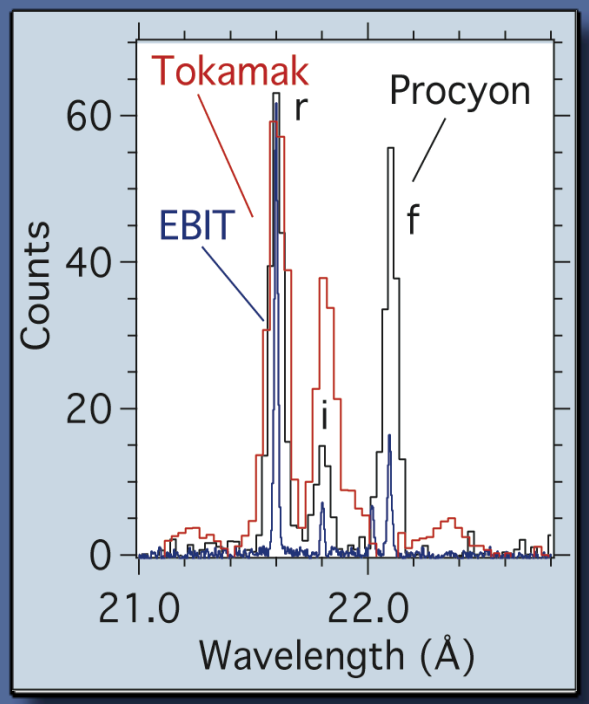
Atomic Physics Measurements in Support of X-ray Astronomy

Physical and Life Sciences Directorate



P. Beiersdorfer

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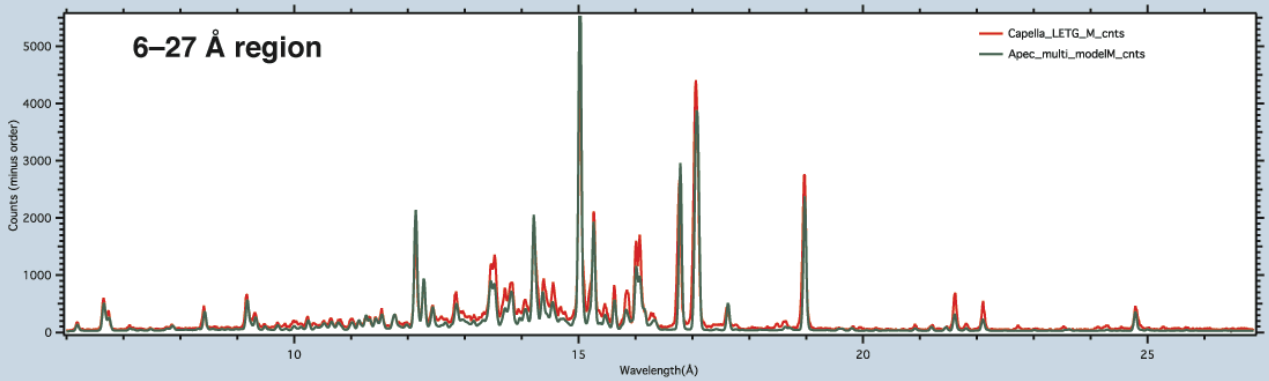
Oct 27, 2010 | Gatlinburg

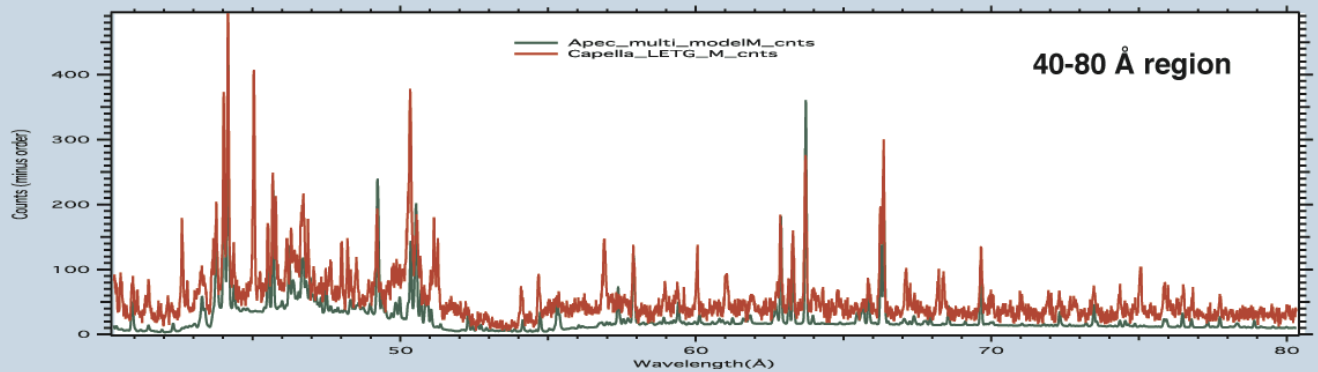
Outline

- Astrophysical needs for emission spectroscopy experiments
  - Progress in laboratory measurements (LLNL EBIT)
- Astrophysical needs for photoabsorption spectroscopy experiments
  - Progress in laboratory measurements (APS, FLASH, BESSY, LCLS light sources)
- Astrophysical needs for ionization equilibrium measurements
  - Progress in laboratory measurements (TSR Storage ring)
- Progress in measurements of radiative transition probabilities, the Fe XVII problem, calibration of electron density diagnostic (LLNL EBIT, tokamaks, new calculations)
- Charge transfer experiments for modeling the X-ray emission from planetary/cometary atmospheres (JPL, Reno, LLNL)
- Summary

High-resolution astrophysical observations illustrate the need for laboratory astrophysics

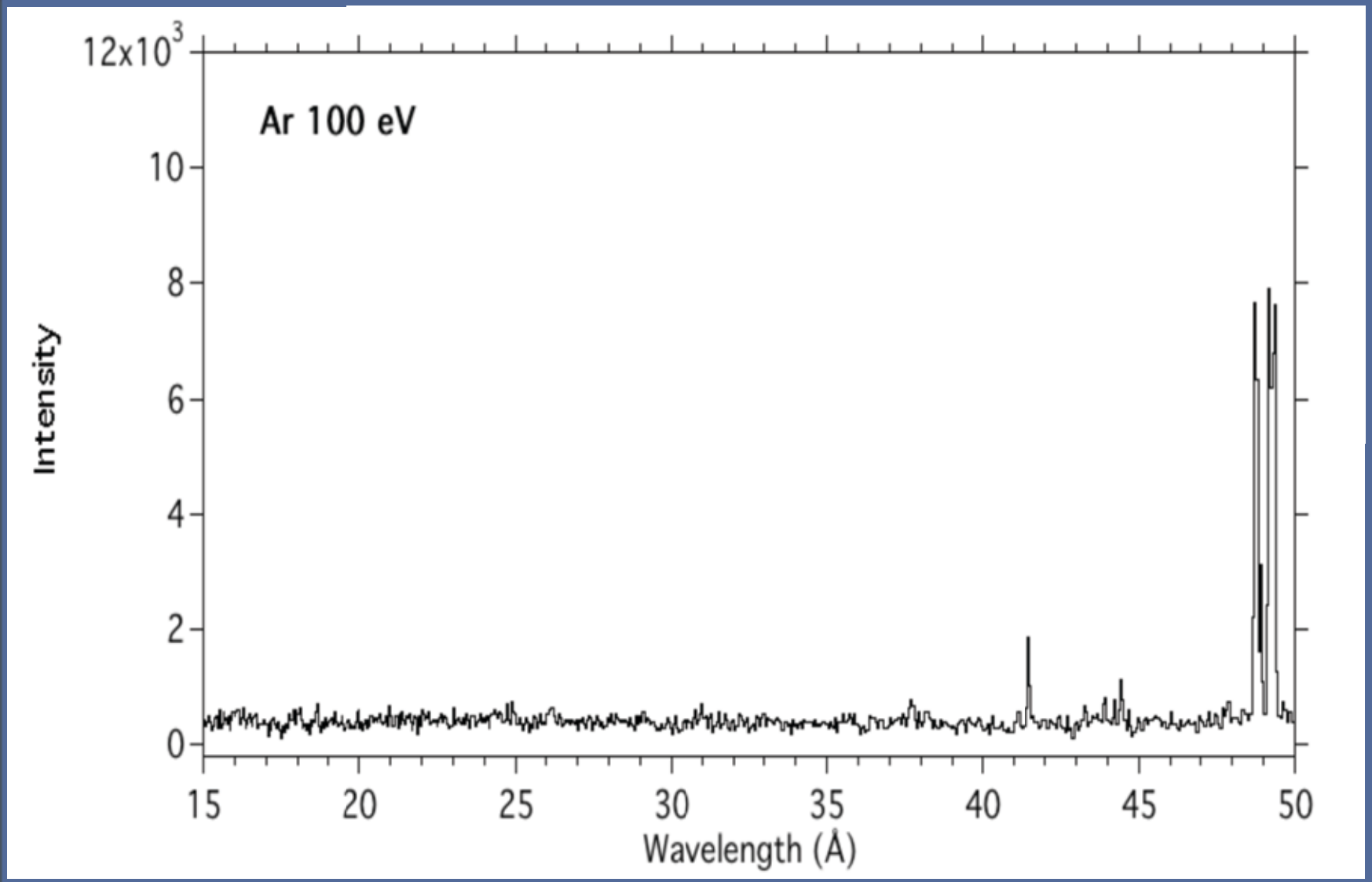
Spectral fits of Capella observations with APEC model





Spectral data bases have been incomplete and cannot identify all lines

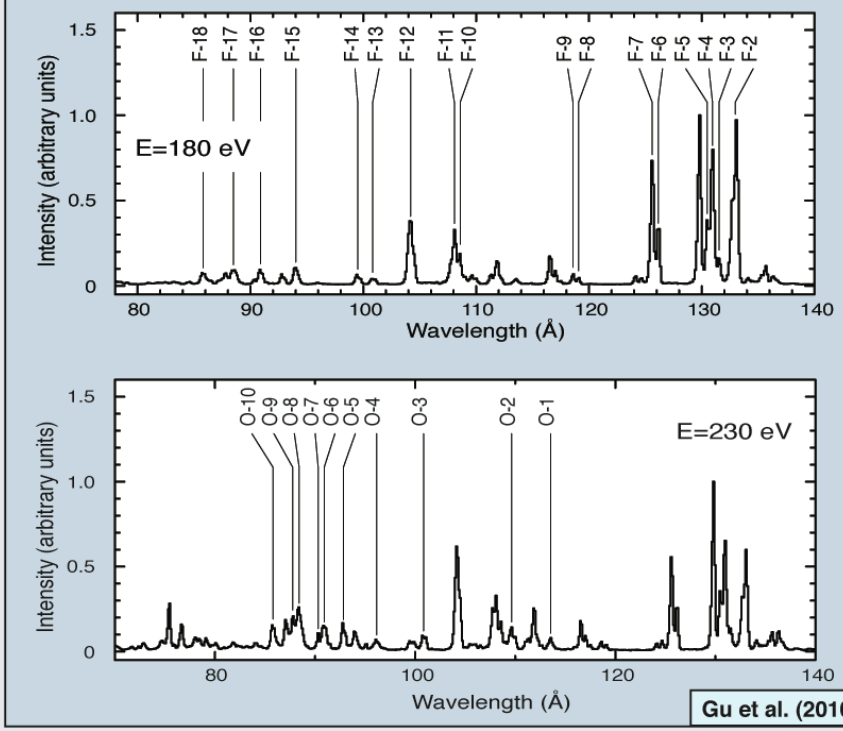
Evolution of argon EUV emission with beam energy



Controlled measurements provide comprehensive spectral catalogues of the lines in the EUV

The measurements yield line identifications, wavelengths, and intensities.

L-shell aluminum emission measured on EBIT-I



Gu et al. (2010)

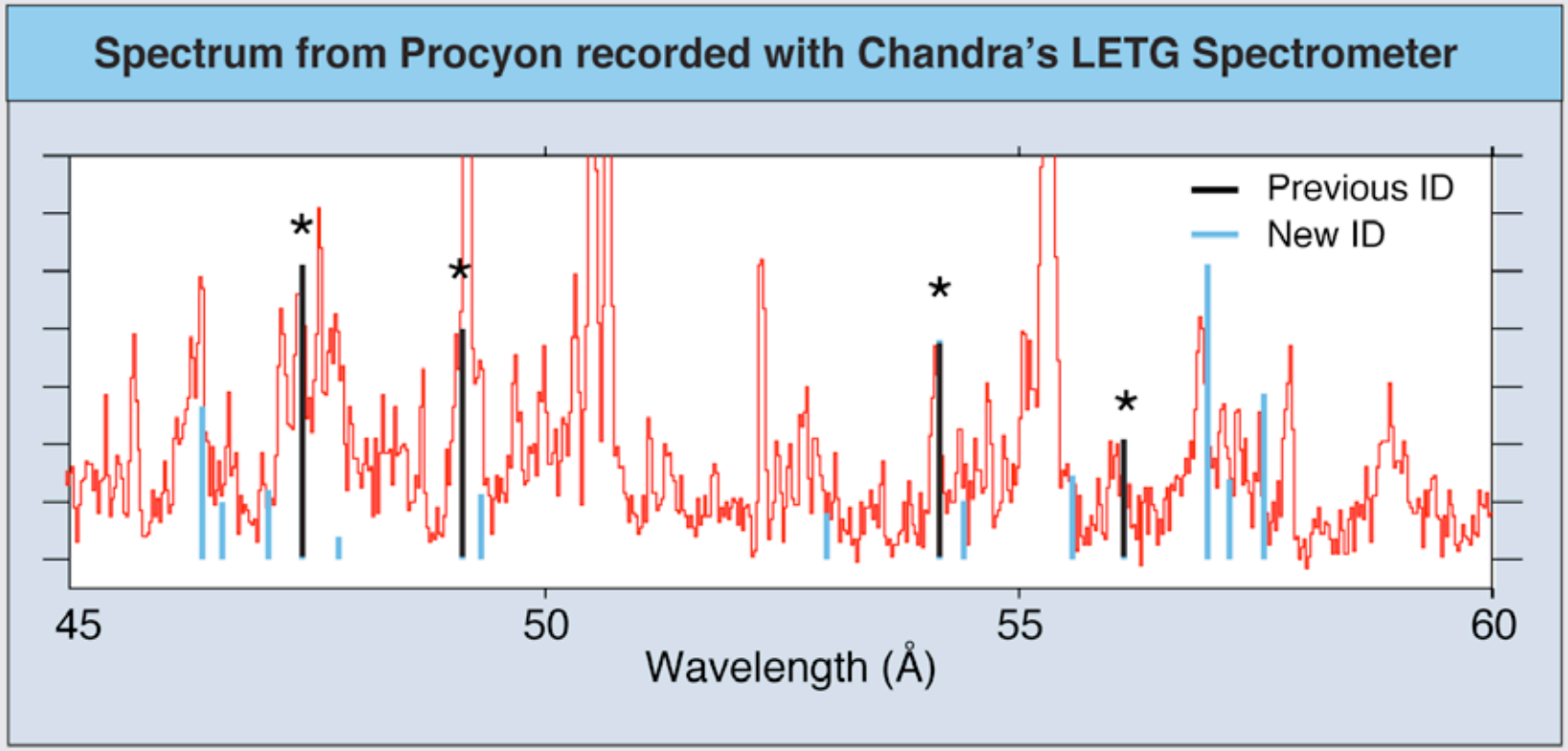
Line list for S VII - S XIV between 20 and 75 Å

Ion	Lab Data EBIT	Present Data Bases MEKAL	CHIANTI
S VII	10	8	0
S VIII	25	8	0
S IX	22	2	0
S X	29	4	1
S XI	14	1	0
S XII	9	0	4
S XIII	10	0	4
S XIV	8	0	13
TOTAL	135	23	22

Lepson et al. ApJ 625, 1045 (2005)

Ne, Mg, Al, Si, S, Ar, Fe, Ni measurements are now complete.

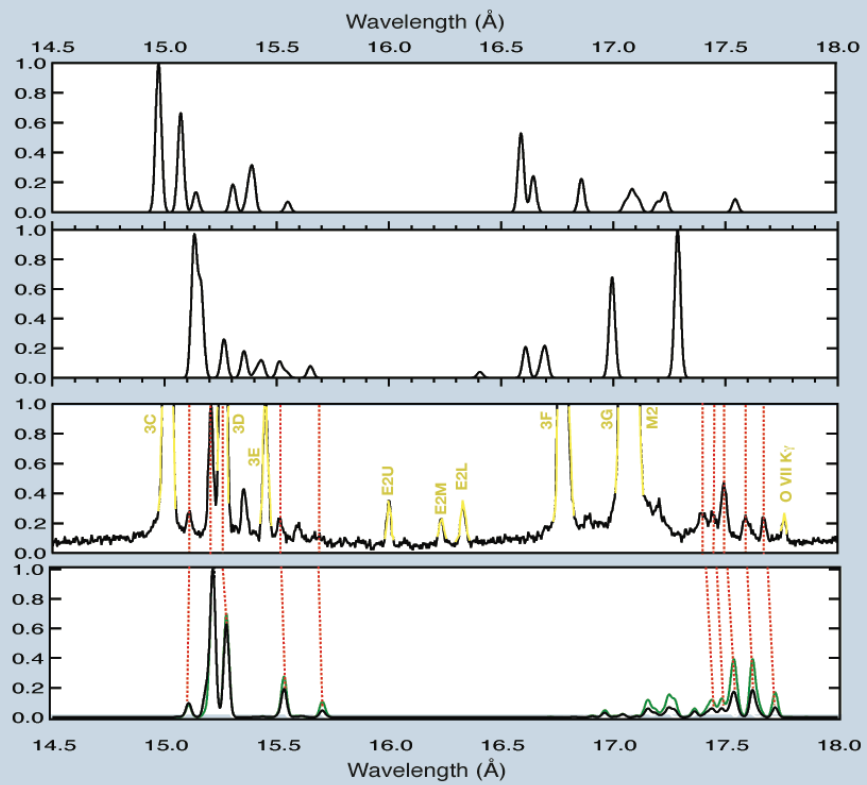
The laboratory data allow us to make new identifications of L-shell lines in stellar coronae



Using the experimental data 10 new S IX lines were identified

Even the Fe L-shell emission spectra still need work

Fe XVI L-shell emission: innershell satellite lines



Cornille et al. A&AS 105,77 (1994)

Phillips et al. A&A324, 381 (1997)

Graf et al. ApJ 695, 818 (2009)

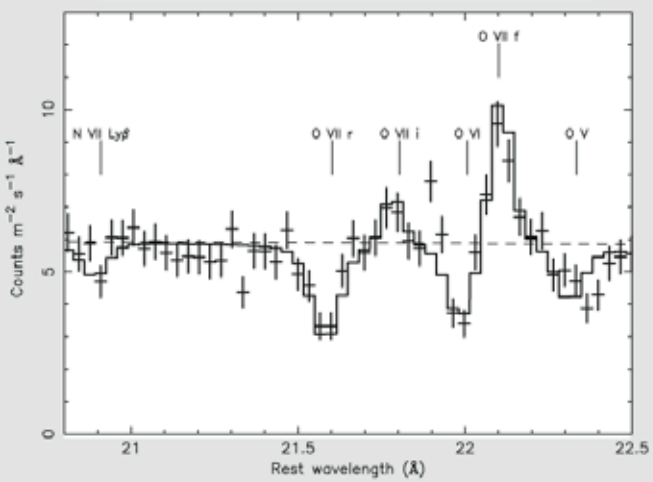
FAC; Graf et al. ApJ 695, 818 (2009)

The Fe XVI spectral features have finally been identified

Accurate measurements are needed to calibrate outflow velocities near active galactic nuclei

Line energies from theory are only good to 700 km/s, while Chandra's accuracy is 120 km/s.

