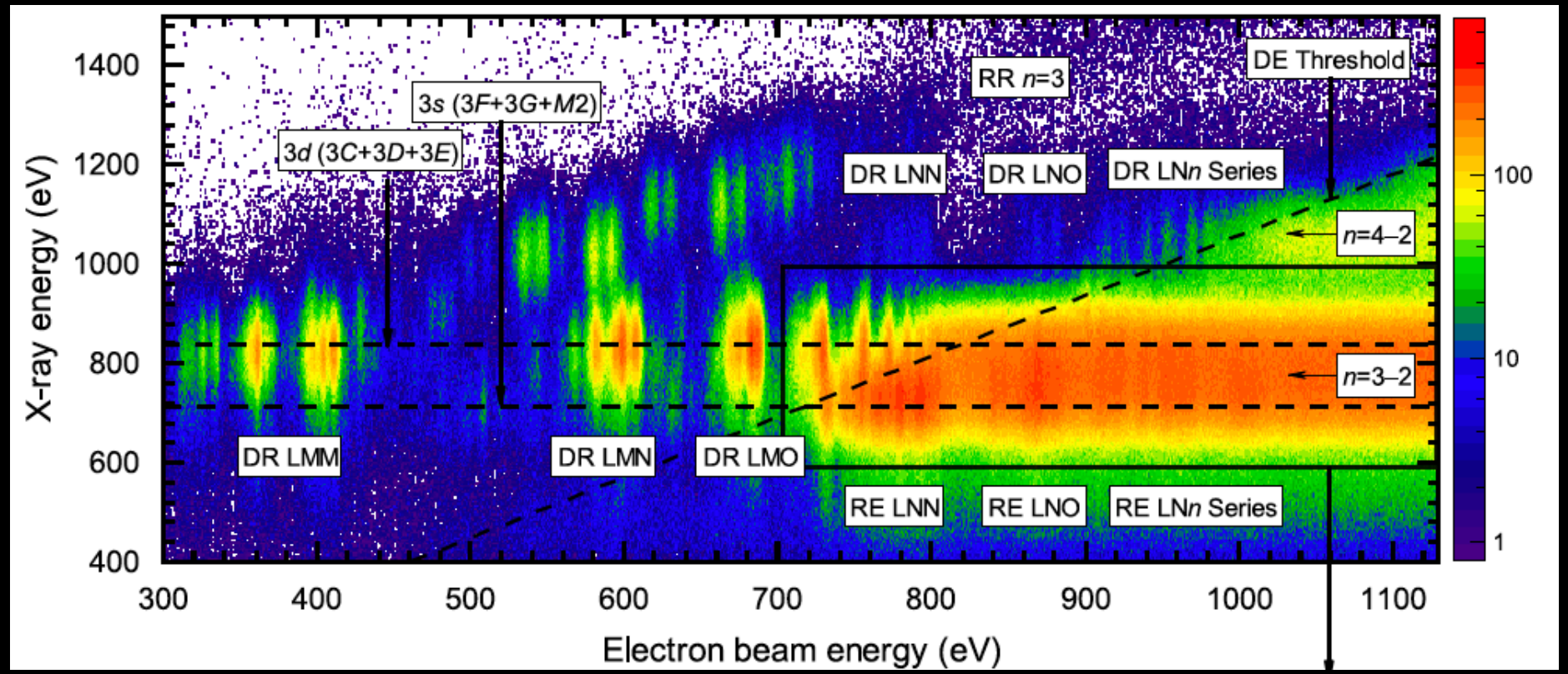
Kühn+Shah et al., Phys. Rev. Lett., **124**, 225001 (2020)

What's next for the Fe XVII problem?

- Improvements in signal to noise ratio

- The present beamtime had very bad signal to noise ratio of 0.05.

- 3C and 3D lines were photoexcited (signal) over electron-impact excitation (background) at 1.6 keV of beam energy.



