Laboratory X-ray studies with trapped ions using EBITs and synchrotrons

Chintan Shah

NASA Goddard Space Flight Center
&
Max Planck Institute for Nuclear Physics, Heidelberg

NASA POSTDOCTORAL PROGRAM
Administered by Universities Space Research Association

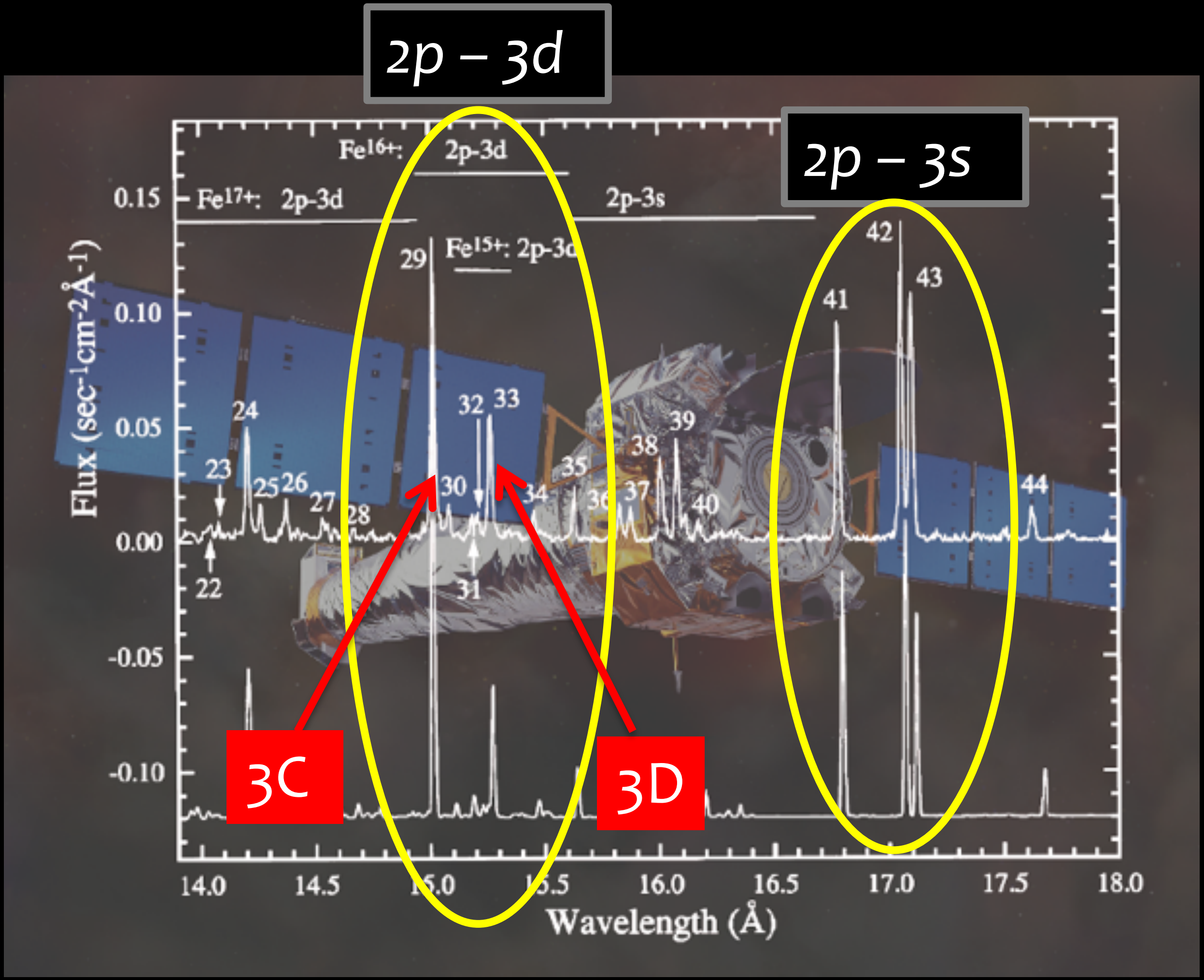
MAX-PLANCK-INSTITUT FÜR KERNPHYSIK

AtomDB workshop
Monday, August 3rd 2020

MAX-PLANCK-GESELLSCHAFT

Fe^{16+} (Fe XVII) line emission problem

Fe^{16+} ions emit strongest soft X-ray diagnostic lines seen in space



Fe XVII 2p – 3d ~15 Å
3C (resonance line)and 3D (intercombination line)