XMM Newton spectrum of NGC 5548



Arav et al., ApJL 590, 174 (2003)

Wavelength predictions for O V resonance line

22.38 Å (Vainshtein & Safronova 1978)
22.41 Å (Chen 1985, 1986)
22.33 Å (Behar & Kahn 2002)
22.35 Å (Pradhan et al. 2003)

Accurate measurements are needed to calibrate outflow velocities near active galactic nuclei

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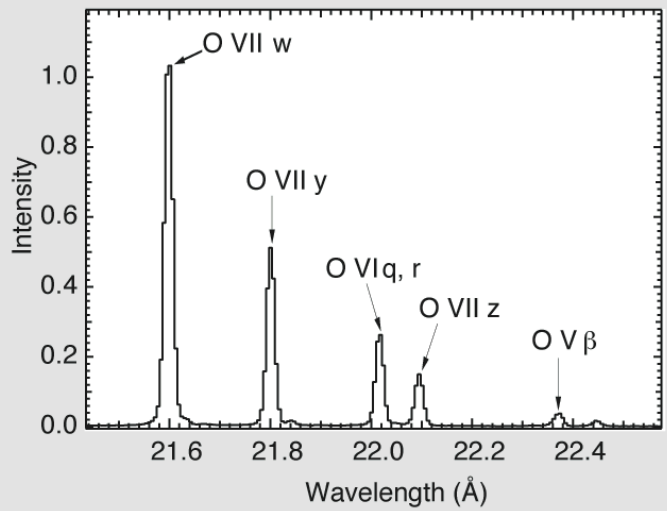
EBIT-I measurement of O K lines



Schmidt et al., ApJL 604, 562 (2004)
Gu et al., ApJ, 627, 1066 (2005)

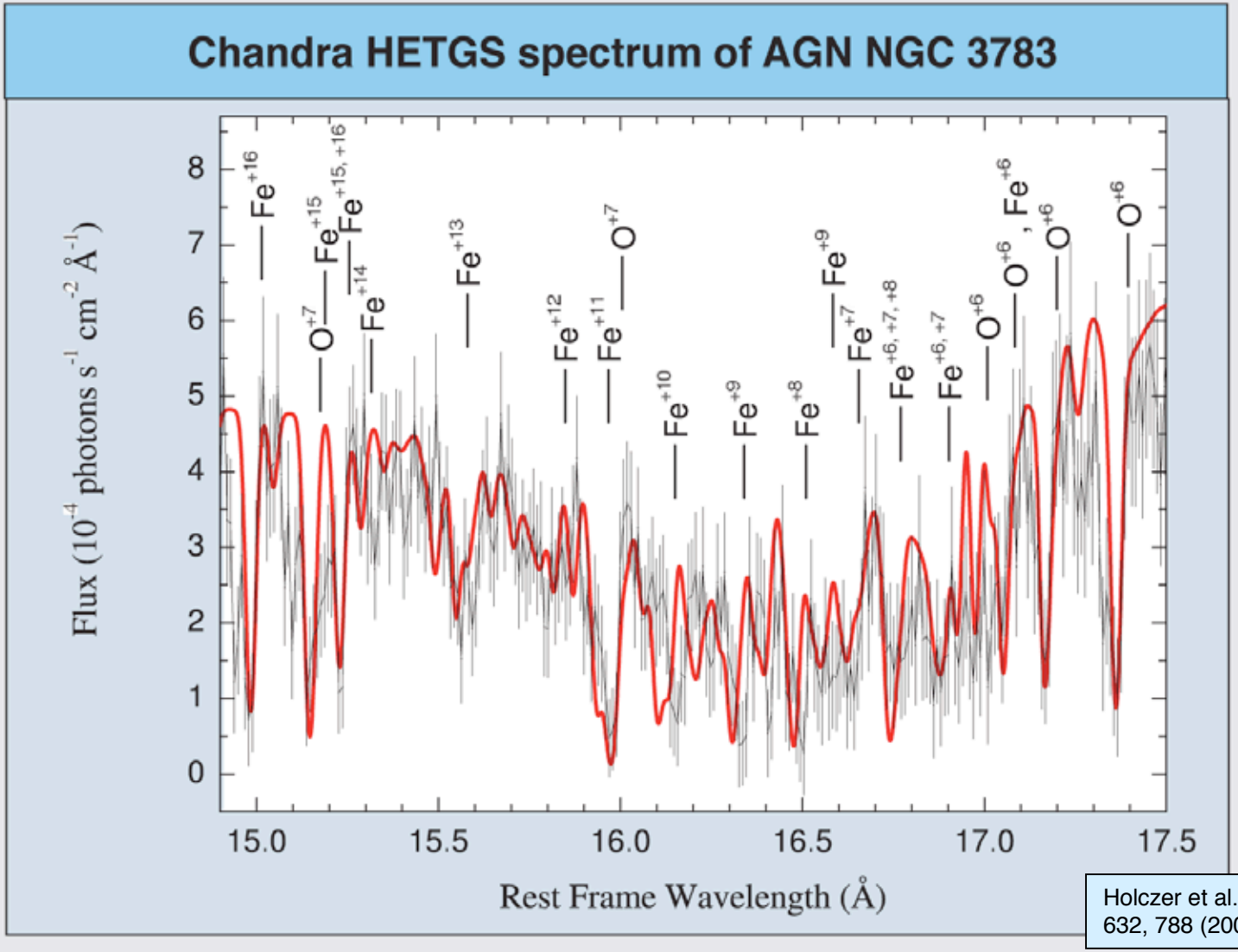
Wavelength predictions for O V resonance line

22.38 Å (Vainshtein & Safronova 1978)
22.41 Å (Chen 1985, 1986)
22.33 Å (Behar & Kahn 2002)
22.35 Å (Pradhan et al. 2003)

22.374 ± 0.003 Å (measured)

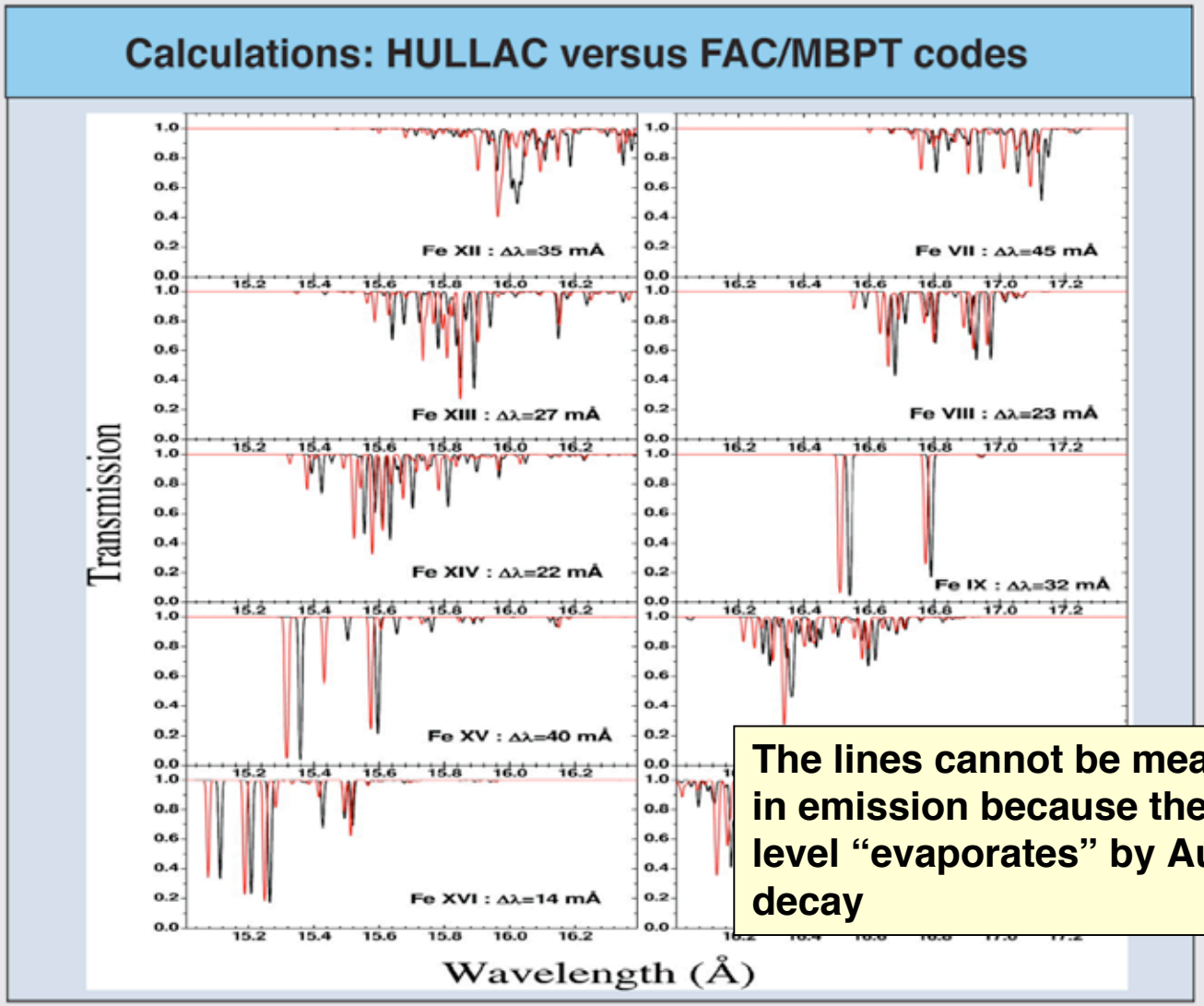
The EBIT-I measurements allow a determination of the gas outflow velocities of typically 500–1000 km/s to within 40 km/s

The iron M-shell region represents an even bigger problem



Holczer et al., APJ 632, 788 (2005)

The calculations do not agree



The lines cannot be measured in emission because the upper level "evaporates" by Auger decay

Advanced light sources coupled with an EBIT can now address these issues

The "First" such deployment was reported in 2010

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Title:	First Deployment of an Electron Beam Ion Trap at an Advanced Source of Hard X-rays
Authors:	Gillaspy, J. D.; Silver, E.; Kanter, E. P.; Brickhouse, N. S.; Dunford, R. W.; Kirby, K.; Lin, T.; McDonald, J.; Schneider, D.; Seifert, S.; Young, L.
Publication:	American Physical Society, APS April Meeting 2010, February 13-16, 2010, abstract #C1.045
Publication Date:	02/2010
Origin:	APS
Bibliographic Code:	2010APS..APR.C1045G

Abstract

We have deployed an Electron Beam Ion Trap (EBIT) at the Advanced Photon Source. The EBIT was cooled to 4K with a cryocooler and mounted on stepper motors to allow precise adjustment relative to the x-ray beam. The electron and x-ray beams crossed at a right angle in the horizontal plane. Spectra of photons emitted off-axis from the incident beams were recorded as Kr26+ and Ar8+ ions were subjected to x-rays up to 18 keV. No heating or other adverse effects on the operation of the cryogenic ion trap were experienced. Spectra and lessons learned for future work will be presented.)

Advanced light sources coupled with an EBIT can now address these issues

The "First" such deployment was reported in 2010

An even earlier such deployment was reported in 2007 (and before)

PRL 98, 183001 (2007) PHYSICAL REVIEW LETTERS week ending 4 MAY 2007

Soft X-Ray Laser Spectroscopy on Trapped Highly Charged Ions at FLASH

S. W. Epp,[1,*] J. R. Crespo López-Urrutia,[1] G. Brenner,[1] V. Mäckel,[1] P. H. Mokler,[1] R. Treusch,[2] M. Kuhlmann,[2] M. V. Yurkov,[2] J. Feldhaus,[2] J. R. Schneider,[2] M. Wellhöfer,[3] M. Martins,[3] W. Wurth,[3] and J. Ullrich[1]

[1]*Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany*
[2]*DESY, D-22607 Hamburg, Germany*
[3]*Institut für Experimentalphysik, Universität Hamburg, D-22761 Hamburg, Germany*

(Received 28 December 2006; published 1 May 2007)

In a proof-of-principle experiment, we demonstrate high-resolution resonant laser excitation in the soft x-ray region at 48.6 eV of the $2\,^2S_{1/2}$ to $2\,^2P_{1/2}$ transition of Li-like Fe^{23+} ions trapped in an electron beam ion trap by using ultrabrilliant light from Free Electron Laser in Hamburg (FLASH). High precision spectroscopic studies of highly charged ions at this and upcoming x-ray lasers with an expected accuracy gain up to a factor of a thousand, become possible with our technique, thus potentially yielding fundamental insights, e.g., into basic aspects of QED.

subjected to x-rays up to 18 keV. No heating or other adverse effects on the operation of the cryogenic ion trap were experienced. Spectra and lessons learned for future work will be presented.)

Advanced light sources coupled with an EBIT can now address these issues

The "First" such deployment was reported in 2010

An even earlier such deployment

PRL 98, 183001 (2007) PHYSICAL RE

Soft X-Ray Laser Spectroscopy on Ti

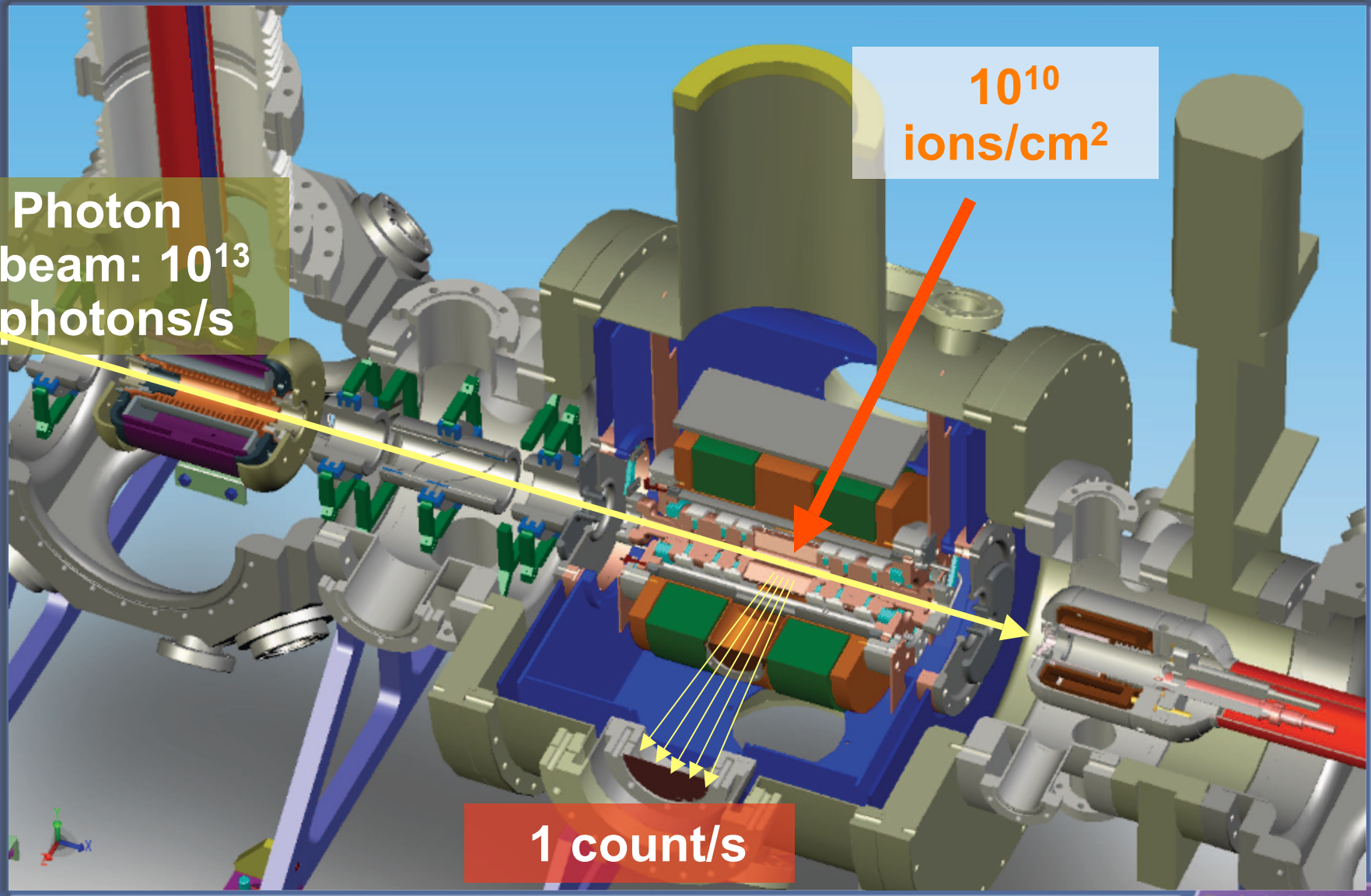
S. W. Epp,[1,*] J. R. Crespo López-Urrutia,[1] G. Brenner,
M. V. Yurkov,[2] J. Feldhaus,[2] J. R. Schneider,[2] M.
[1]*Max-Planck-Institut für Kernph*
[2]*DESY, D-22607*
[3]*Institut für Experimentalphysik, Univers*
(Received 28 December

In a proof-of-principle experiment, we demonstr
x-ray region at 48.6 eV of the $2\,^2S_{1/2}$ to $2\,^2P_{1/2}$ tran
ion trap by using ultrabrilliant light from Free E
spectroscopic studies of highly charged ions at this
gain up to a factor of a thousand, become po
fundamental insights, e.g., into basic aspects of Q