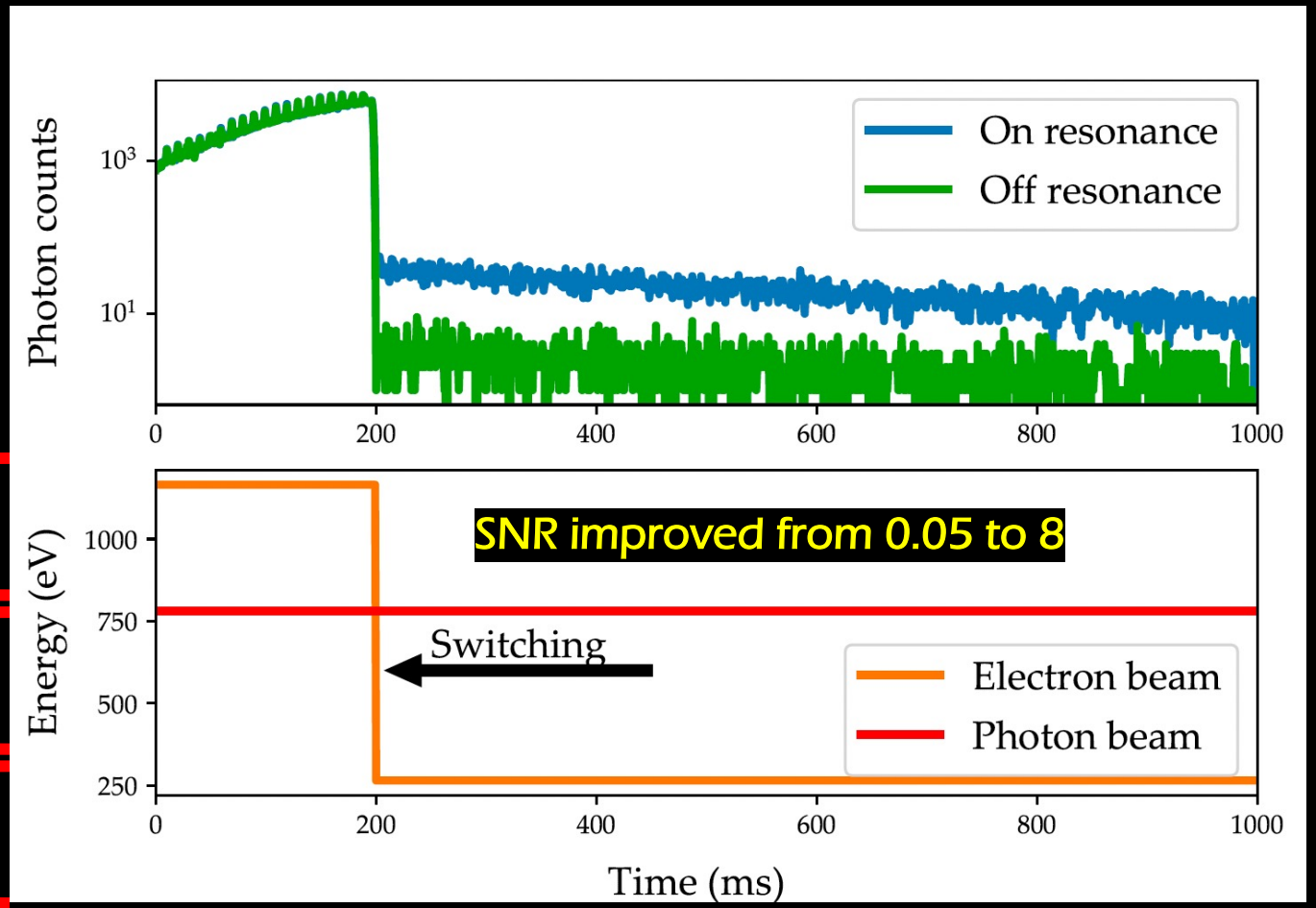
Improving signal to noise ratio (2019 campaign)

- Implemented fast switching power supplies - enable us to measure 3C and 3D photoexcited resonances below the beam energy (Eb), where electronically-excited background is zero.