Fe XVII 2p – 3s ~17 Å
3F + 3G
and
M2 (forbidden line)

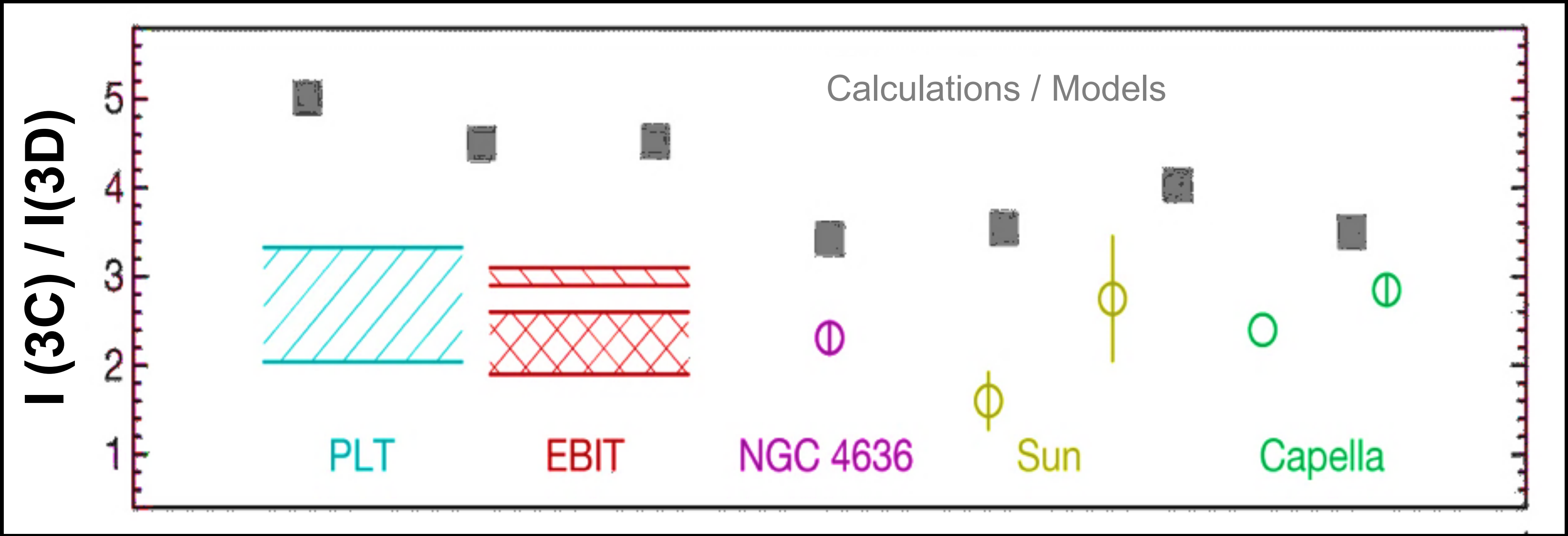
Very Crucial for
- plasma temperature
- density
- turbulence velocity
- plasma opacity

diagnostics…

Image: Chandra Space Telescope, NASA/CXC/NGST   Spectrum: E. Behar et al., ApJ (2001)

Disagreements between Observations and Models and between Experiments and Theoretical calculations.