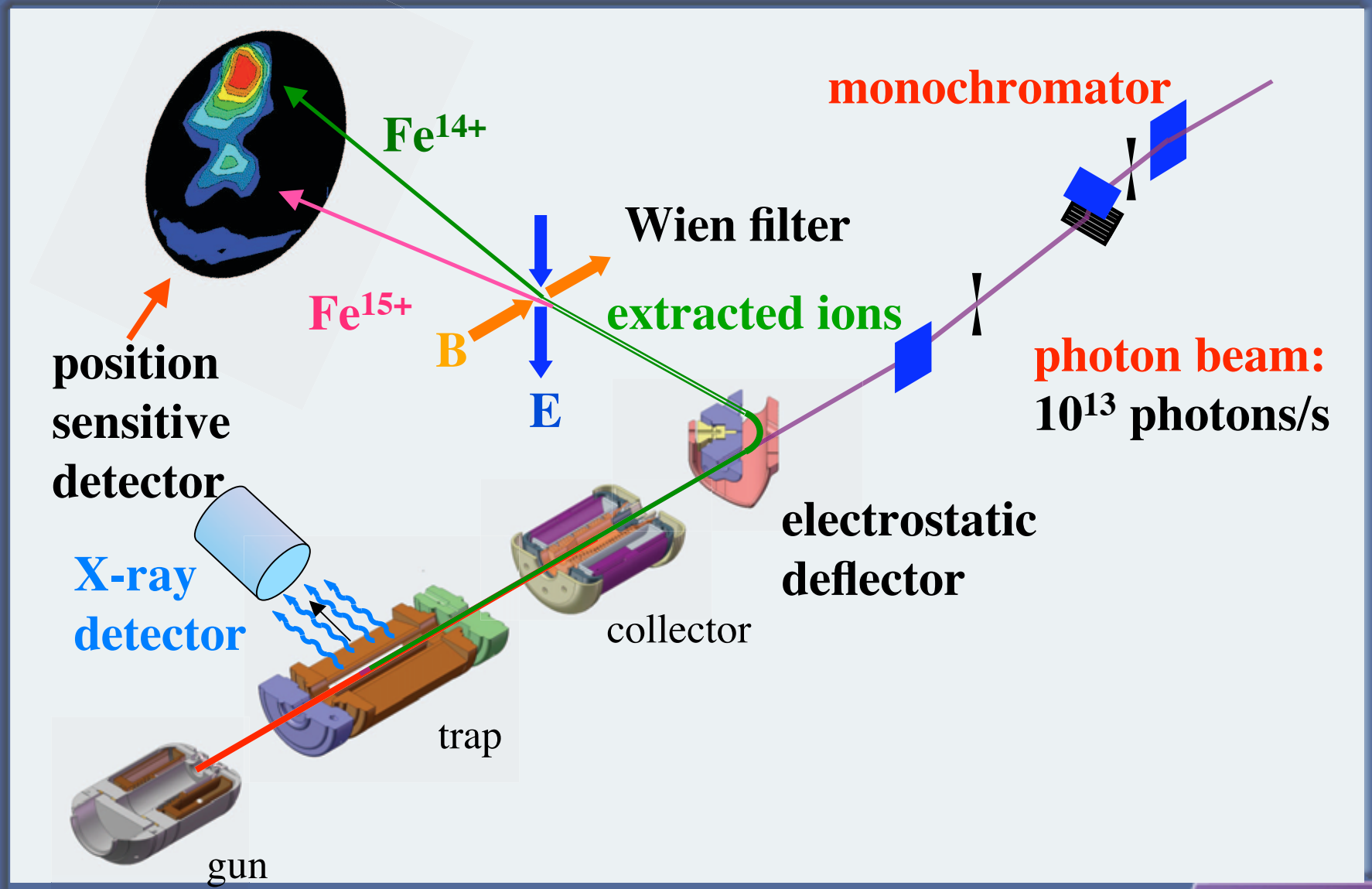
subjected to x-rays up to 18 keV. No heating or other adverse effects on the operation of the cryogenic ion trap were experienced. Spectra and lessons learned for future work will be presented.)

- **Resonance excitation of Fe XXIV was the first successful measurement using an EBIT at an advanced light source (FLASH)**
  [Epp et al., PRL 98, 183001 (2007)]
- **An extension to Cu XXVII was recently reported (using FLASH)**
  [Epp et al., JPhysB 43, 194008 (2010)]
- **Photoionization of N IV and Ar IX has also been reported by the Heidelberg group (using BESSY)**
  [Simon et al., JPhysB 43, 065003 (2009)]
- **Photoionization data of Fe XV and Fe XVI are now in press (using BESSY)**
  [Simon et al., PRL, in press (2010)]

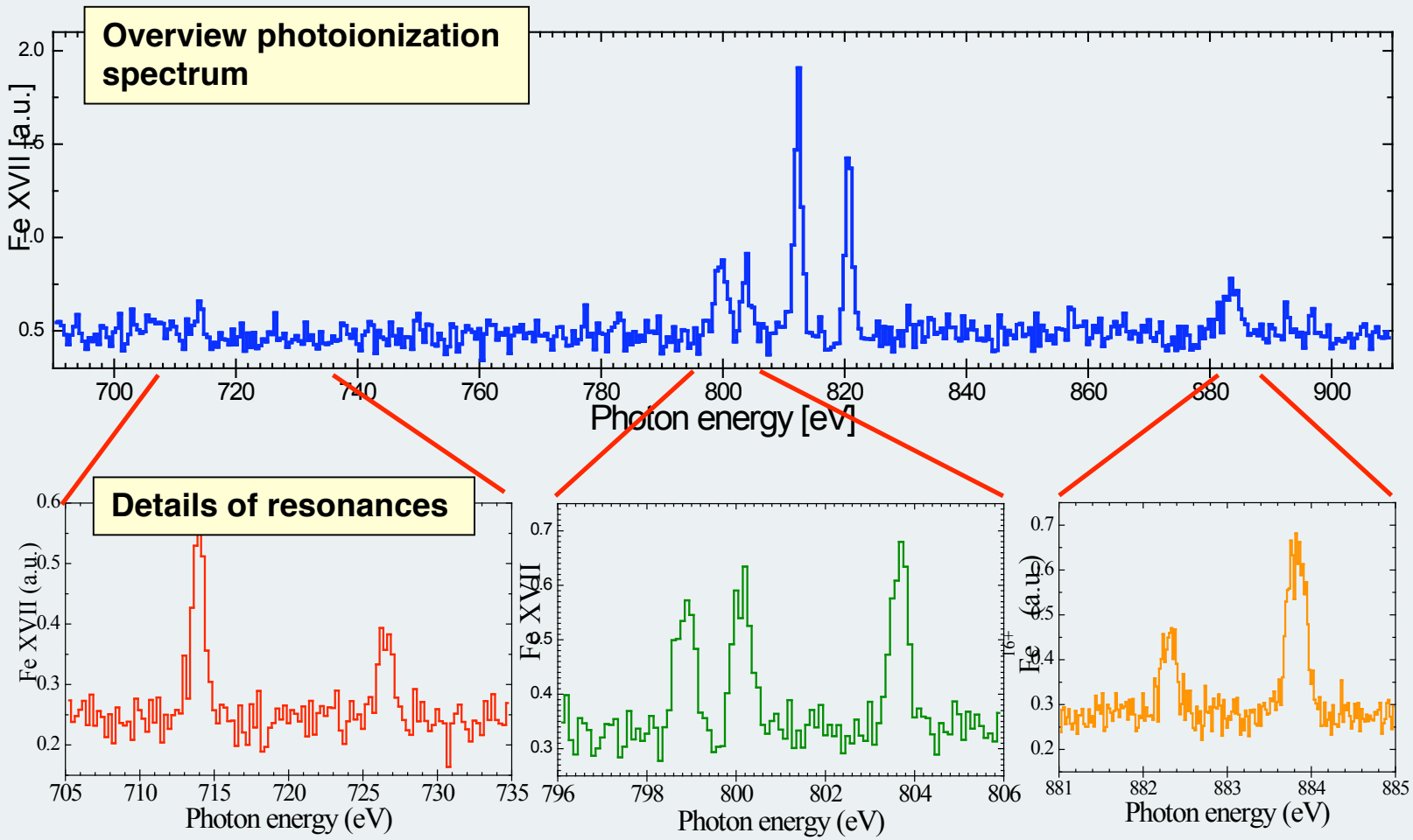
Schematic of the Heidelberg EBIT interacting with a photon beam



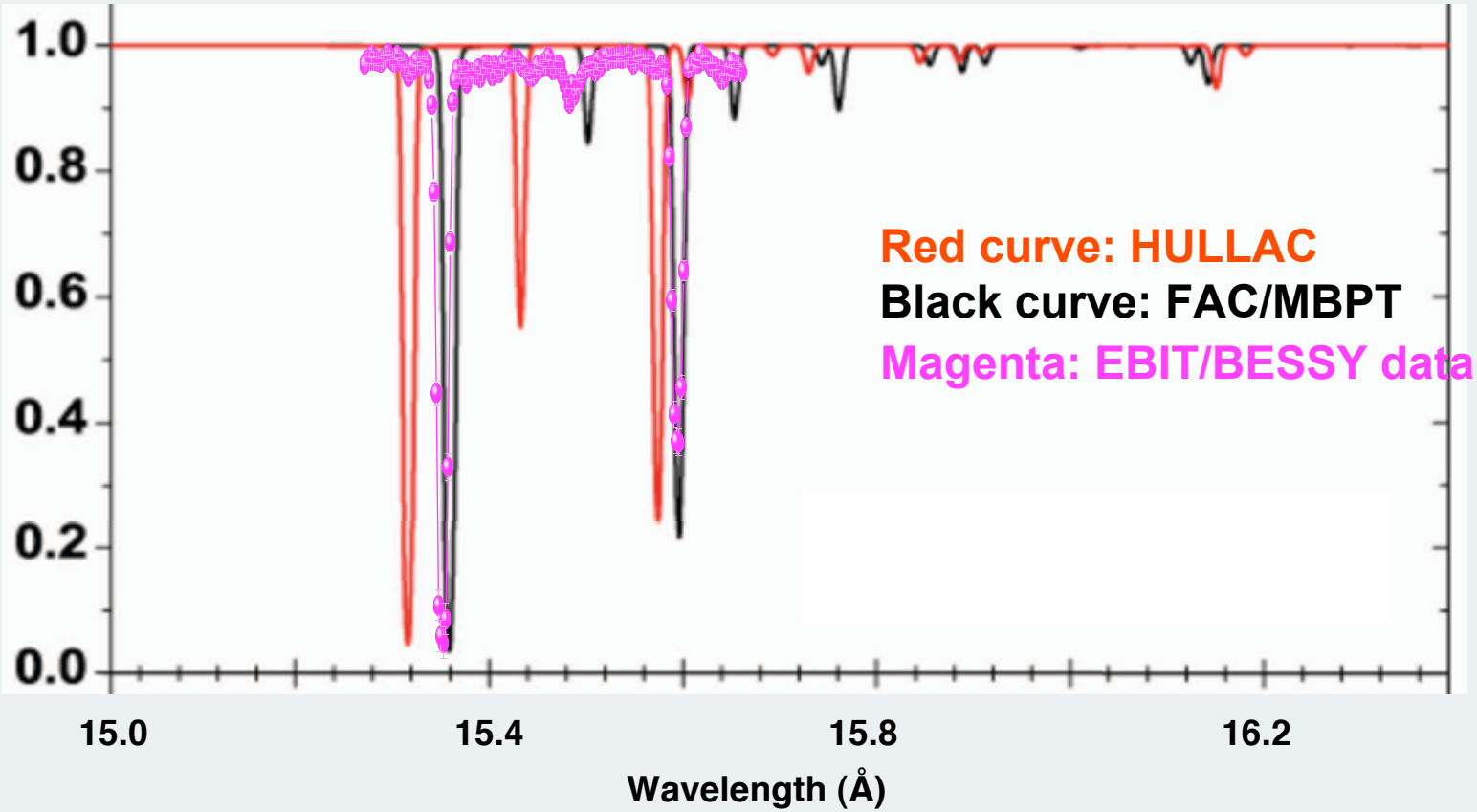
Measurements of the photoionization cross sections of Fe X[illegible]ies on ion extraction and charge analysis



Results of Fe XVI photoionization measurements on the BESSY light source



The comparison of Fe XV results with theory favors the recent FAC/MBPT calculations



Interfacing the HD EBIT with an advanced light source can be done rather rapidly

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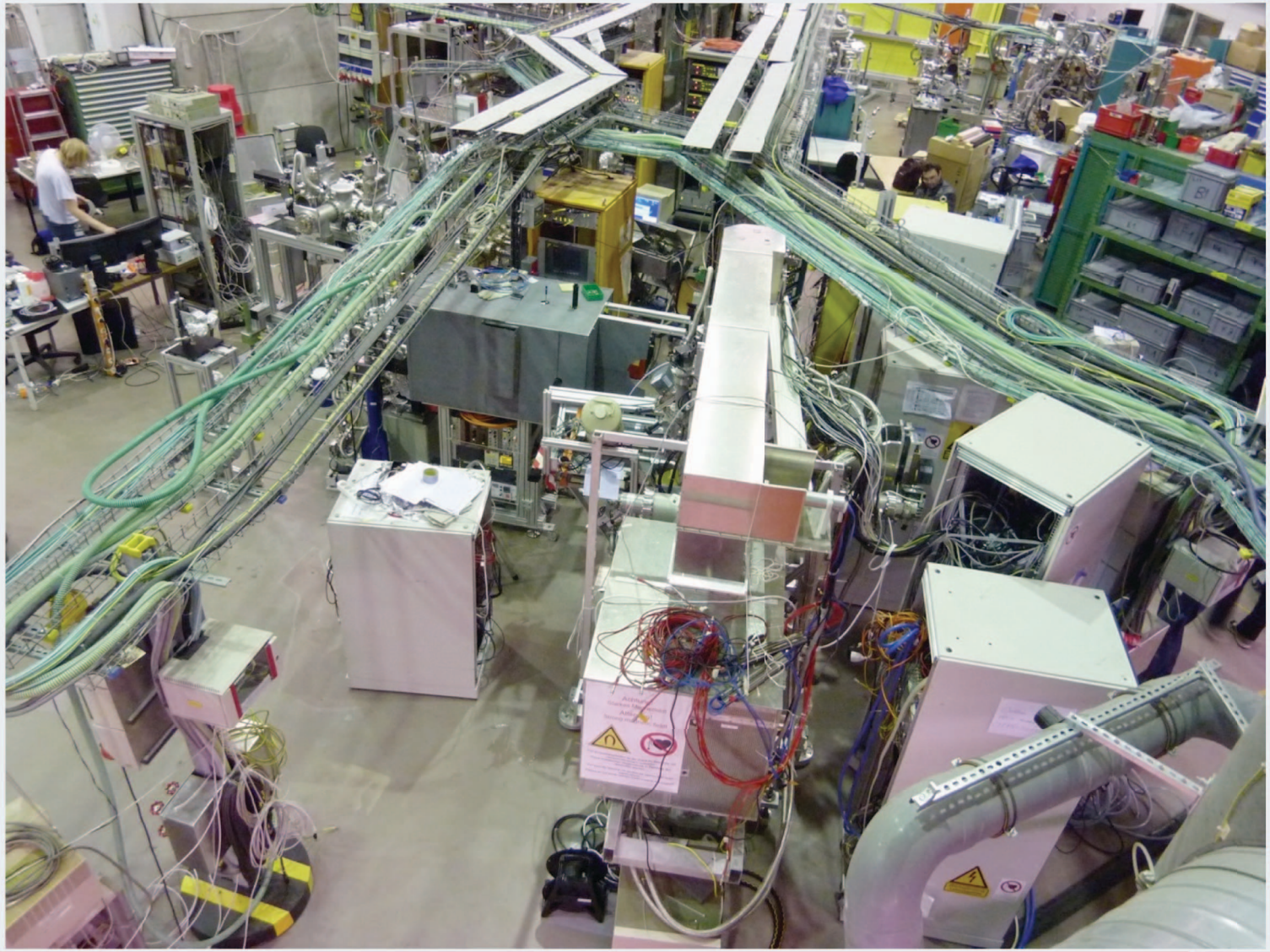
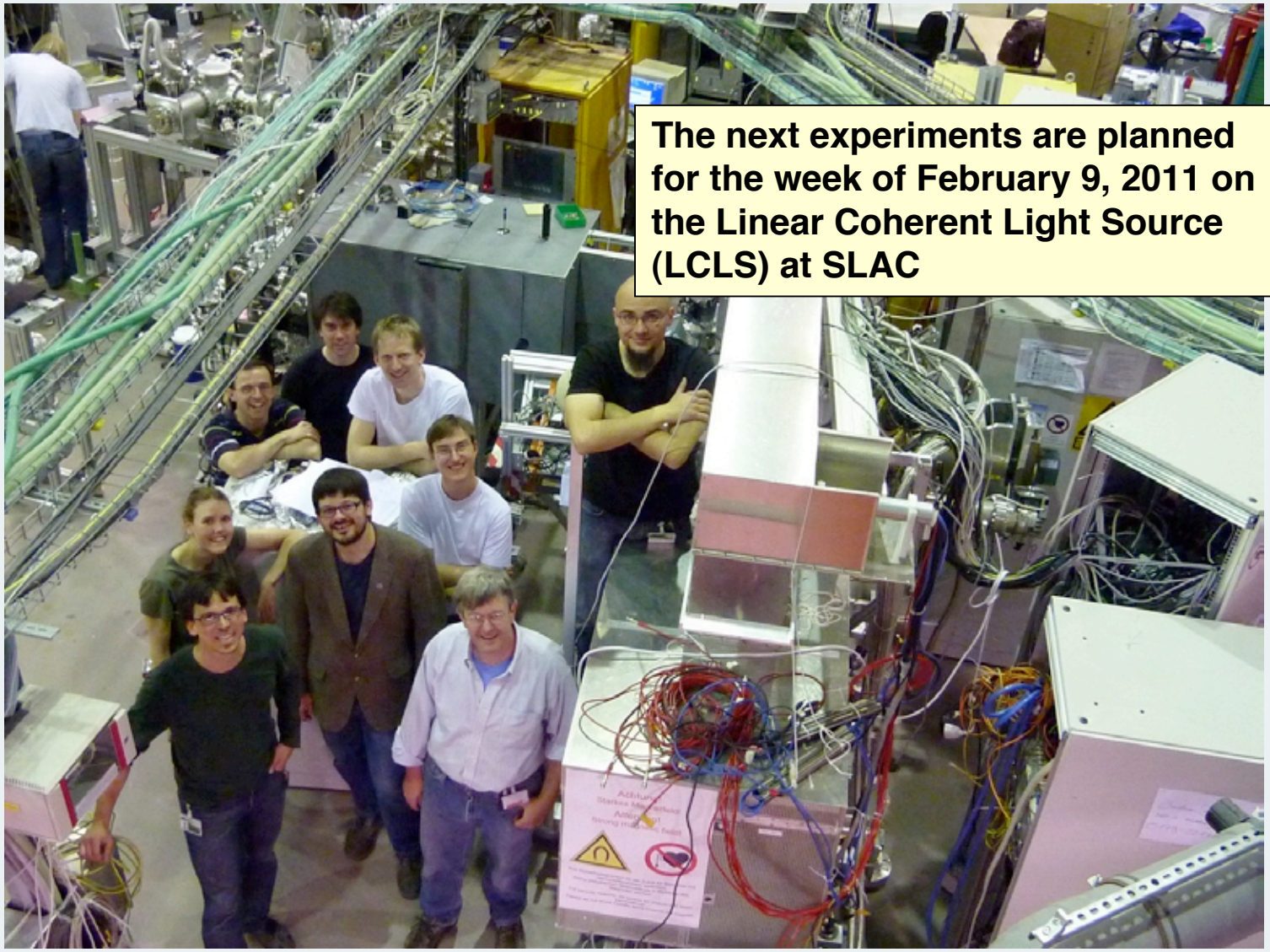