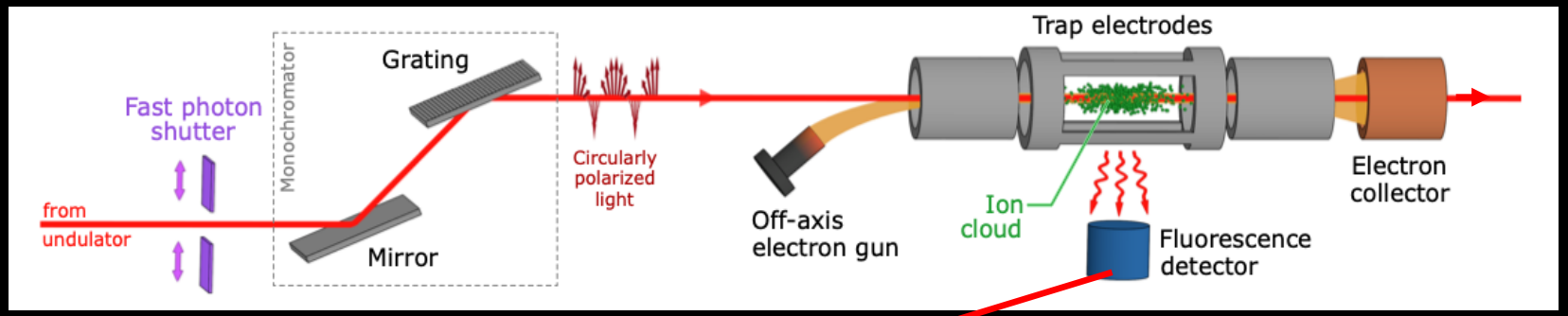
Bkg. from DE +RE

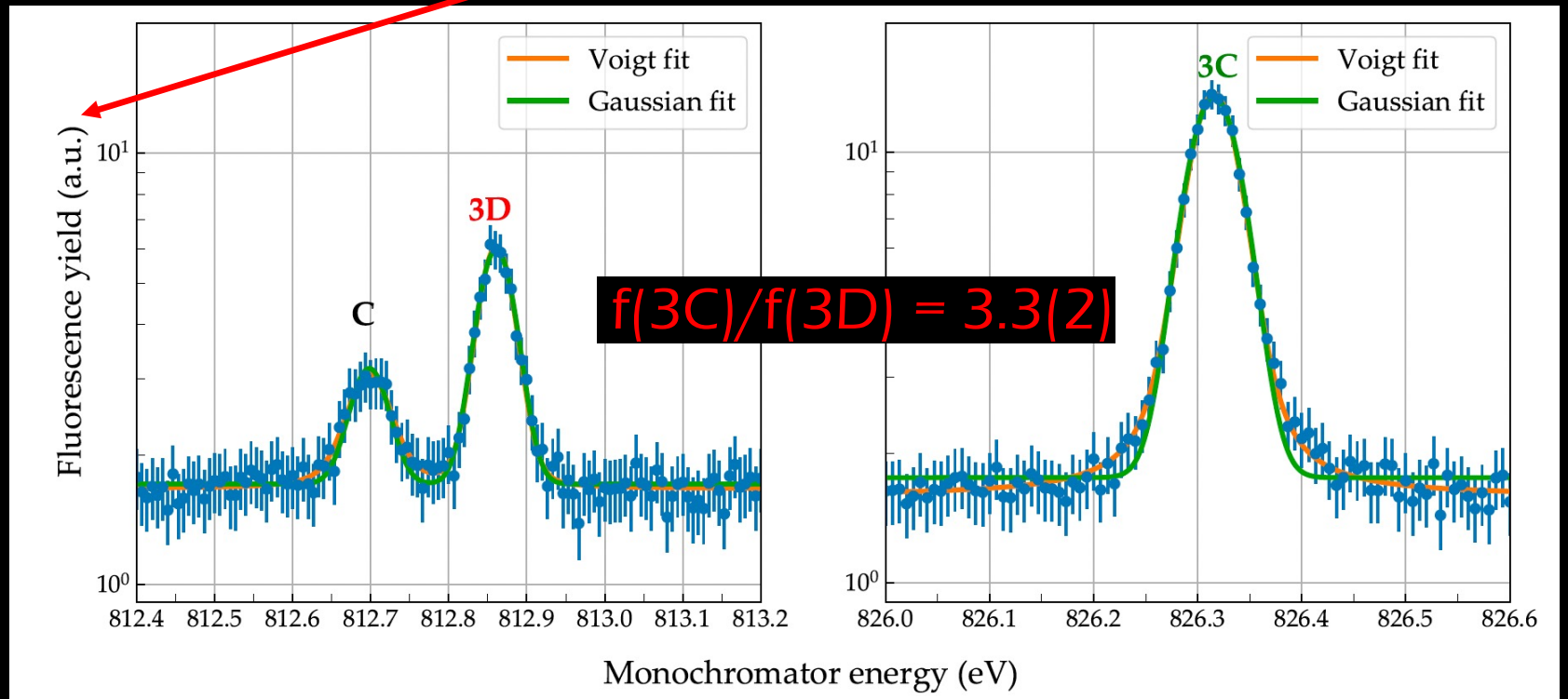
Bkg. from DR

No Bkg.