Interfacing the HD EBIT with an advanced light source can be done rather rapidly



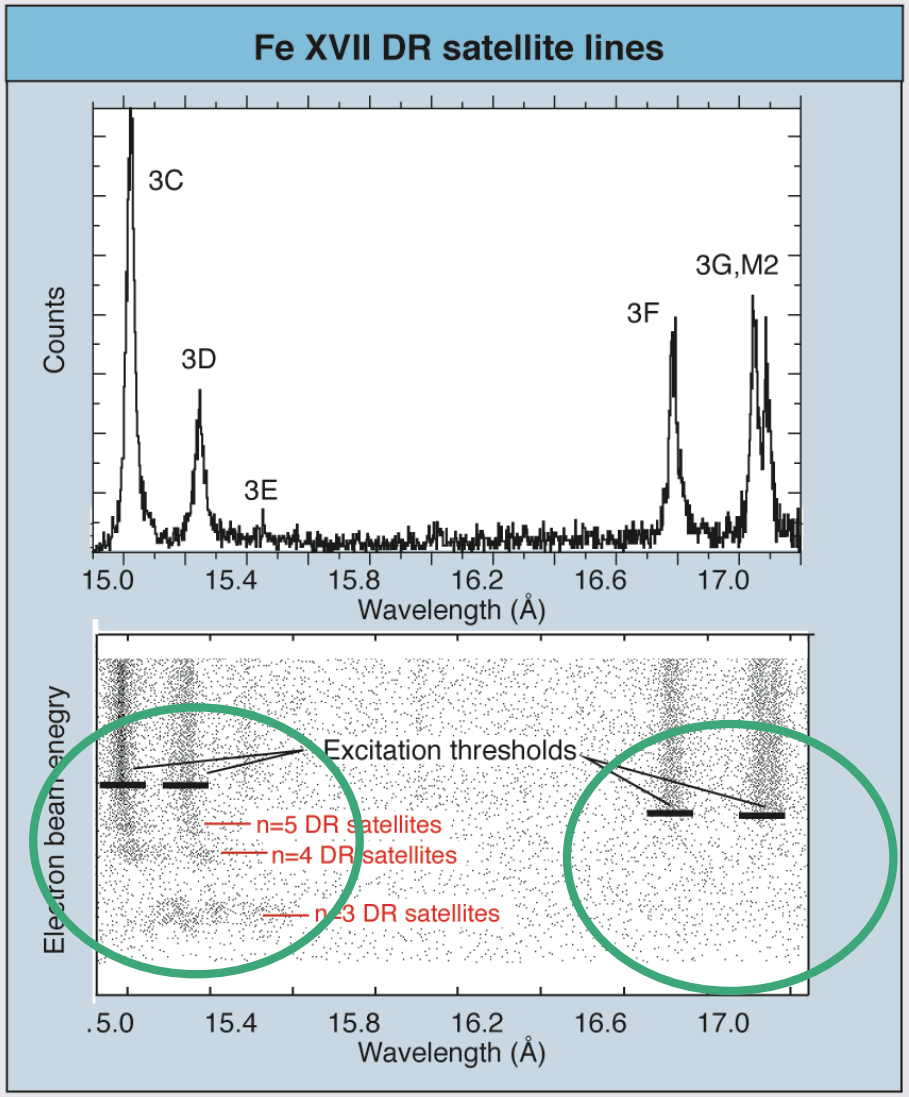
The next experiments are planned for the week of February 9, 2011 on the Linear Coherent Light Source (LCLS) at SLAC

Fe XVI lines produced by dielectronic recombination (DR)

$1s^2 2s^2 2p^6 + e^-$

$\rightarrow 1s^2 2s^2 2p^5 3\ell n\ell'$

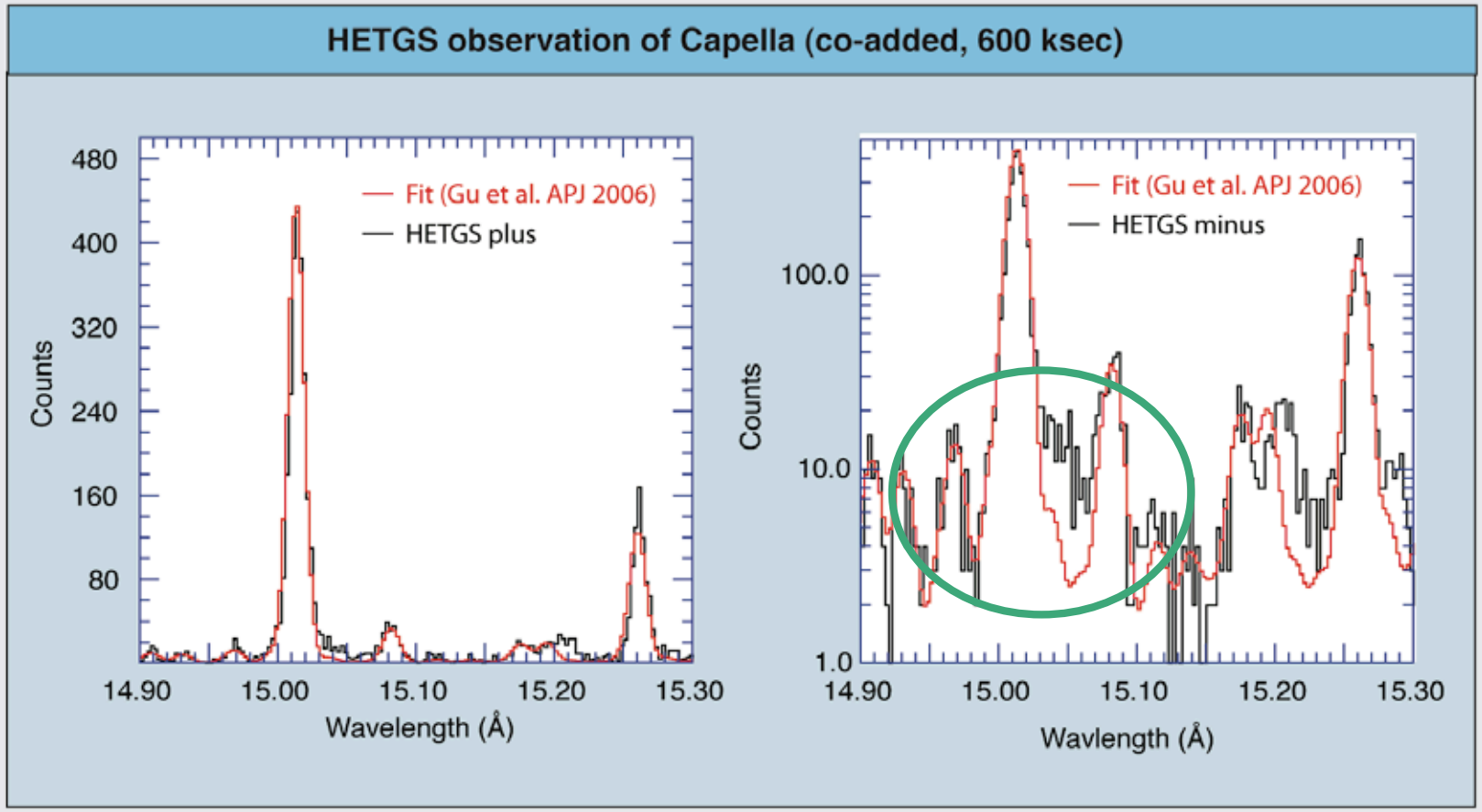
$\rightarrow 1s^2 2s^2 2p^6 n\ell' + h\nu$



3d —> 2p DR satellite lines

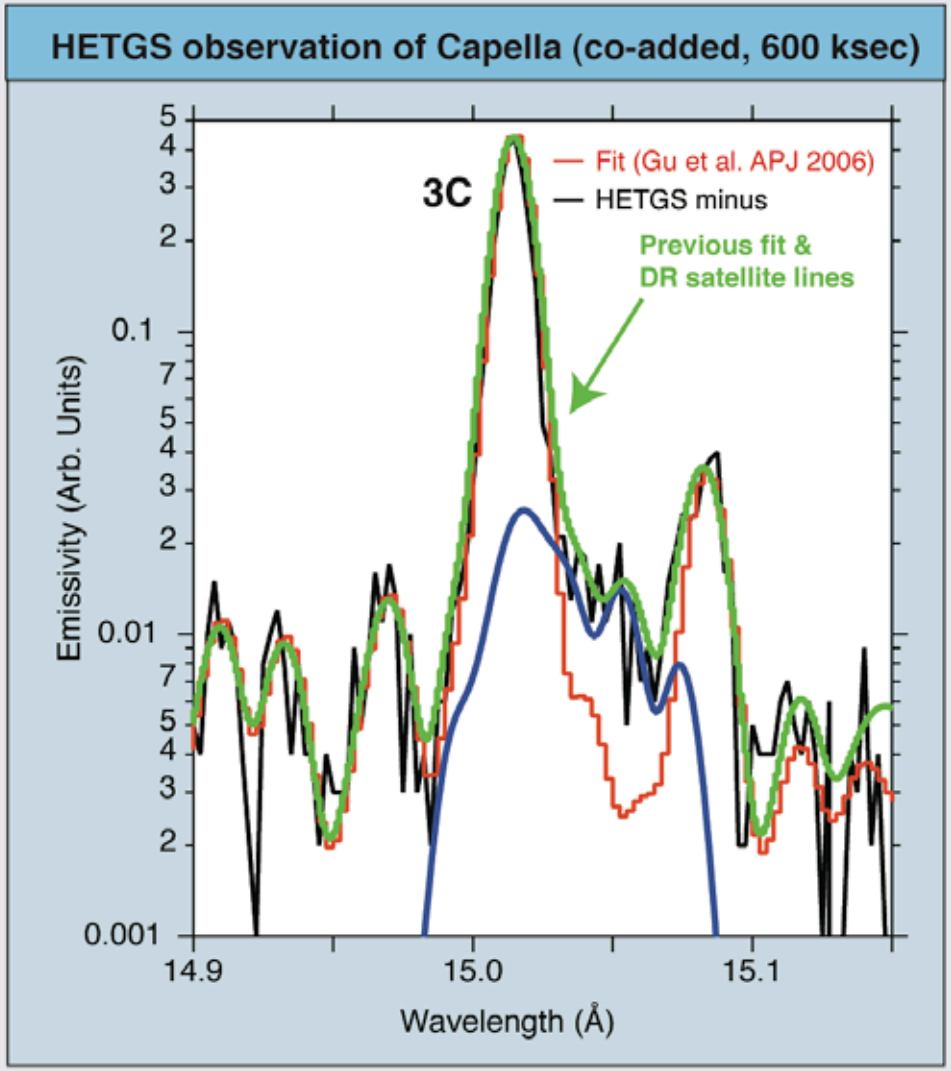
No 3s —> 2p DR satellite lines

Fe XVI DR satellites are important for Chandra HETGS observations



Excess flux, not fitted with FAC/APEC, is seen next to FeXVII line 3C

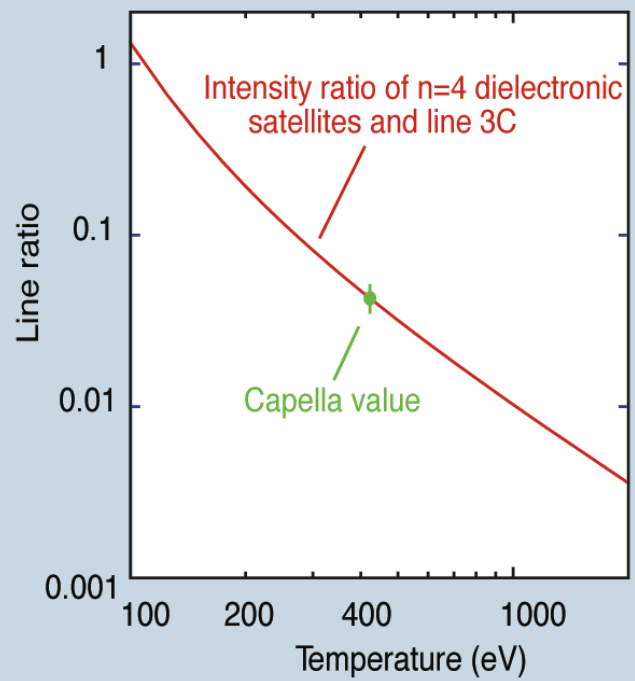
The DR satellite lines are needed for best fit



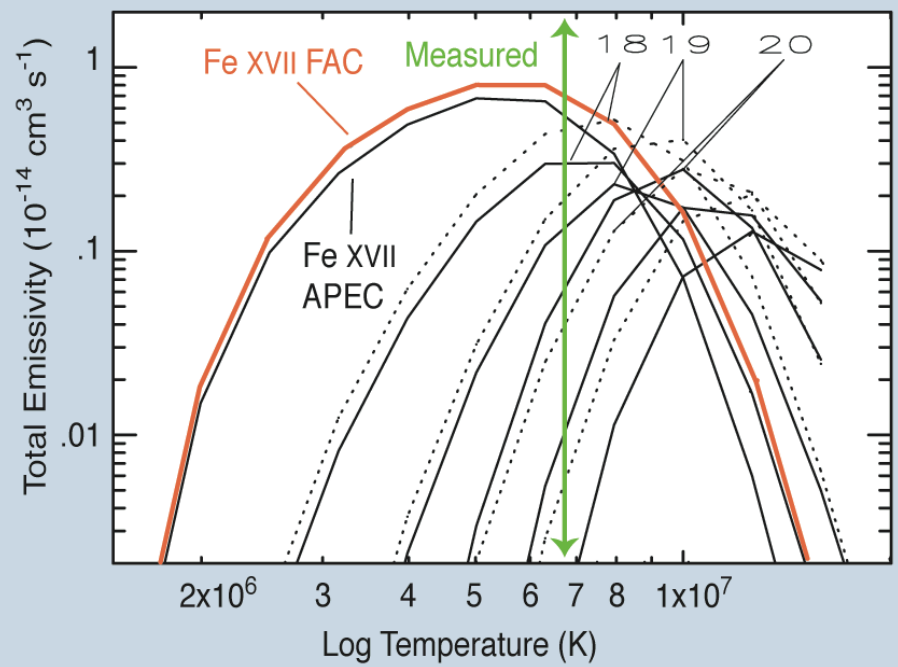
Beiersdorfer et al., Bull. AAS 42, 685 (2010)

The DR satellite line intensity depends on temperature and can be used to get the Fe XVII emission temperature

Temperature dependence of DR lines



Fe XVII emission occurs above predicted peak T

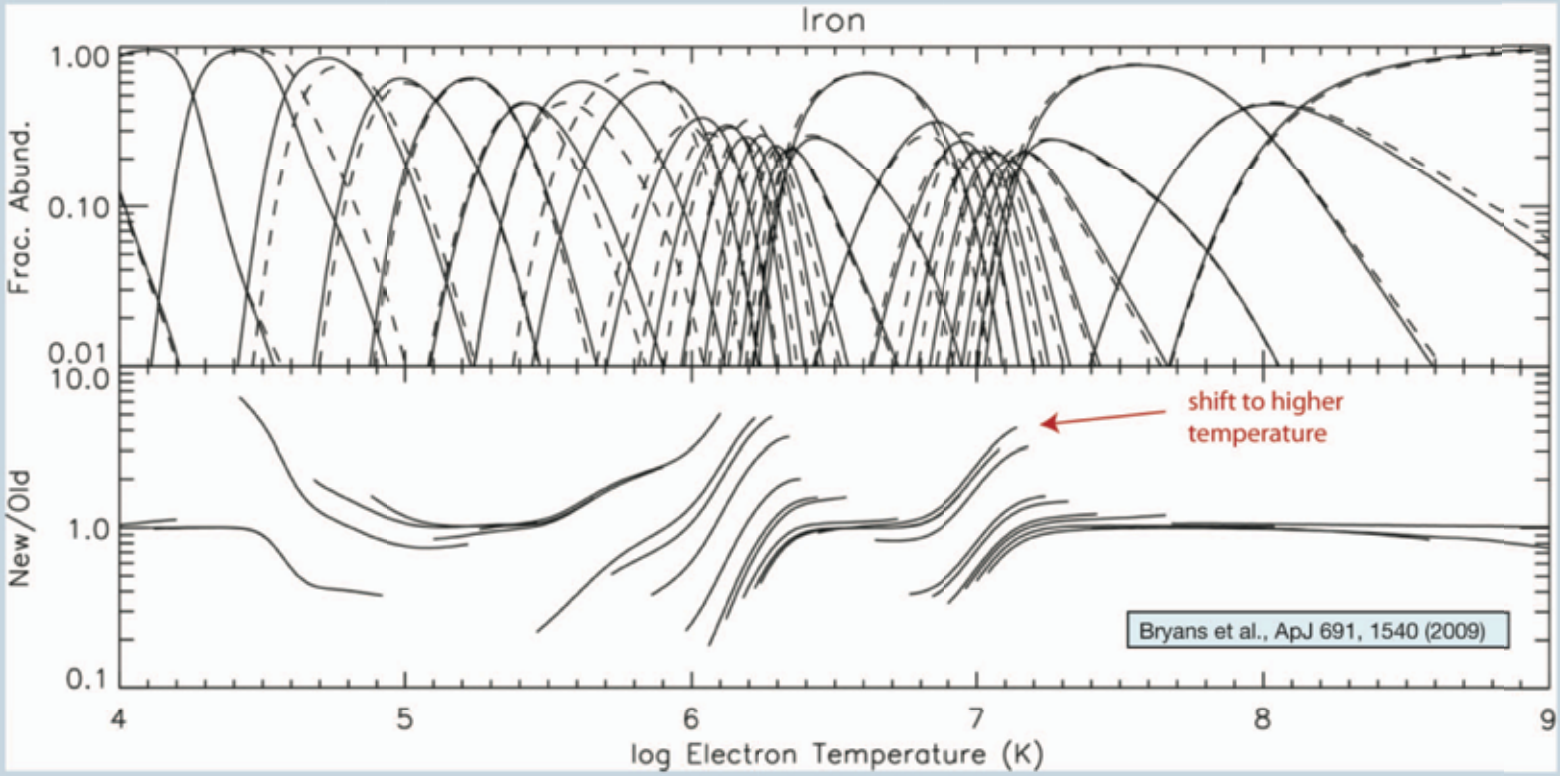


Beiersdorfer et al., Bull. AAS 42, 685 (2010)

The DR method is very potent and yields log(T)=6.67 ±0.026 K

Ionization fractions are also being investigated theoretically and experimentally

New calculations of Fe ionization fraction vs T compared to Mazzotta et al.



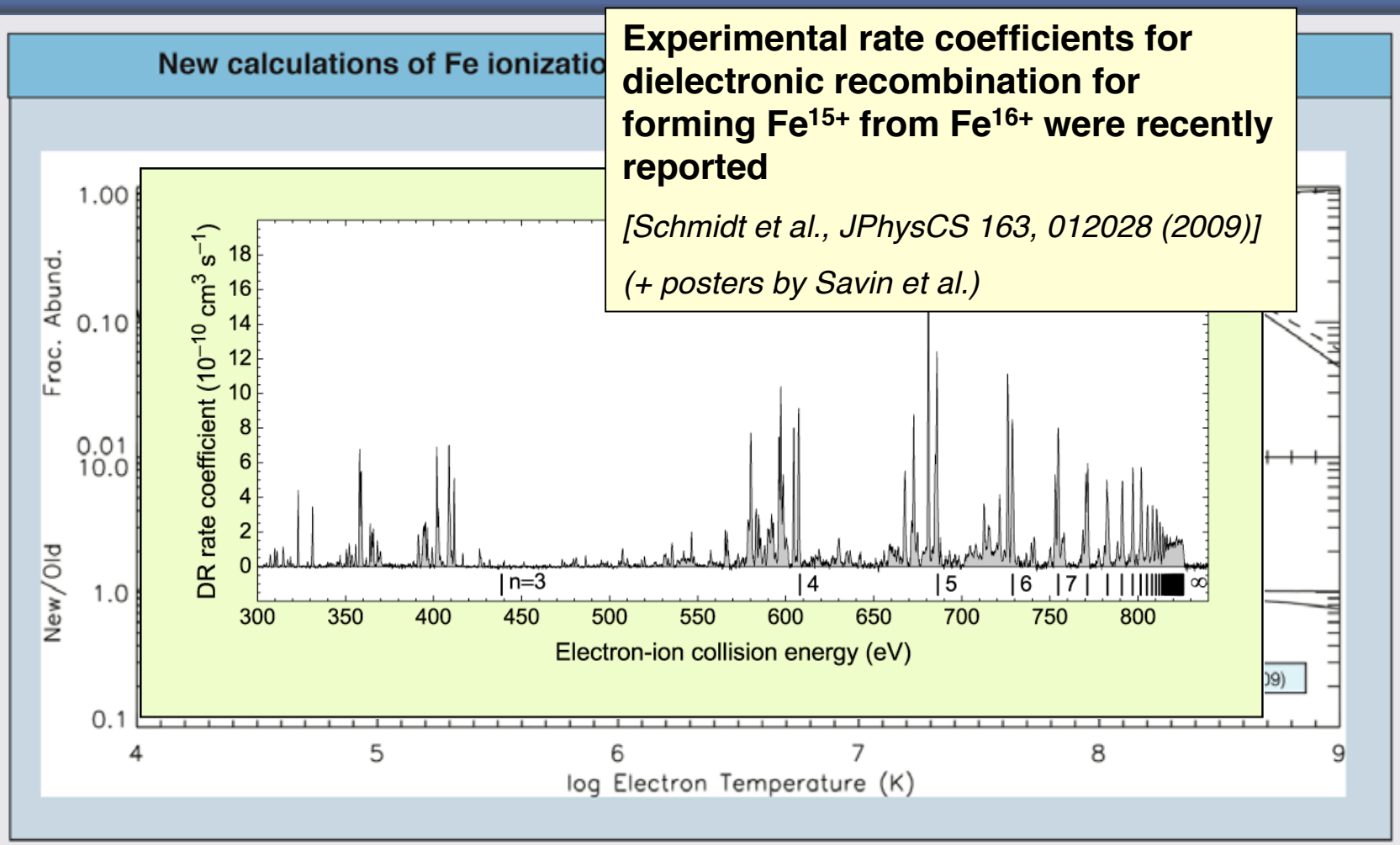
The new calculated ionization fractions have shifted considerably

Ionization fractions are also being investigated theoretically and experimentally

Experimental rate coefficients for dielectronic recombination for forming Fe^{15+} from Fe^{16+} were recently reported

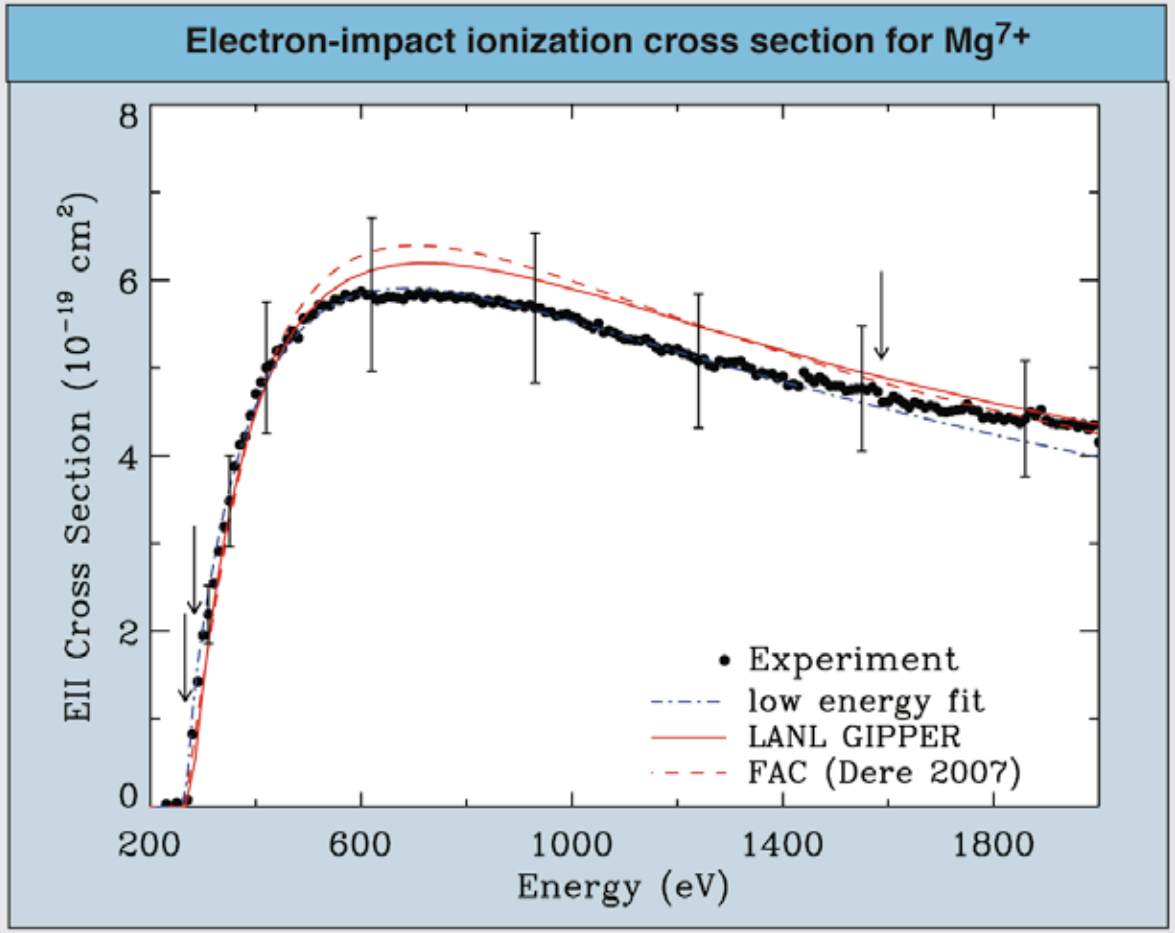
[Schmidt et al., JPhysCS 163, 012028 (2009)]

(+ posters by Savin et al.)



The new calculated ionization fractions have shifted considerably

Storage ring measurements provide new rates for both ionization and recombination

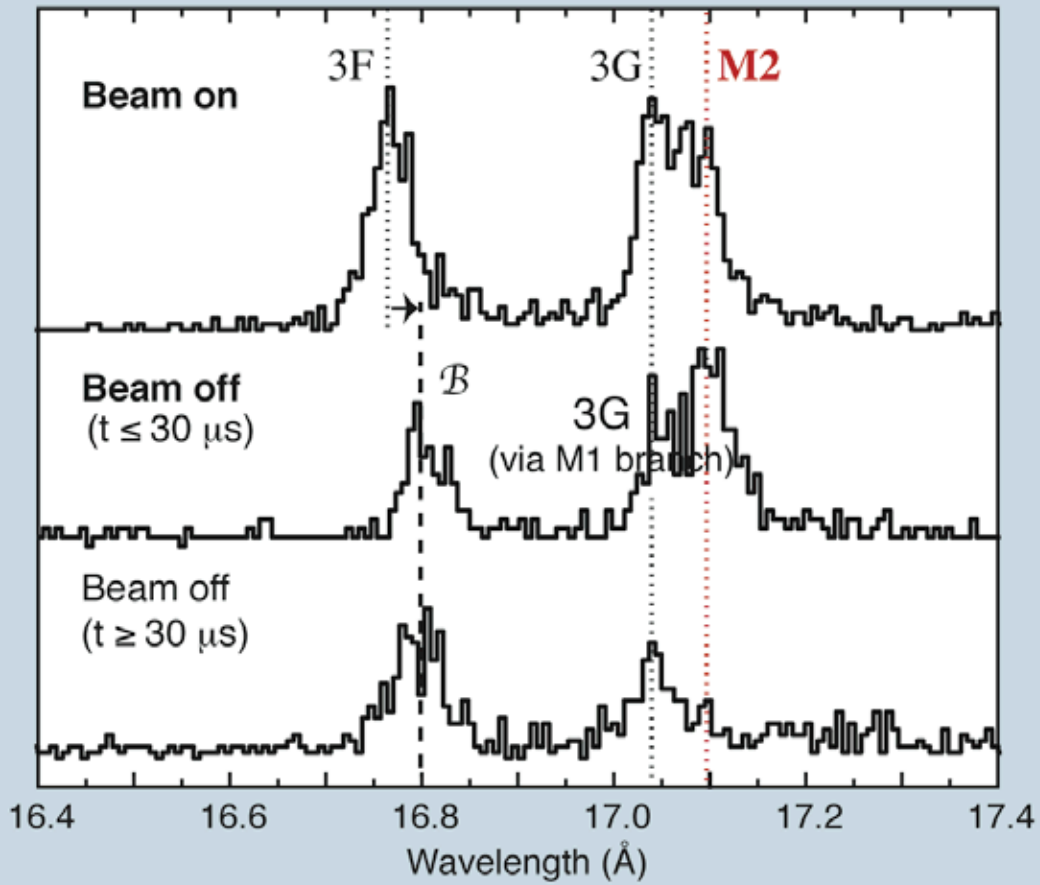


Hahn et al.,
ApJ 711, 1166 (2010)

Ionization and recombination rates are both needed to determine the ionization balance

Time-dependent measurements of the Fe XVII spectrum allow us to measure radiative lifetimes

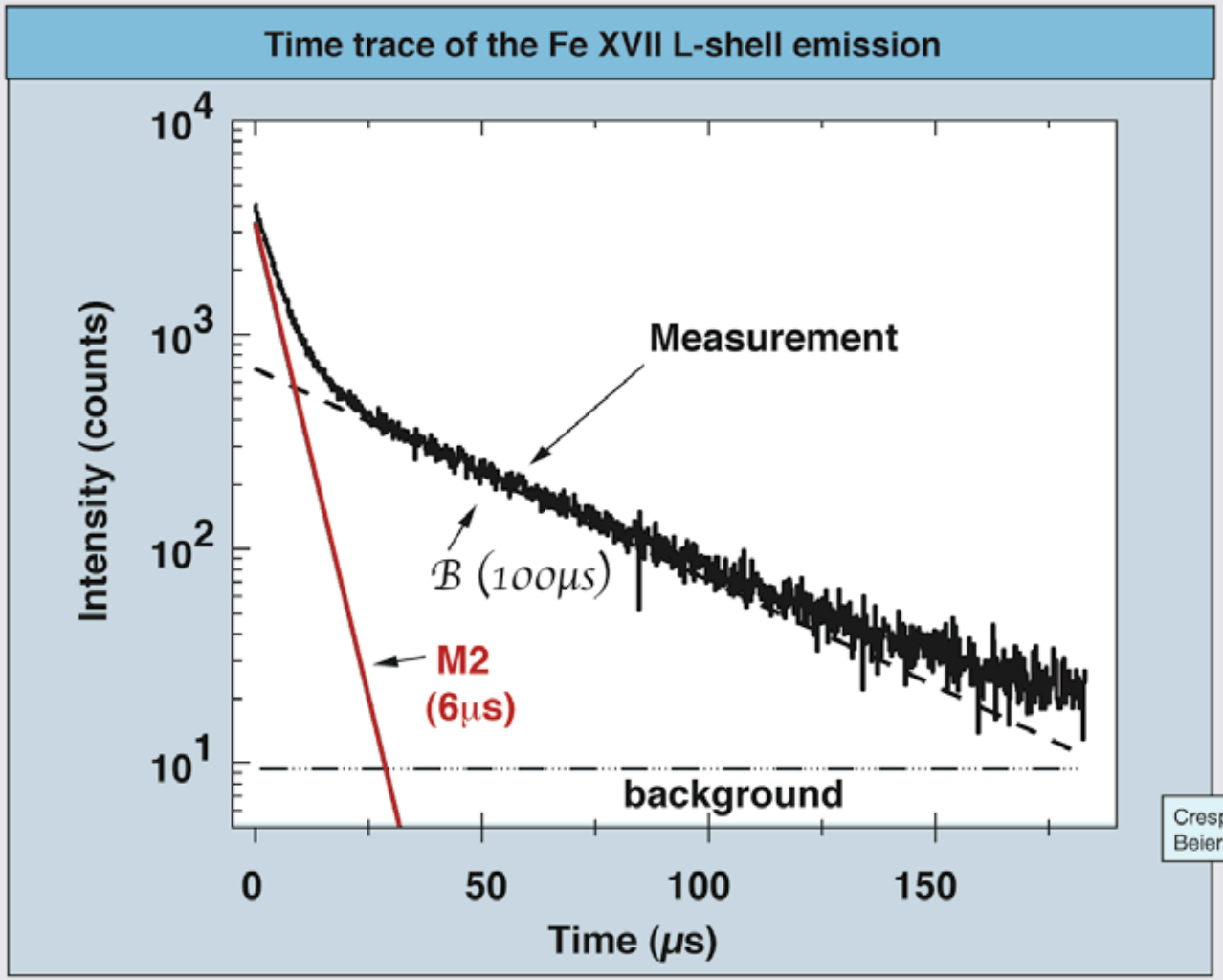
Fe XVII spectrum showing the 3s→2p transitions



Crespo López-Uruttia & Beiersdorfer, ApJ 721, 576 (2010)

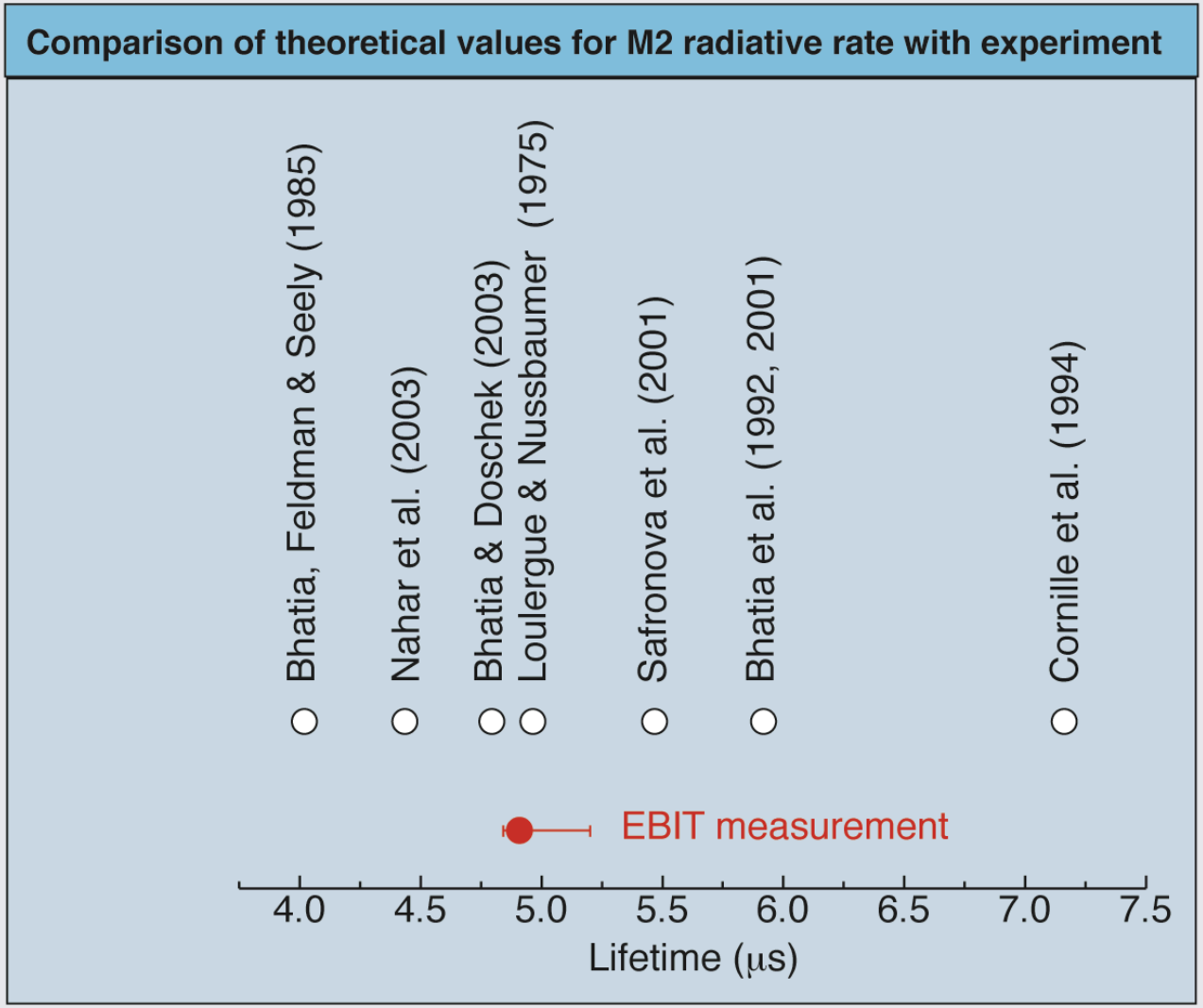
The line ratios clearly change as a function of time

Time-dependent measurements of the Fe XVII spectrum allow us to measure radiative lifetimes