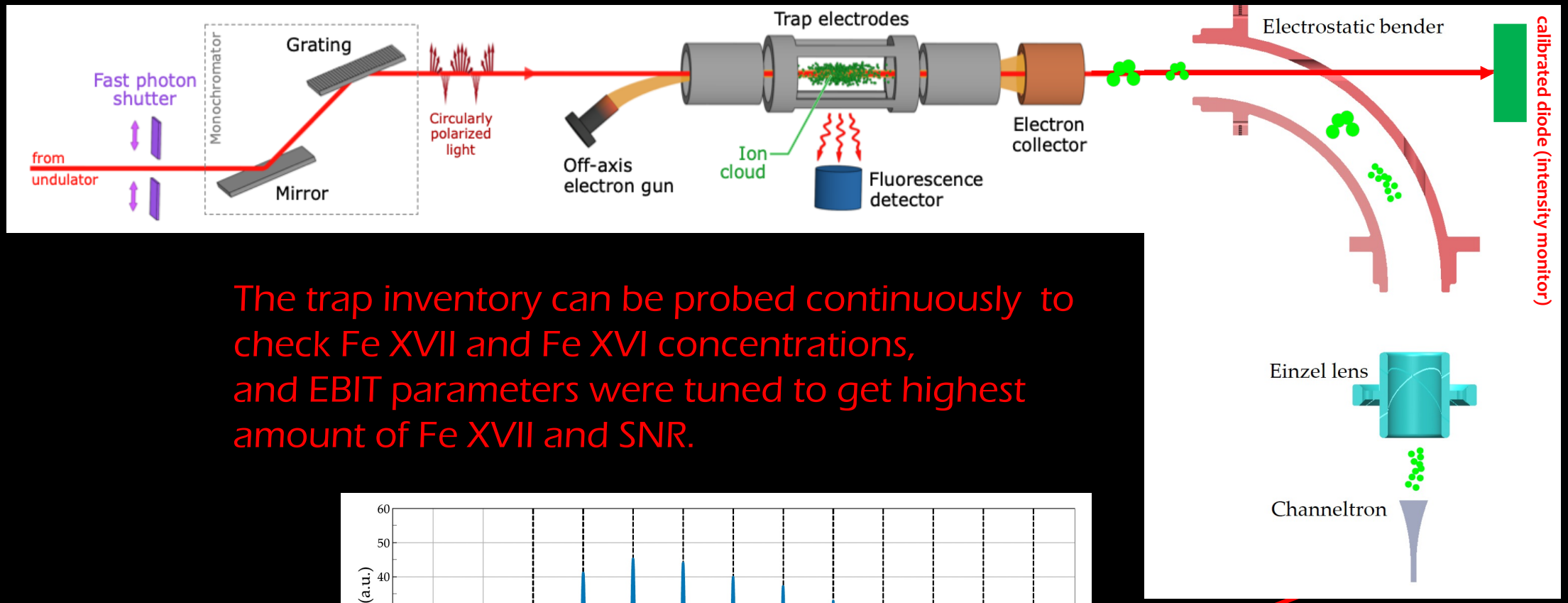


Improving resolving power to 14000 (2019 campaign)

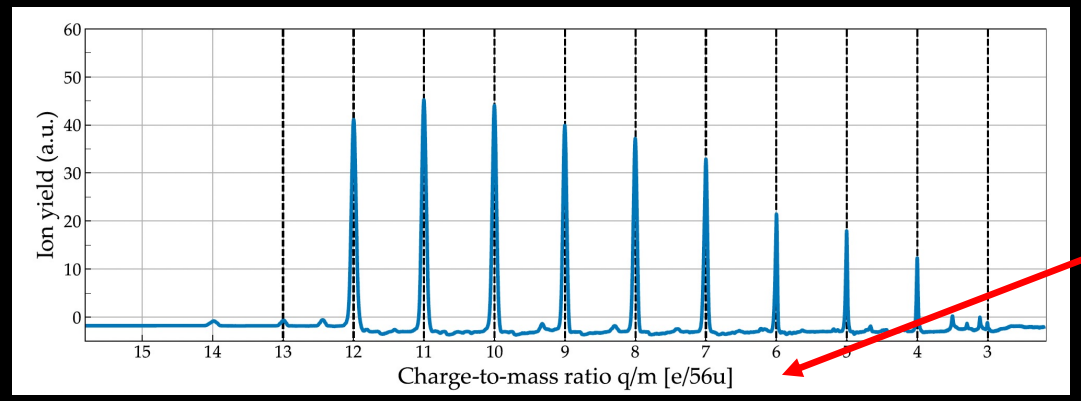




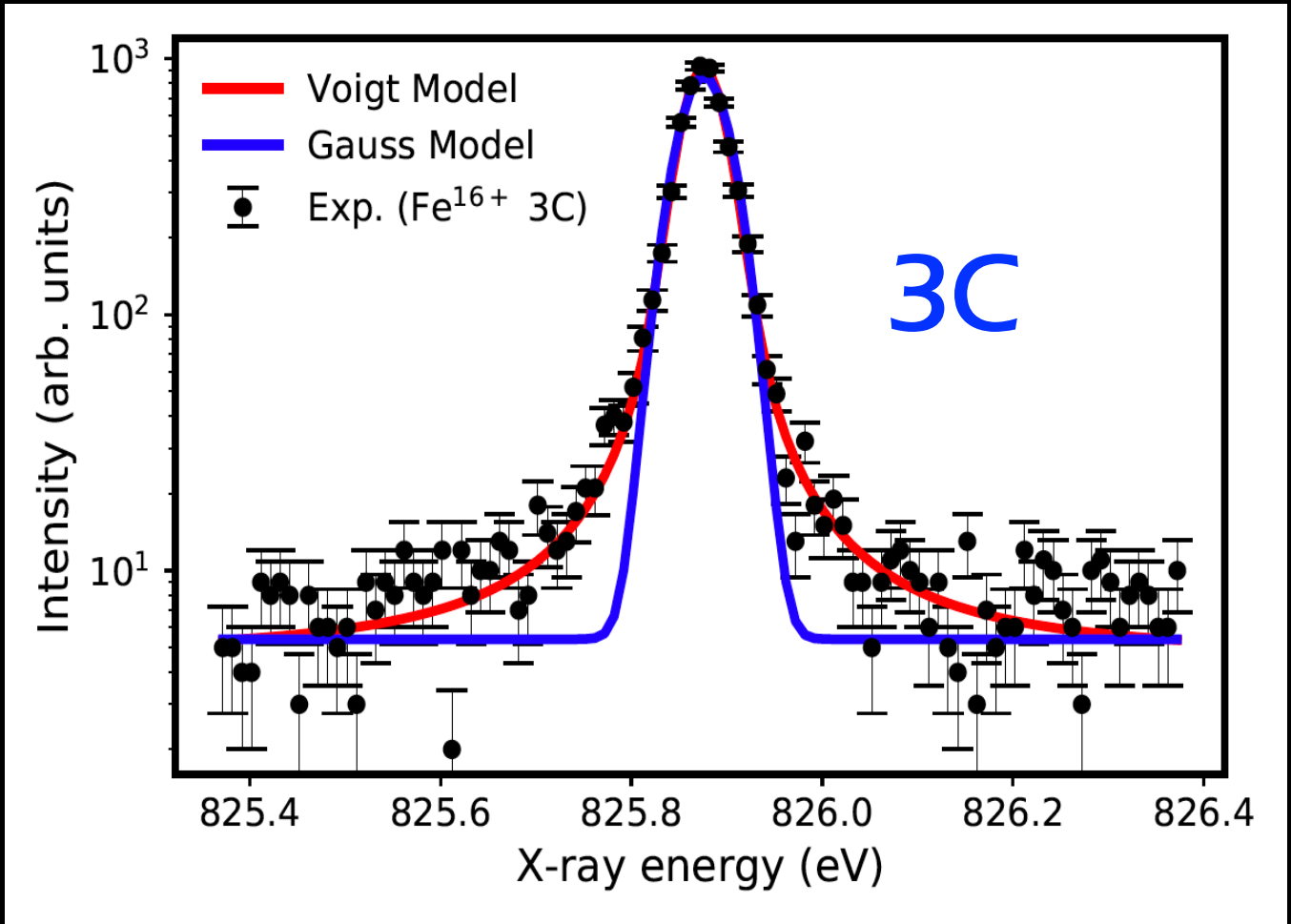
Further improvements (5x) in SNR by installing ion extraction system (2020 campaign)