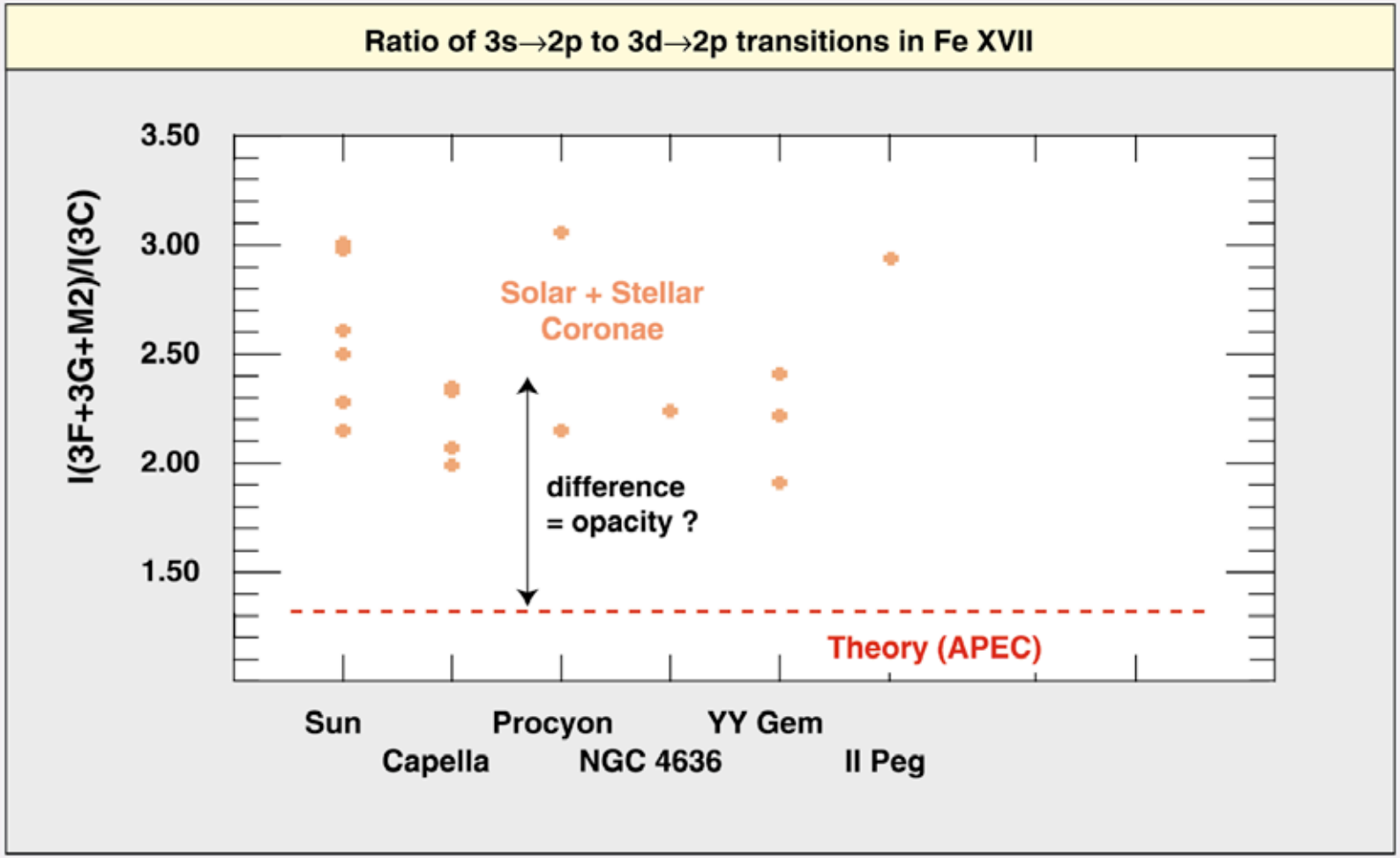
Crespo López-Uruttia & Beiersdorfer, ApJ 721, 576 (2010)

The measurement distinguishes among a spread of theoretical results for the Fe XVII M2 radiative rate



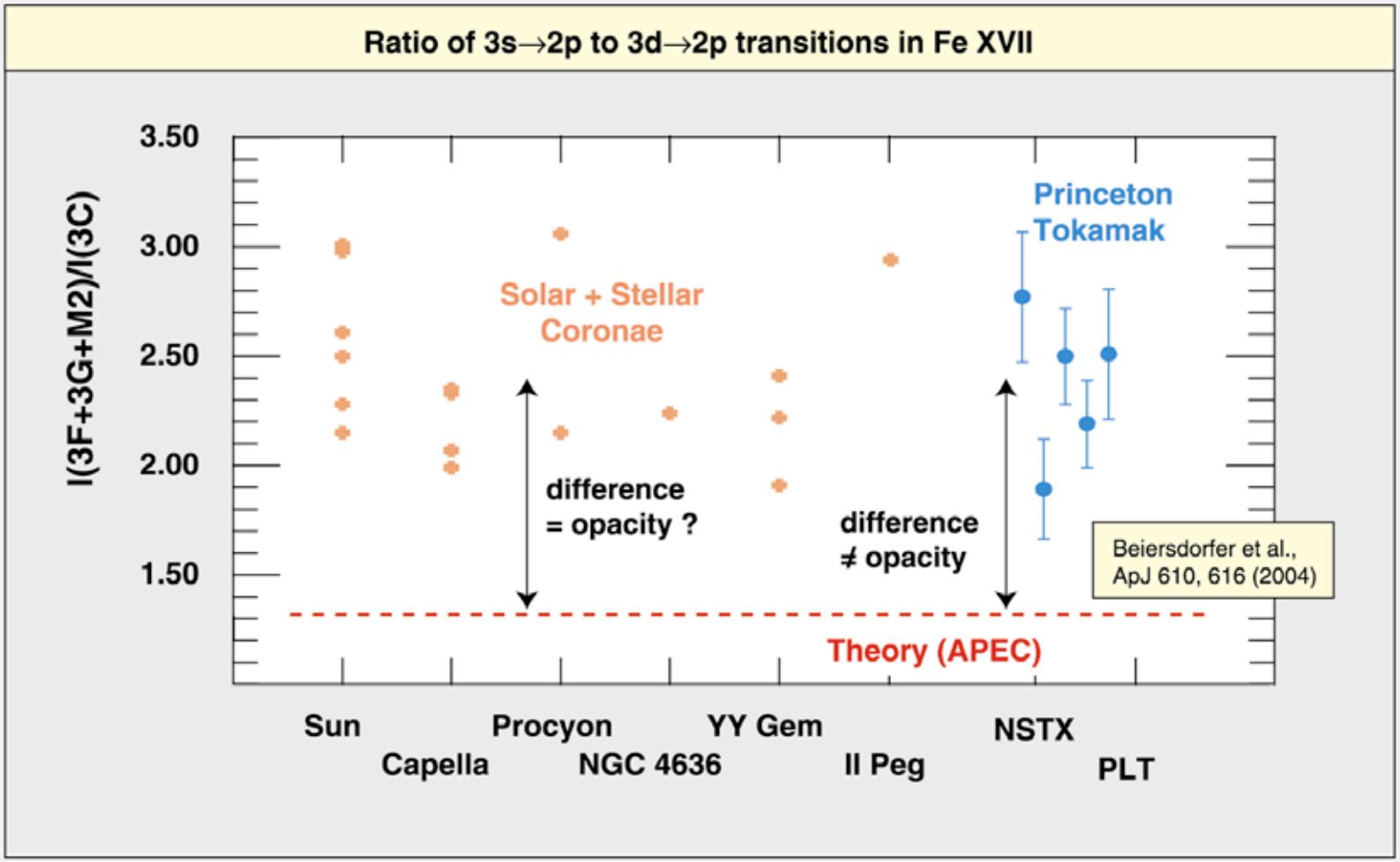
Crespo López-Uruttia & Beiersdorfer, ApJ 721, 576 (2010)

Astrophysical Fe XVII spectra have been puzzling



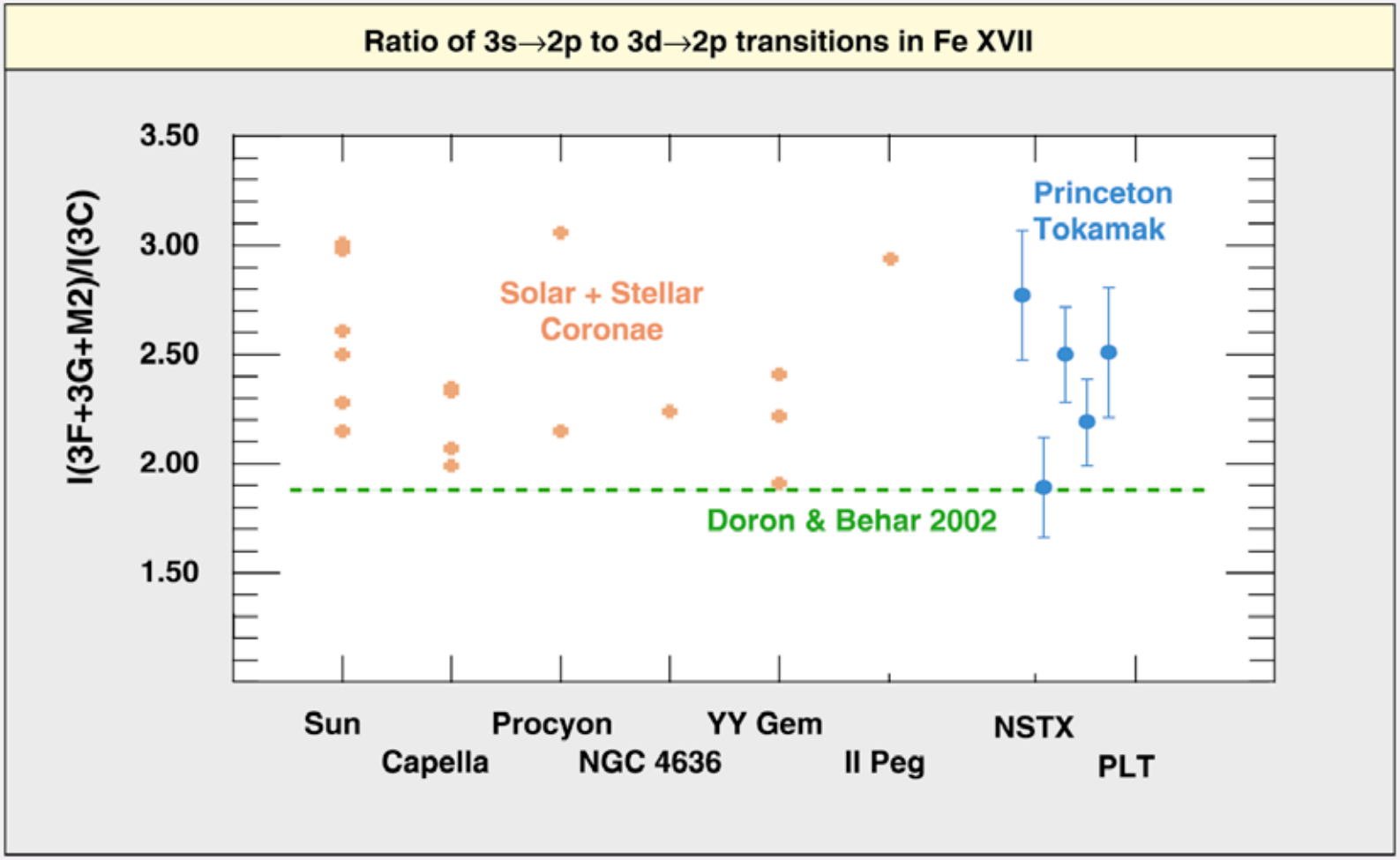
The difference between observed line ratios and spectral calculations was attributed to opacity effects

Astrophysical Fe XVII spectra have been puzzling



Our tokamak and EBIT laboratory data reproduced space observations and showed that spectral models are inadequate

Astrophysical Fe XVII spectra have been puzzling



Most recent models still miss the data by 20–30%

Numerous theoretical papers have tried to address these issues since the first measurements in the 70!s

PHYSICAL REVIEW A **71**, 012717 (2005)

Resolution of the long-standing overprediction of the resonance to intercombination line-intensity ratio in mid-Z neonlike ions

Kevin B. Fournier and Stephanie B. Hansen
Lawrence Livermore National Laboratory, P.O. Box 808, L-473, Livermore, California 94550, U
(Received 15 September 2004; published 31 January 2005)

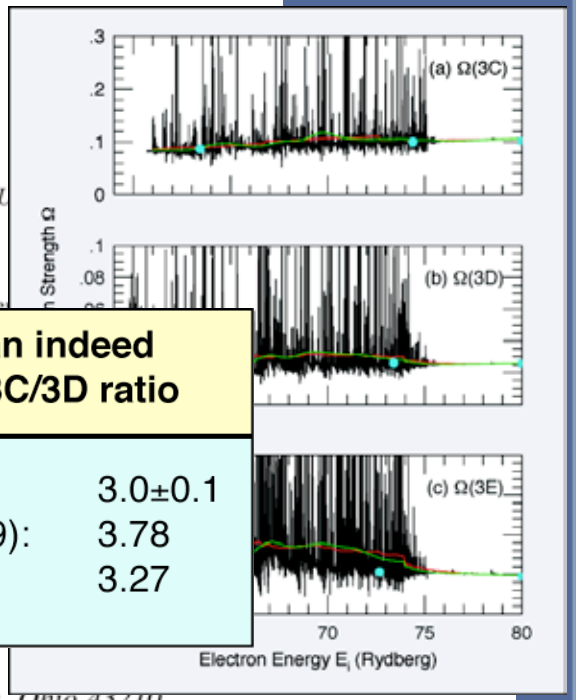
The Ne-like resonance $2p^6\,{}^1S\,2p^5 3d\,{}^1P\,(3C)$ to intercombination $2p^6\,{}^1S\,2p^5 3d\,{}^3D\,(3D)$ line-inte
tio, $R(3C/3D)$
structure and
physics codes
coronal-density

VOLUME 89, NUM

Influ

Guo Xin Chen and Anil K. Pradhan
Department of Astronomy, The Ohio State University, Columbus, Ohio 43210
(Received 24 January 2002; published 17 June 2002)

New theoretical results from large-scale relativistic close coupling calculations reveal the precise effect of resonances in collisional excitation of x-ray lines of Ne-like Fe XVII. By employing the Breit-Pauli R-matrix method and an 89-level eigenfunction expansion, including up to $n = 4$ levels, significant resonance enhancement of the collision strengths of forbidden and intercombination transitions is shown. The present results should help resolve long-standing discrepancies; in particular, the present line ratios of three benchmark diagnostic lines $3C$, $3D$, and $3E$ at 15.014, 15.265, and 15.456 Å, respectively, are in excellent agreement with two independent measurements on electron-beam ion traps. Strong energy dependence in cross sections due to resonances is demonstrated.

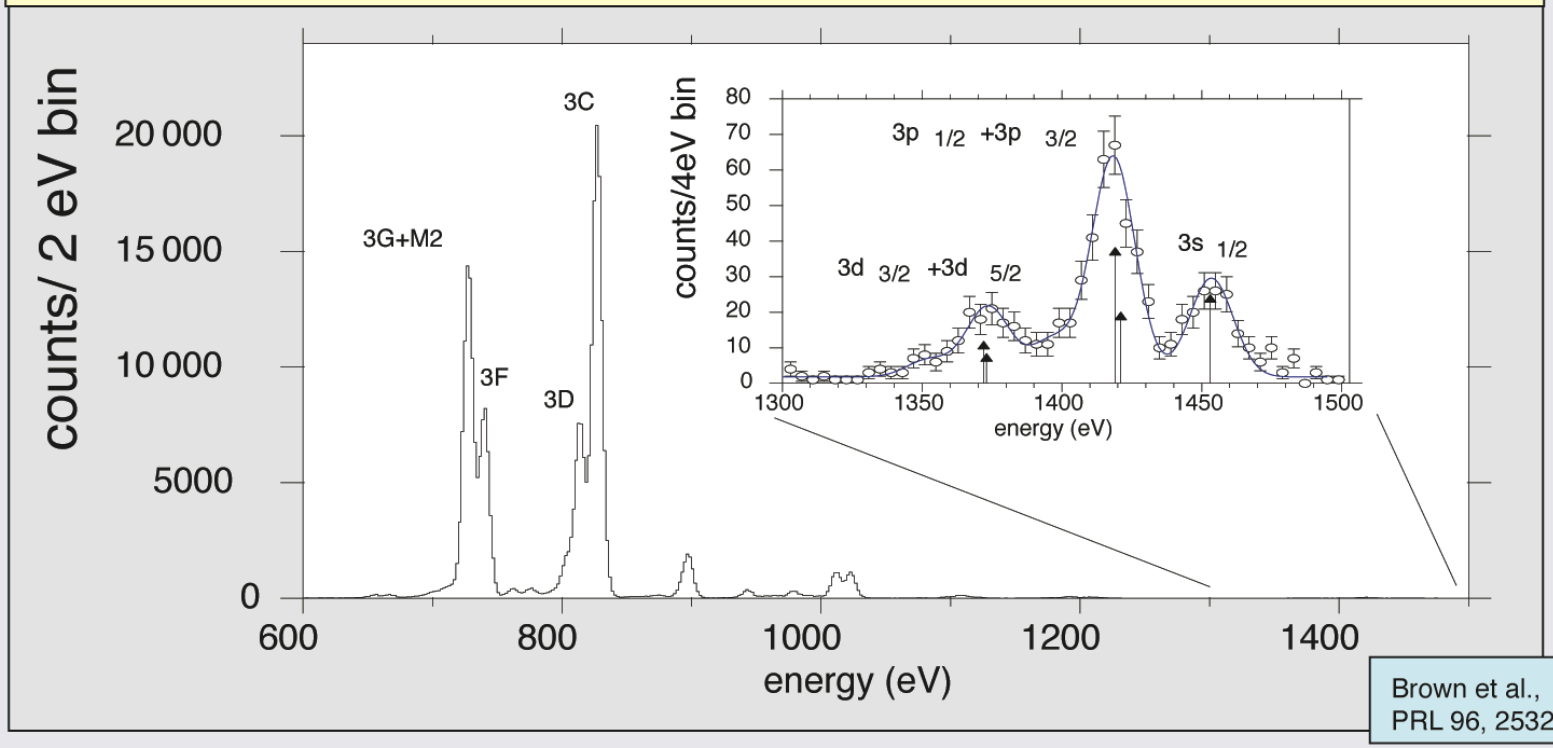


R-matrix calculations of GX Chen and Pradhan indeed gave the best agreement with the measured 3C/3D ratio

EBIT value (Brown et al., APJ 1998):	3.0±0.1
Distorted-wave value (Zhang & Sampson 1989):	3.78
R-matrix value (Chen & Pradhan, PRL 2002):	3.27

In 2006 the Livermore group went beyond line ratios and measured excitation cross sections

Fe XVII cross section measurement with the NASA Goddard XRS X-ray calorimeter



Brown et al., PRL 96, 253201 (2006)

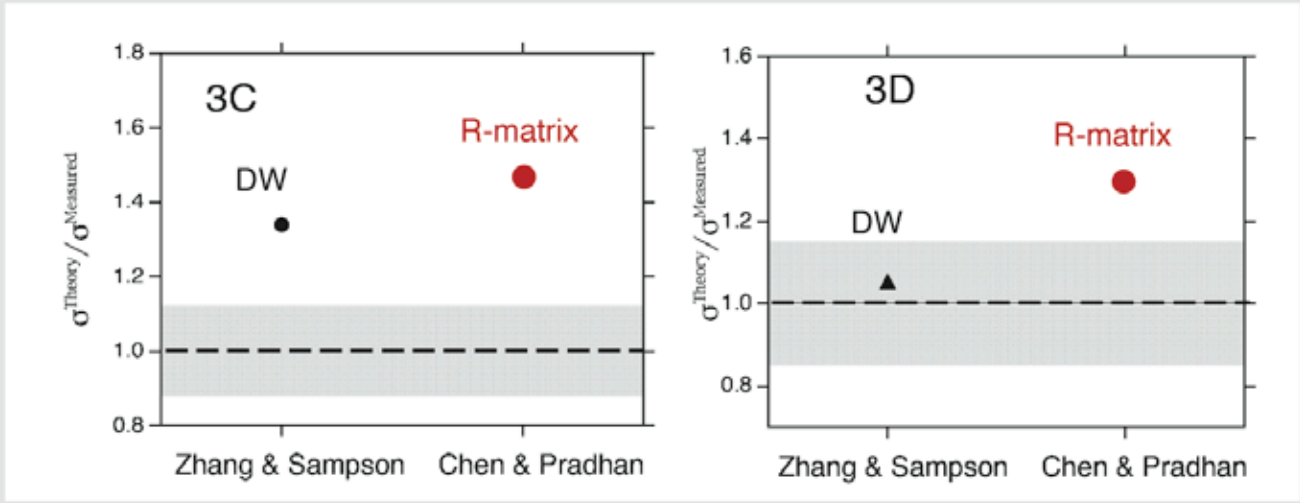
The Fe XVII excitation cross section measurements on Livermore's EBIT-I facility provided crucial information not provided by line ratio measurements

The Livermore cross section measurements raised the bar for theory

R-matrix calculations of GX Chen and Pradhan indeed gave the best agreement with the measured 3C/3D ratio

EBIT value (Brown et al., APJ 1998):	3.0±0.1
Distorted-wave value (Zhang & Sampson 1989):	3.78
R-matrix value (Chen & Pradhan, PRL 2002):	3.27

Comparison of calculated with measured cross sections



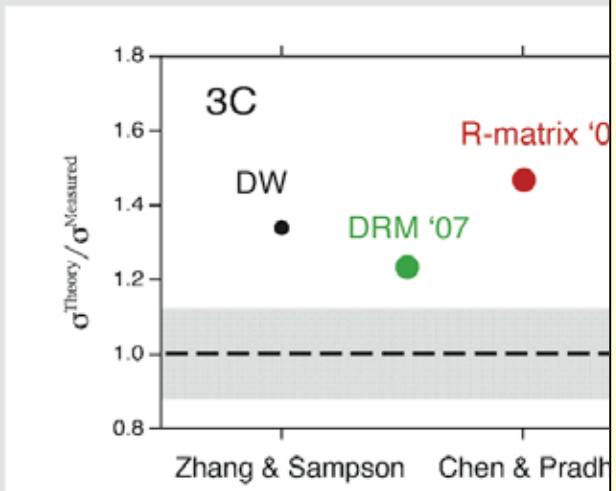
The disagreement in the cross sections is actually worse

A new calculation quickly changed the R-matrix results to values that agree better with measurement

R-matrix calculations of GX Chen and Pradhan indeed gave the best agreement with the measured 3C/3D rati

EBIT value (Brown et al., APJ 1998):	3.0
Distorted-wave value (Zhang & Sampson 1989):	3.7
R-matrix value (Chen & Pradhan, PRL 2002):	3.2

Comparison of calculated



- **A subsequent paper GX Chen confirmed his 2007 calculations and suggest the measured value to be in error**
  [GX Chen, PRA 77, 022701, (2008)]
- **In a companion paper GX Chen finds the theoretical values used for normalization of the measurement to be wrong by 24% - if so, this would bring experiment into agreement with his own numbers**
  [GX Chen, PRA 77, 022703, (2008)]
- **Most recently, GX Chen et al. find that the previous calculations of the X-ray line polarization to be off by 30% or more**
  [GX Chen et al., PRA 79, 062715 (2009)]

The disagreement in the cross sections got smaller

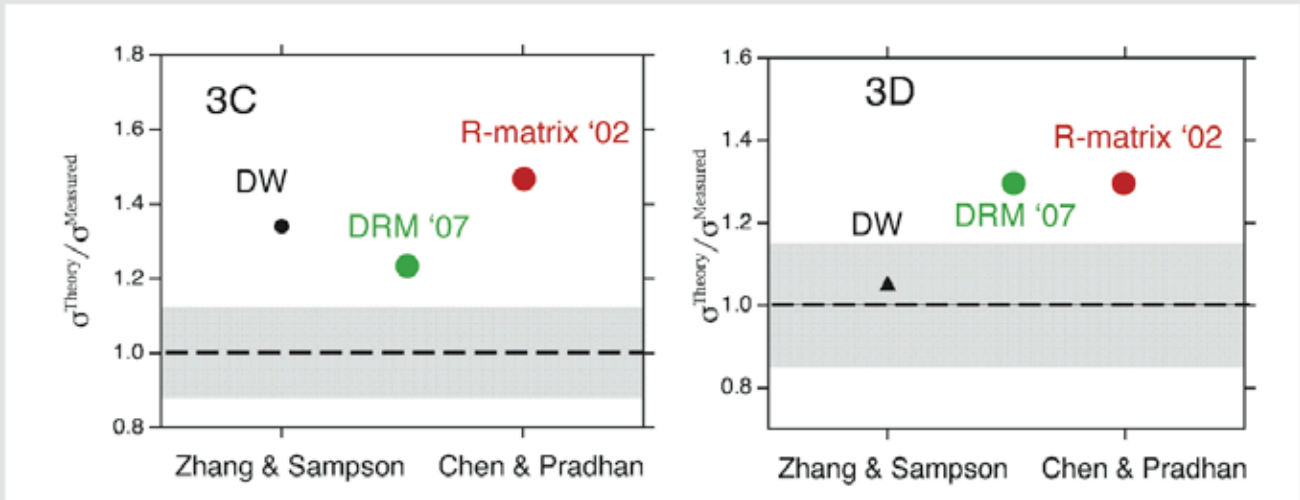
The Fe XVII saga continues: What if GX Chen!s 2007 & 2008 calculations were correct?

R-matrix calculations of GX Chen and Pradhan indeed gave the best agreement with the measured 3C/3D ratio

EBIT value (Brown et al., APJ 1998):	3.0±0.1
Distorted-wave value (Zhang & Sampson 1989):	3.78
R-matrix value (Chen & Pradhan, PRL 2002):	3.27
Dirac R-matrix value (Chen, PRA 76 2007):	**2.74**

Measured ratio = 2.98

Comparison of calculated with measured cross sections



These calculations would reproduce the measured cross sections, but they would contradict the line ratio measurements

MF Gu!s paper hints at what aspect of theory needs to be improved

arXiv:0905.0519v1 [astro-ph.SR] 5 May 2009

New Benchmark of X-ray Line Emission Models of Fe XVII

M. F. Gu

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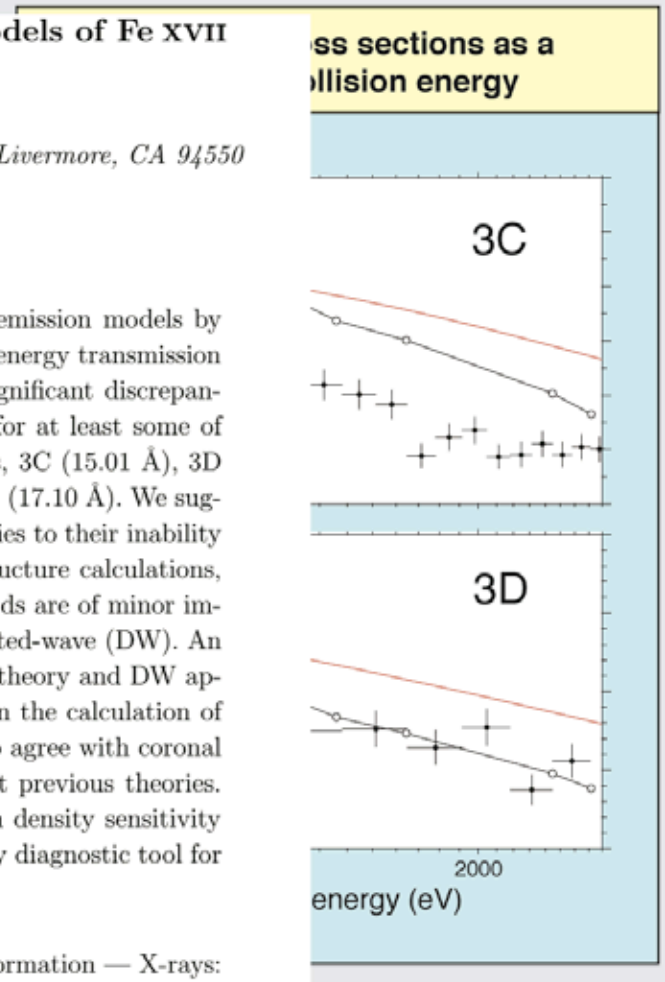
ABSTRACT

We review the accuracy of existing Fe XVII X-ray line emission models by comparing them with an extensive analysis of *Chandra* high energy transmission grating (HETG) observations of stellar coronae. We find significant discrepancies between most theoretical predictions and observations for at least some of the intensity ratios involving the six principal Fe XVII lines, 3C (15.01 Å), 3D (15.26 Å), 3E (15.45 Å), 3F (16.78 Å), 3G (17.05 Å), and M2 (17.10 Å). We suggest that the main problem of most previous theoretical studies to their inability to fully include electron correlation effects in the atomic structure calculations, while any deficiencies in the scattering approximation methods are of minor importance, regardless of it being close-coupling (CC) or distorted-wave (DW). An approximate method based on the many-body perturbation theory and DW approximation is proposed to include such correlation effects in the calculation of collisional excitation cross sections. The results are shown to agree with coronal observations and laboratory measurements better than most previous theories. Using the new atomic data, we then investigate the electron density sensitivity of the M2/3G intensity ratio and provide an improved density diagnostic tool for astrophysical observations.

Subject headings: atomic data — atomic processes — line: formation — X-rays: general



The Fe XVII saga continues

PHYSICAL REVIEW A **79**, 062715 (2009)

Dirac *R*-matrix method for the calculation of x-ray line polarization

G. X. Chen,[1,2] K. Kirby,[1,2] N. S. Brickhouse,[2] T. Lin,[2] and E. Silver[2]
[1]*ITAMP, Harvard–Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138, USA*
[2]*Harvard–Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138, USA*
(Received 9 December 2008; published 30 June 20

We have developed a method within the Dirac *R*-matrix theory to calculate x
from electron-impact excitation to excited-state magnetic sublevels of complex
the excitation of two well-known x-ray lines of Fe XVII, 3*C* (λ=15.015 Å) an
strong resonance effects which contribute to complicated energy dependence i
show large differences, up to 30% or more, from earlier theoretical work, and th
experimental measurement of the 3*C* and 3*D* line polarizations and further the

PHYSICAL REVIEW A **82**, 03670

Comment on "Dirac *R*-matrix method for the calcu

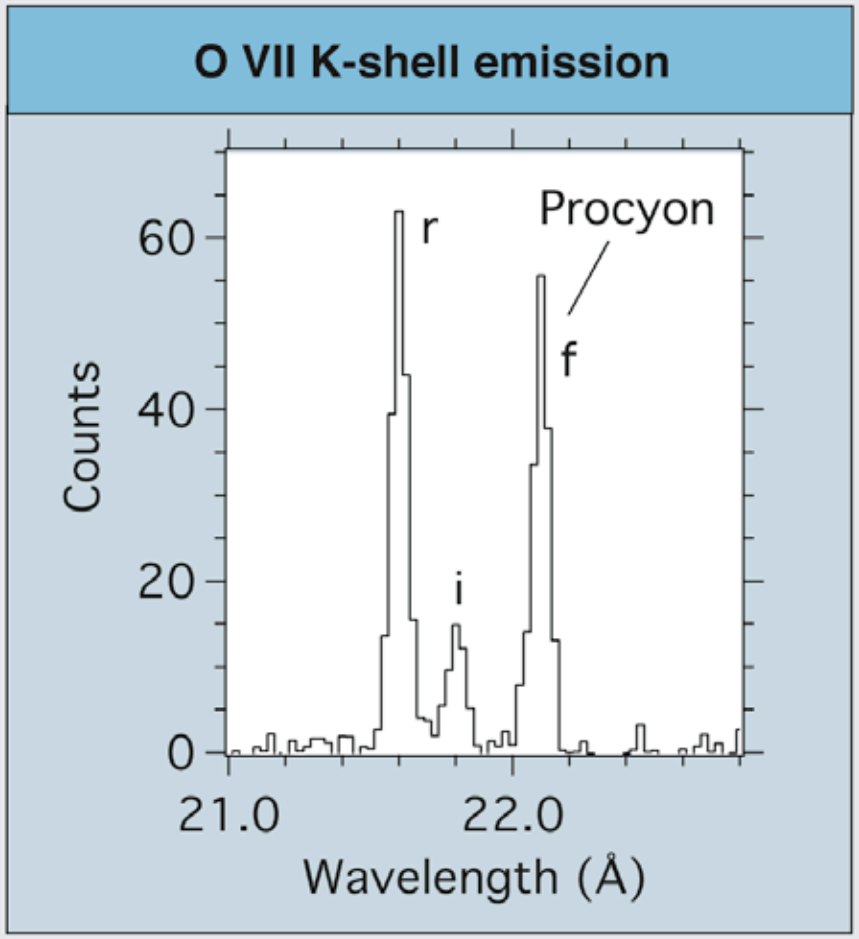
Hong Lin Zhang* and Christopher J. Fontes†
Computational Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

Connor P. Ballance‡
Department of Physics, Auburn University, Auburn, Alabama 36849, USA
(Received 10 May 2010; published 22 September 2010)

In a recent article by Chen *et al.* [Phys. Rev. A **79**, 062715 (2009)], reference is made to magnetic sublevel collision strengths in an earlier relativistic distorted-wave (RDW) article by Zhang *et al.* [Phys. Rev. A **41**, 198 (1990)]. In the former reference, Chen *et al.* carried out Dirac *R*-matrix calculations that suggest the polarization of the 3*C* and 3*D* lines of Fe XVII, which can be computed from the magnetic sublevel collision strengths, differ from RDW results by as much as 20%. We have recently carried out a variety of RDW and Dirac *R*-matrix calculations of the 3*C* and 3*D* polarizations that demonstrate this quantity to be relatively insensitive to the size and details of the atomic model. Moreover, the polarizations obtained from these recent RDW and Dirac *R*-matrix calculations agree well, and they also agree well with the polarizations that can be obtained from the fundamental collision data published by Zhang *et al.* This good agreement between RDW and Dirac *R*-matrix polarizations contradicts the behavior reported by Chen *et al.*

- **Last month Zhang, Fontes & Ballance showed the result of GX Chen et al. to be wrong and reaffirmed the 1990 results of Zhang et al. concerning X-ray line polarization**
  [Zhang et al., PRA 82, 036701, (2010)]

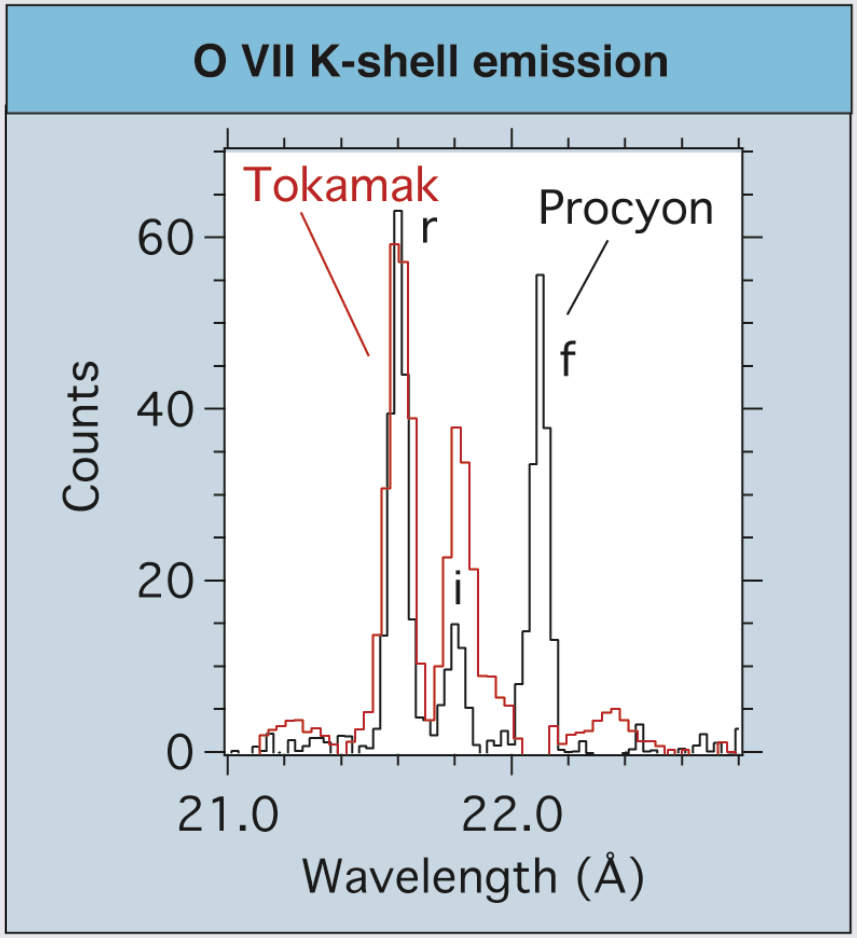
EUV lines also provide crucial electron density diagnostics



Procyon: $n_e \leq 10^{11} cm^{-3}$

EUV lines are used for electron density and temperature diagnostics; emission measures; abundances; velocity measurements.

EUV lines also provide crucial electron density diagnostics

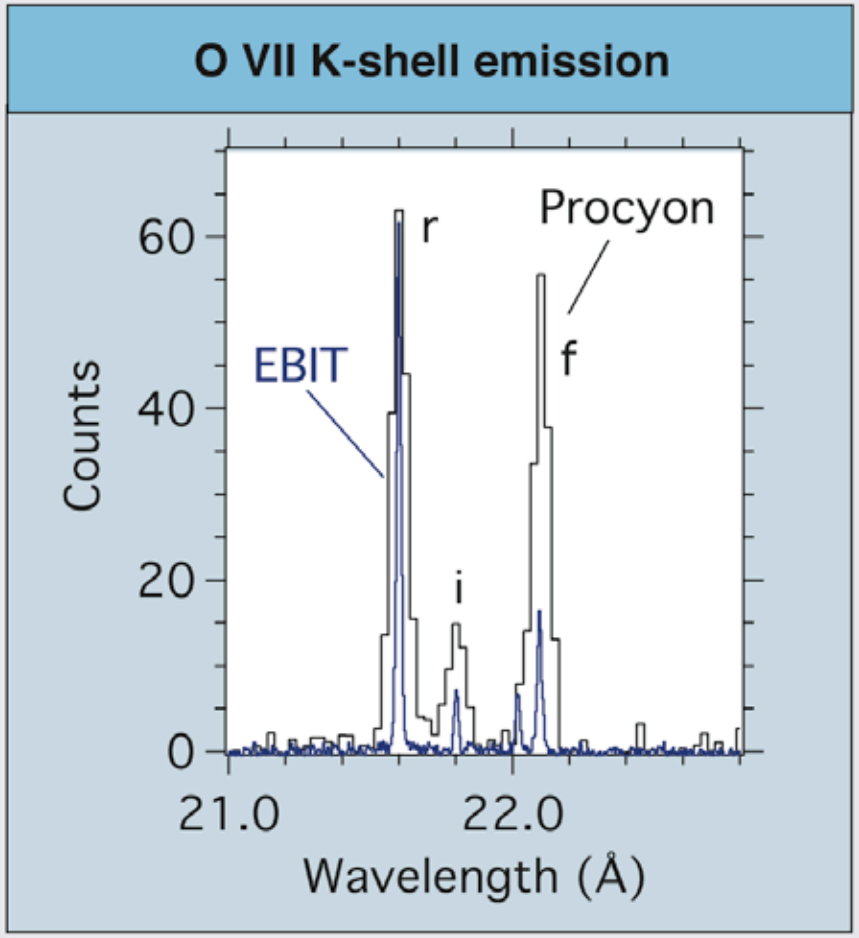


Procyon: $n_e \leq 10^{11} cm^{-3}$

Tokamak: $n_e \geq 10^{13} cm^{-3}$

EUV lines are used for electron density and temperature diagnostics; emission measures; abundances; velocity measurements.