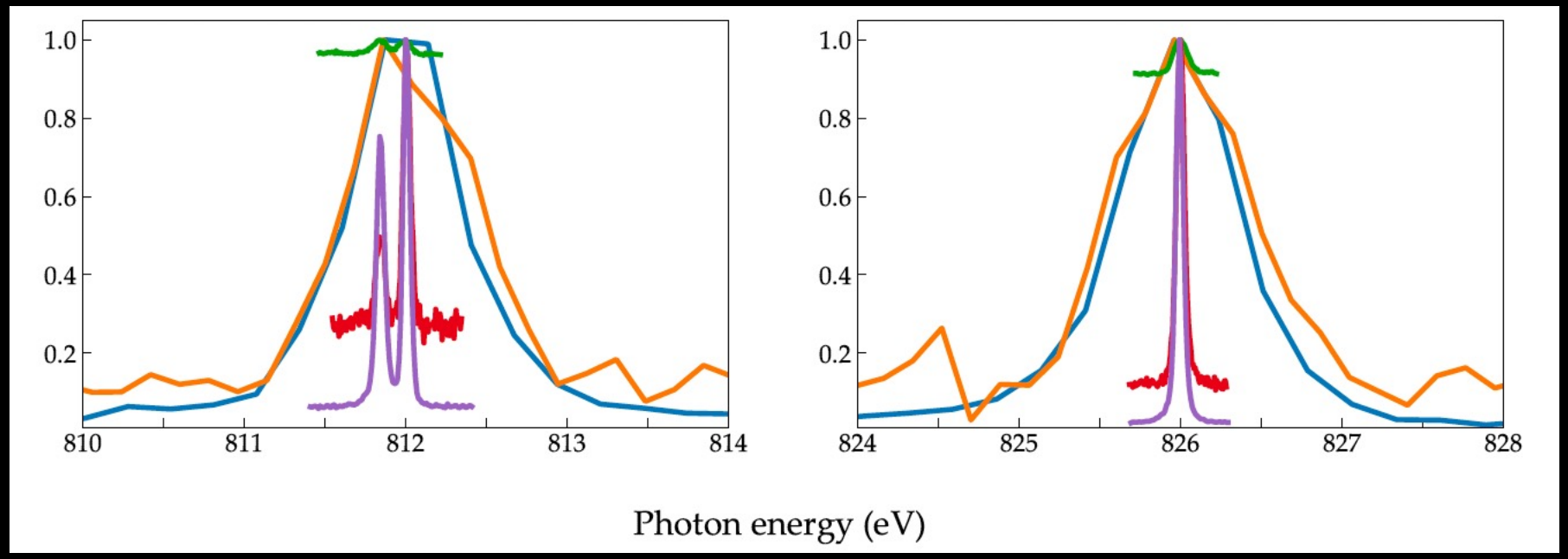
The trap inventory can be probed continuously to check Fe XVII and Fe XVI concentrations, and EBIT parameters were tuned to get highest amount of Fe XVII and SNR.



Improving resolving power to 20000 (2020 campaign)



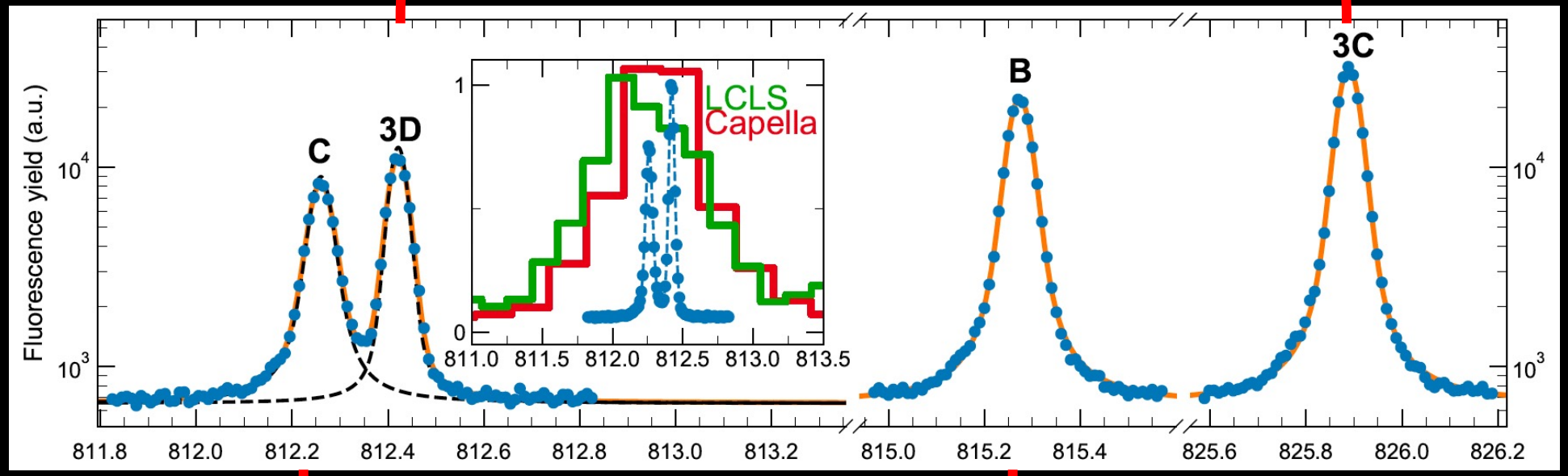
Comparing signal-to-noise and resolution achieved in during PETRA III beamtimes 2018 - 2020



Capella LCLS P04 2018 P04 2019 P04 2020

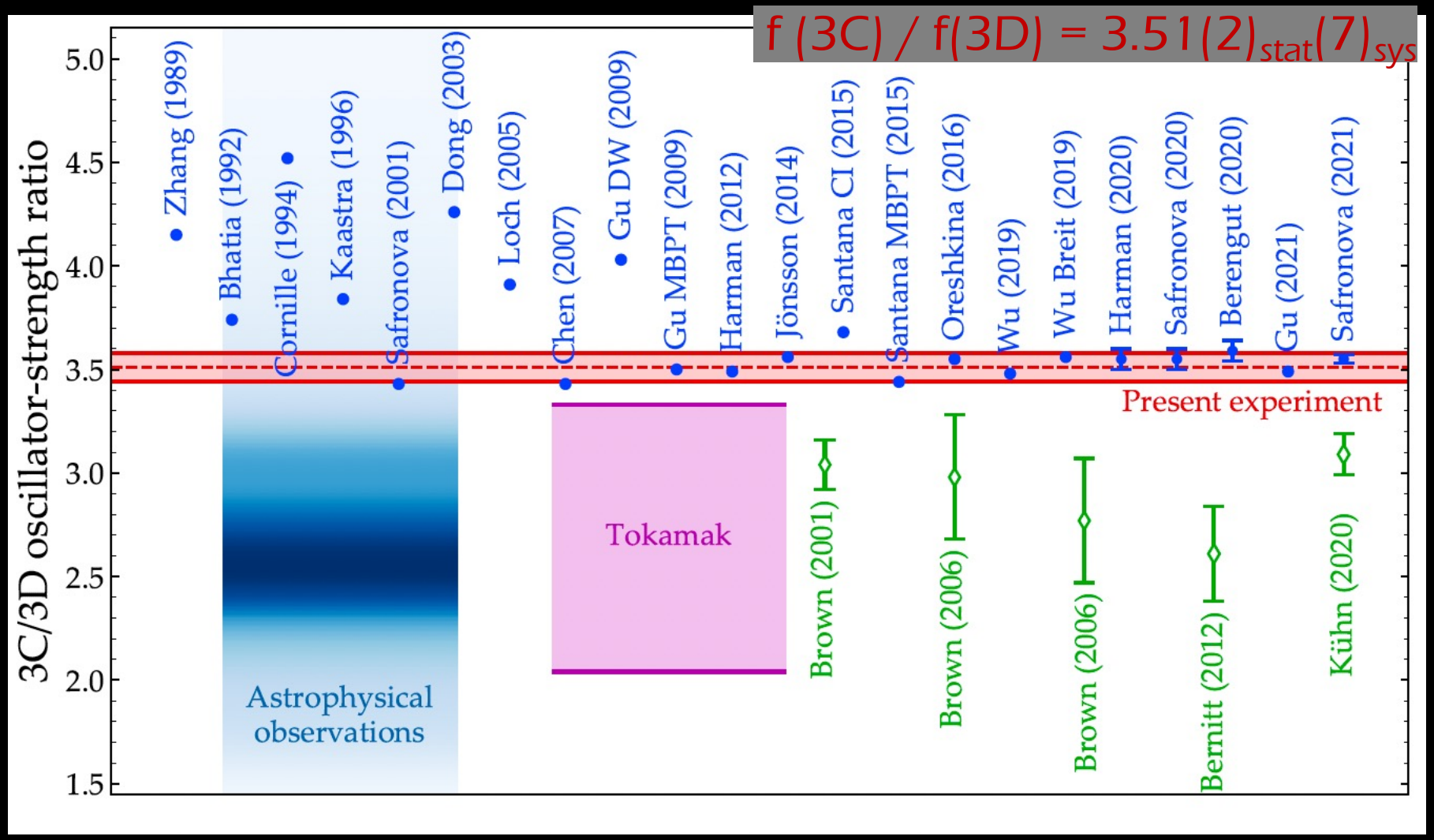
Improving resolving power to 20000 (2020 campaign)