EUV lines also provide crucial electron density diagnostics



Procyon: $n_e \leq 10^{11} cm^{-3}$

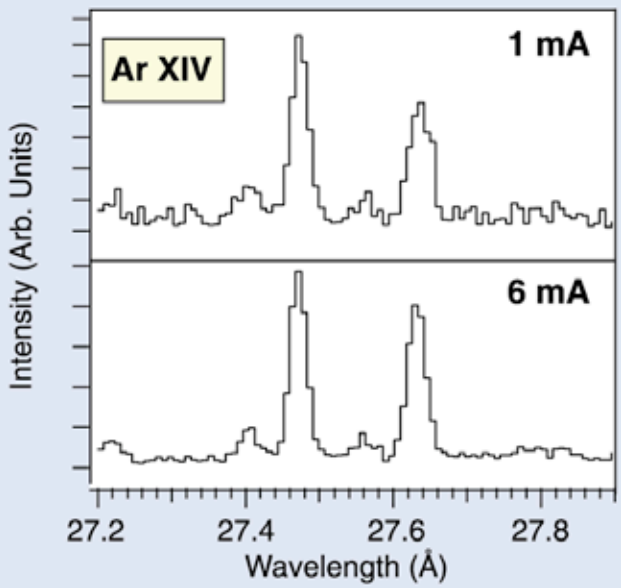
Tokamak: $n_e \geq 10^{13} cm^{-3}$

EBIT: $T \geq 1.5$ keV

EUV lines are used for electron density and temperature diagnostics; emission measures; abundances; velocity measurements.

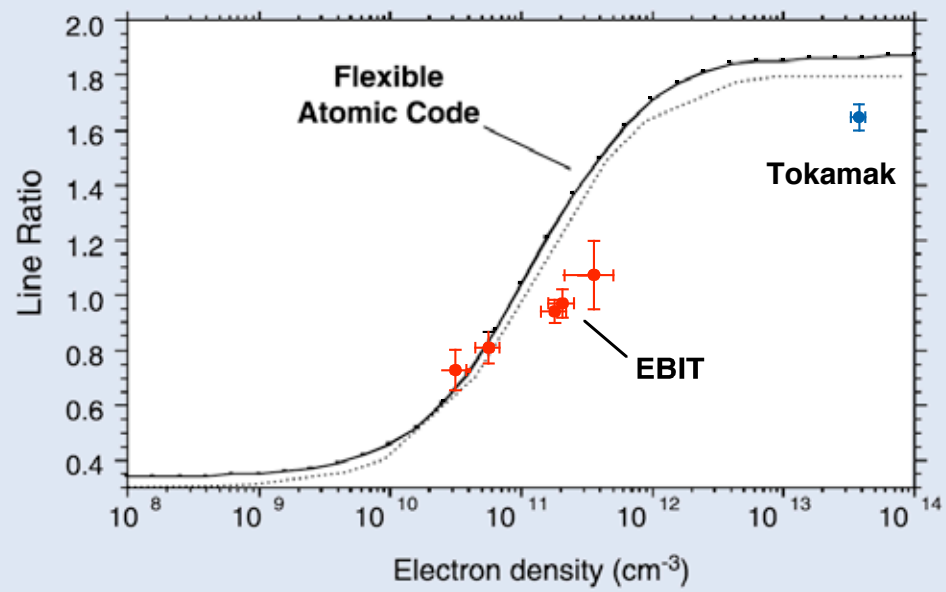
Laboratory calibration of density-sensitive line ratios

3d → 2p transitions in C-like Ar XIV



Chen et al. ApJ 625, 1045 (2005)

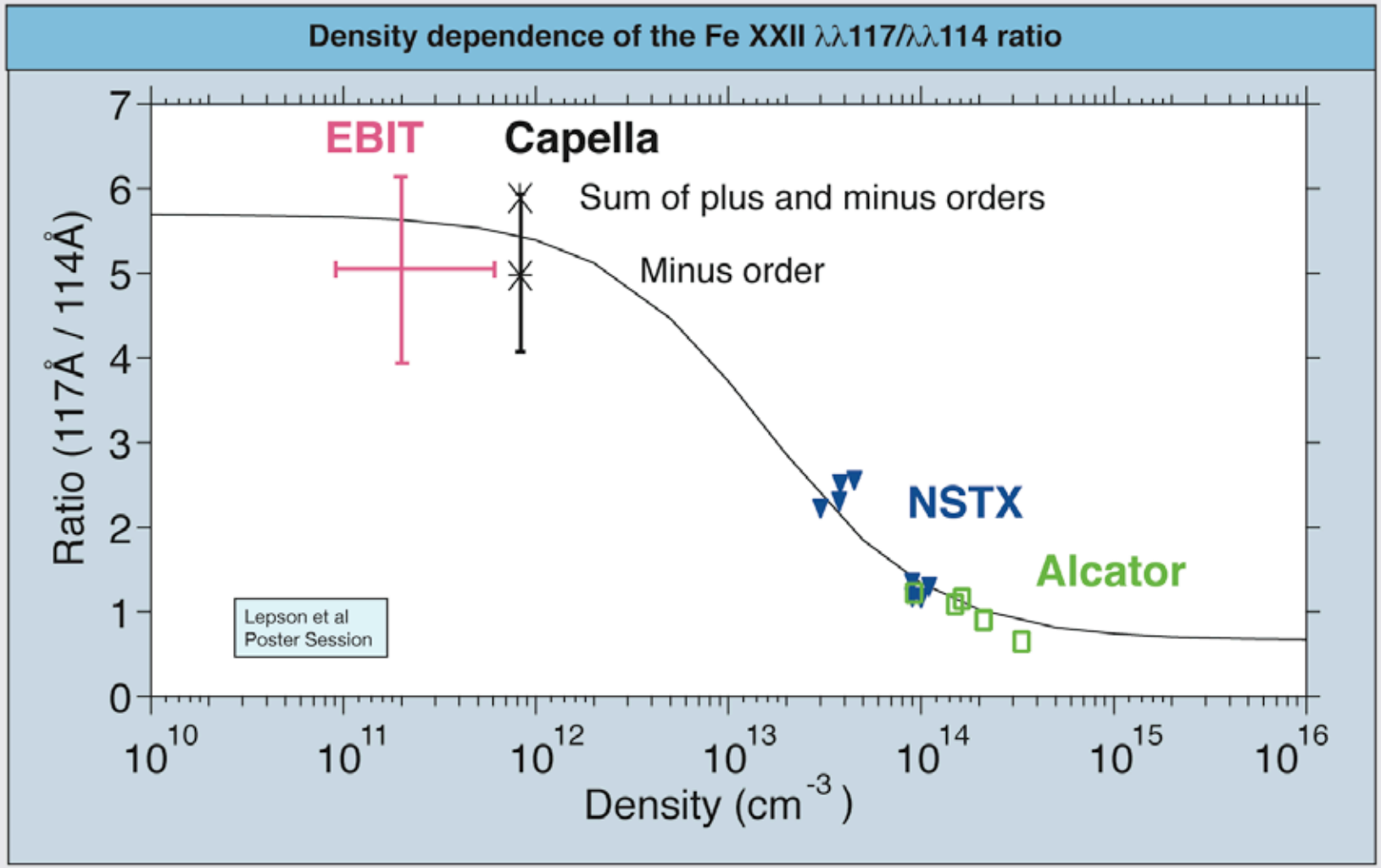
Laboratory measurements versus theory



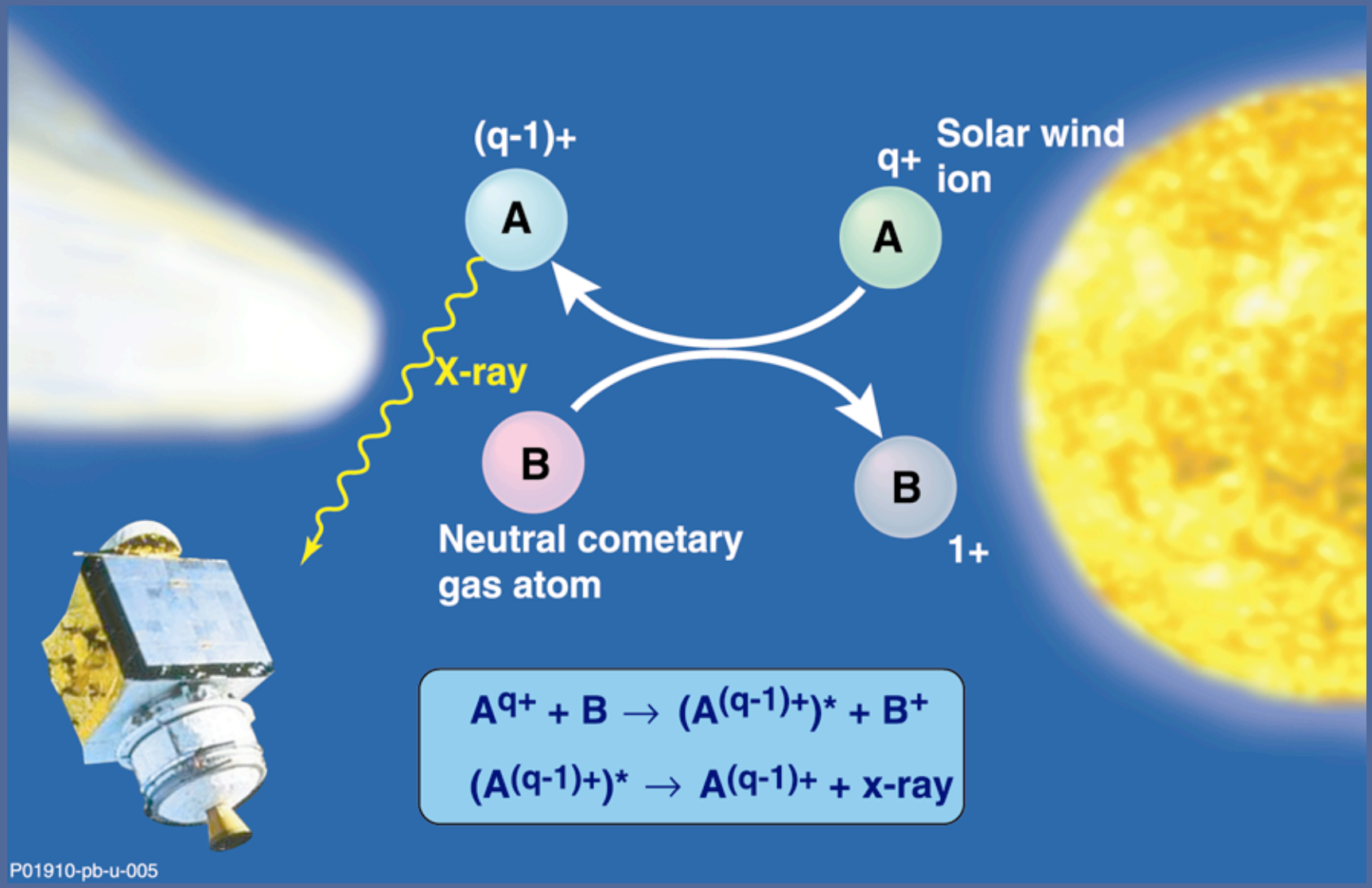
Lepson et al., Can. J. Phys 86, 175 (2008)

Laboratory data spans multiple decades of density

Laboratory calibration of density-sensitive line ratios: Comparison with Capella LETGS observation



Charge exchange between heavy solar ions and neutrals in a comet!s coma



Some recent articles on charge exchange

Cross sections

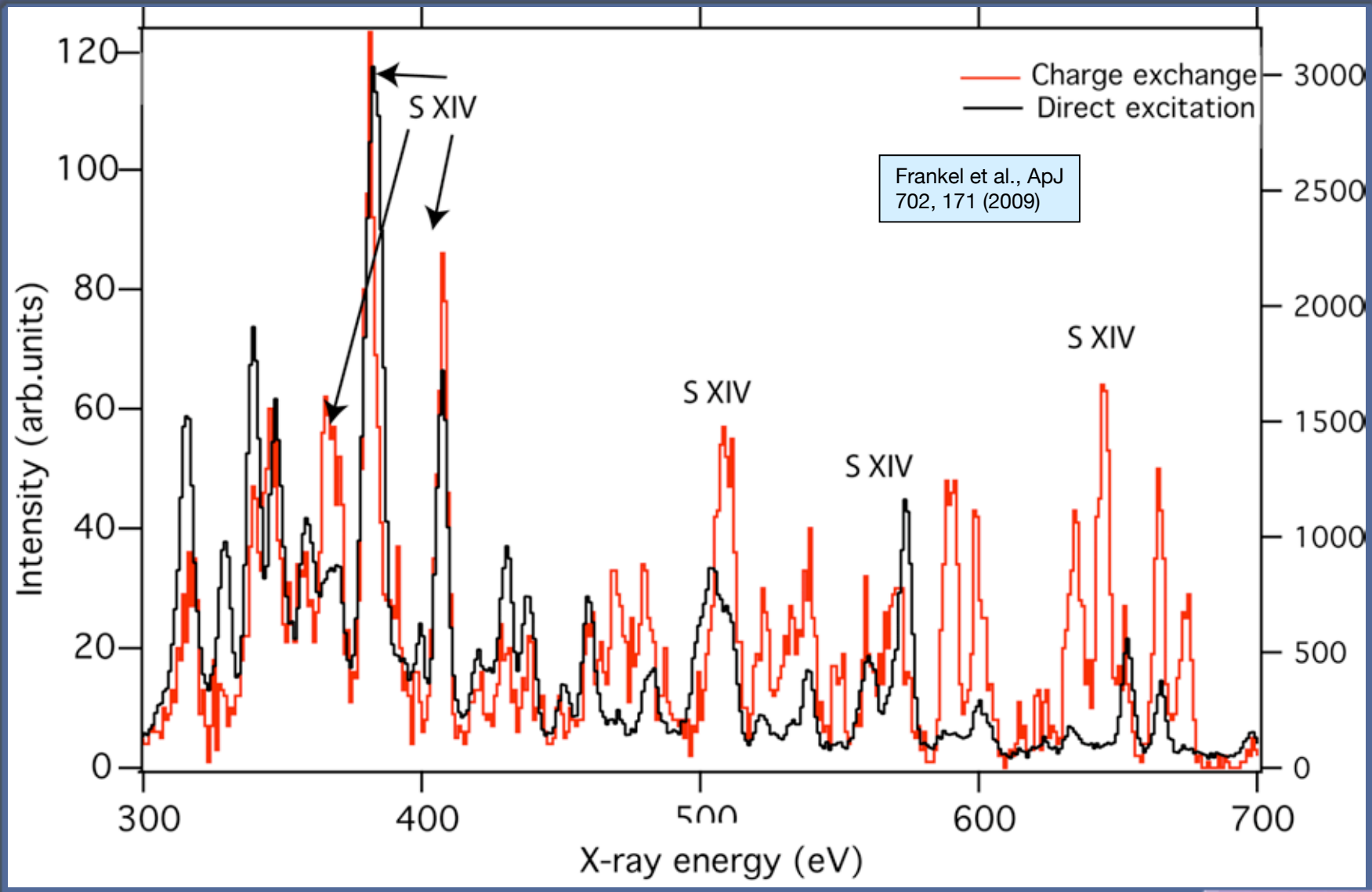
- **C^{q+}, O^{q+}, Ne^{q+} ions colliding with H_2O, CO, and CO_2** *[Mawhorter et al., PRA 75, 032704 (2007)]*
- **C^{q+}, N^{q+}, O^{q+} ions colliding with CH_4** *[Djuric et al., ApJ 679, 1661 (2008)]*
- **Fe^{q+} ions colliding with CO and CO_2** *[Simcic et al., PRA 81, 062715 (2010)]*
- **Fe^{q+} ions colliding with H_2O** *[Simcic et al., ApJ 722, 485 (2010)]*

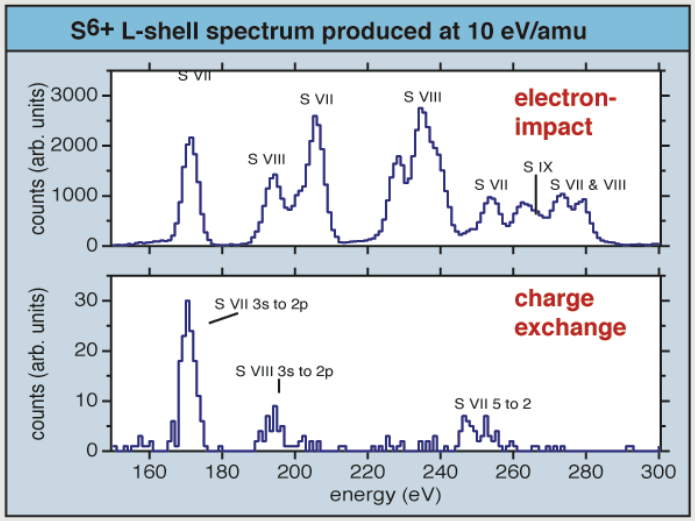
X-ray spectra

- **Fe^{q+} ions colliding with N_2** *[Beiersdorfer et al., ApJ 672, 726 (2008)]*
- **S^{10+}, S^{11+}, S^{12+}, S^{13+} ions colliding with SF_6** *[Frankel et al., ApJ 702, 171 (2009)]*
- **Ne^{10+} ions colliding with He, Ne, Ar** *[Ali et al., ApJ 716, L95 (2010)]*
- **Ar^{17+}, Ar^{18+}, P^{14+}, P^{15+} ions colliding with H_2** *[Leutenegger et al., PRL 105, 063201 (2010)]*

+ measurements (ORNL) and calculations - posters + next talk by Phil Stancil

Differences between collisional and charge exchanged induced spectra: L-shell sulfur emission



Summary

- Much progress has been made to complete the line lists of importance for describing the emission of collisional plasmas
- Measurements to produce line lists of importance for describing absorption features of photoexcited plasmas have been started
- Radiative rates, electron-impact excitation rates, ionization rates, dielectronic recombination rates are being measured
- The ionization balance is now being checked in multiple ways
- Many issues, such as emission produced by charge exchange, require further investigations
- The Fe XVII spectrum still cannot be calculated to the needed accuracy