Fe XVII 3C & 3D

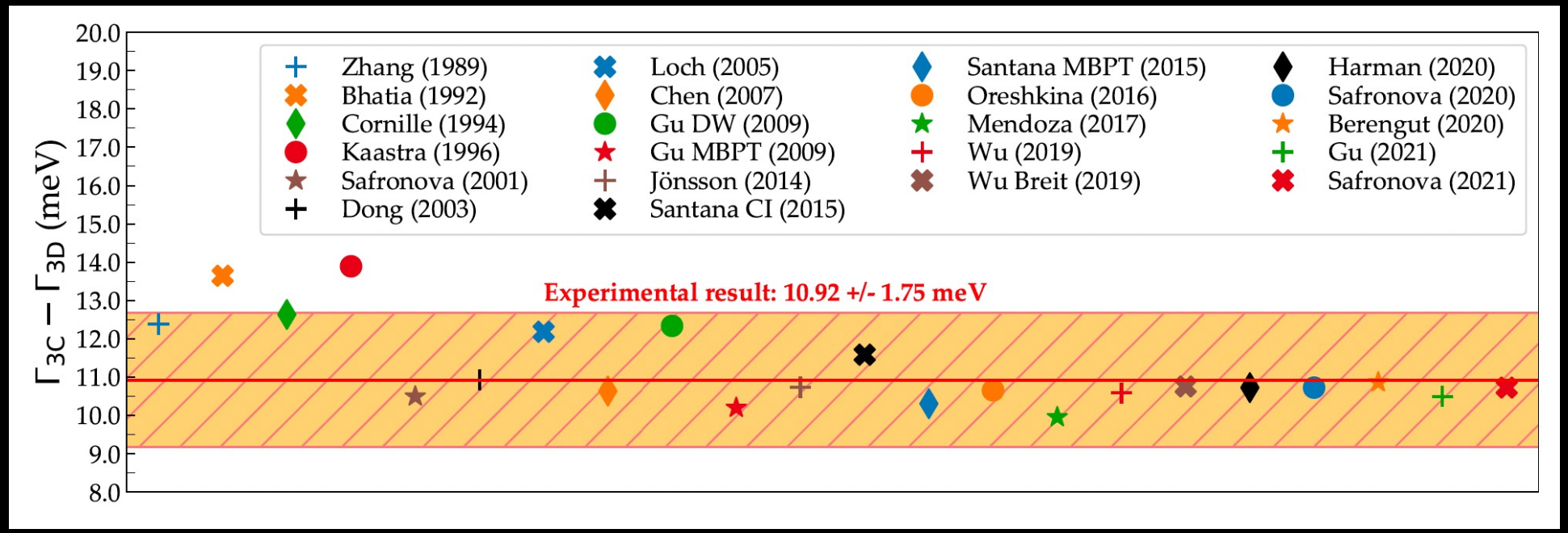


Fe XVI B & C

Final results: 3C/3D ratio (2020 campaign)



Final results: 3C & 3D natural linewidth measurement



$$\Gamma_{3C} = \frac{\Delta\Gamma_{3C-3D}}{1 - \frac{1}{\frac{f(3C)}{f(3D)} \cdot \left(\frac{E_{3C}}{E_{3D}}\right)^2}}$$

$$\Gamma_{3D} = \frac{\Delta\Gamma_{3C-3D}}{\frac{f(3C)}{f(3D)} \cdot \left(\frac{E_{3C}}{E_{3D}}\right)^2 - 1}.$$

Line	Experiment (meV)	Theory (meV)
3C - 3D	10.92(175)	10.71(2)
3C	15.27(247)	14.74(1)
3D	4.22(68)	4.028(15)
B	16.42(301)	14.43†
C	20.52(380)	23.10†

Comparing signal-to-noise and resolution achieved in different PETRA III beamtimes

Campaign	2018	2019	2020
Number of scans	6 + 11	74	60
Resolving Power $E/\Delta E$ (FWHM)	8250	14000	20000
Signal-to-noise ratio	≈ 0.05	≈ 8.5	≈ 45
Model used	Gaussian	Voigt	Voigt
3C/3D oscillator-strength ratio	3.09	3.1-3.5	3.51
Statistical uncertainty	±2.58%	±1.00%	±0.57%
Systematical uncertainties			
ROI selection	±1.8%	X	X
Background instabilities	±1.0%	X	X
Photon flux variation	±2.0%	X	X
Area underestimation of Gaussian profiles fitted to Voigt lines	+4%	X	X
Detection efficiency uncertainty	±0.13%	±0.13%	±0.13%
Asymmetric line shape	X	X	±0.003%
Monochromator interpolation errors	±2.0%	±2.0%	±2.0%
Charge-state equilibrium changes	X	X	X
Final 3C/3D oscillator-strength ratio	$3.09^{+0.18}_{-0.13}$	3.3(2)	3.51(7)

Final remarks on Fe XVII

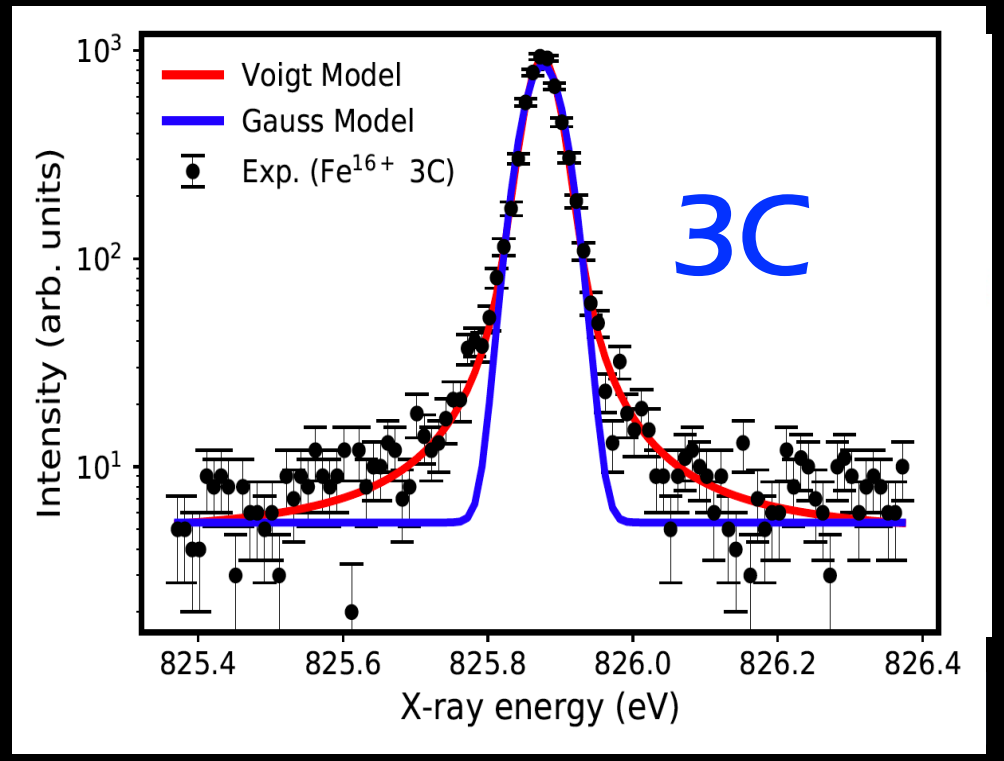
- ✓ Several improvements in our experiments enabled us to achieve lowest uncertainty in measuring 3C/3D oscillator strengths - that agree with very large-scale CI (converged) calculations

- ✓ **Finally, the Fe XVII 3C/3D oscillator-strength ratio problem is resolved!**

- ✓ Most important remark:

- Our work exposes how critical is to understand "non-Gaussian lineshapes"
- When resolving power is comparable to line width - line wings are lost in the background.

This may falsify the intensity ratio.



What’s next

- While the 3C/3D *oscillator strength* ratio problem is solved, the *collision strengths* now need another look (experiment **and** theory)
- The Fe XVII oscillator strength measurement was not a wild goose chase! The theory community came together and produced converged calculations that agree with each other and with experiment. Calculations from > 10 years ago were often not converged. We now know what it takes to get structure right!
- We can still push linewidth measurements further: need improved characterization of monochromator line shape, and continuous monitoring of relative wavelength shift (drift, encoder errors)

Lessons learned

- There’s a lot of insight to be gained by pushing the state of the art in developing new experiments to help answer old questions
- But you have to be prepared to pay the price of developing these techniques
- To have productive benchmarks of theory, it’s best to have collaboration between multiple different theory groups comparing to available experiments, with the aim of constructively diagnosing issues in both theory and experiment

What's next for the Fe XVII problem?