3C/3D ratio have defied atomic and plasma theory for nearly 40 years

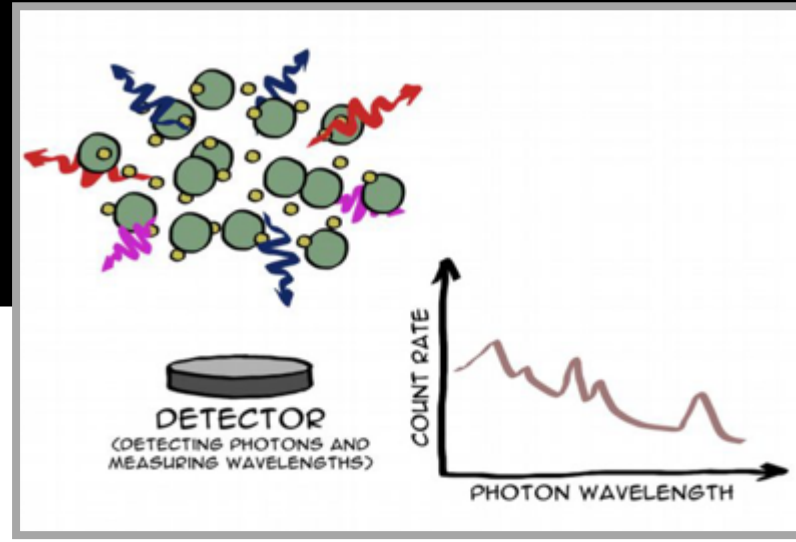


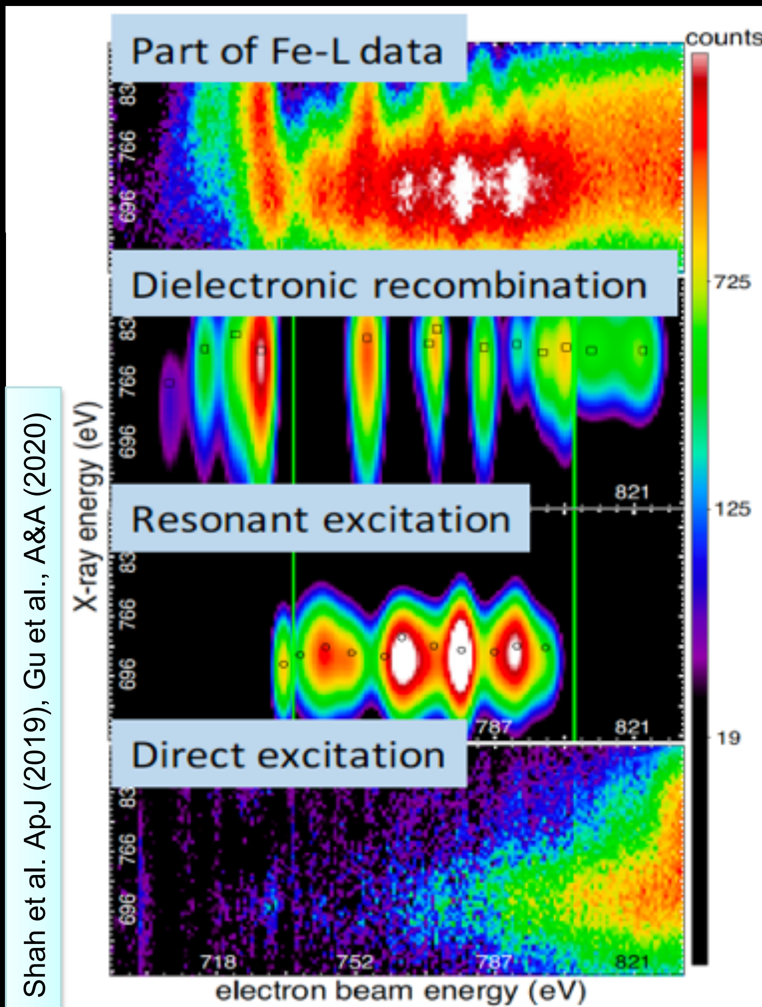
Is theory/Model wrong? Which part?

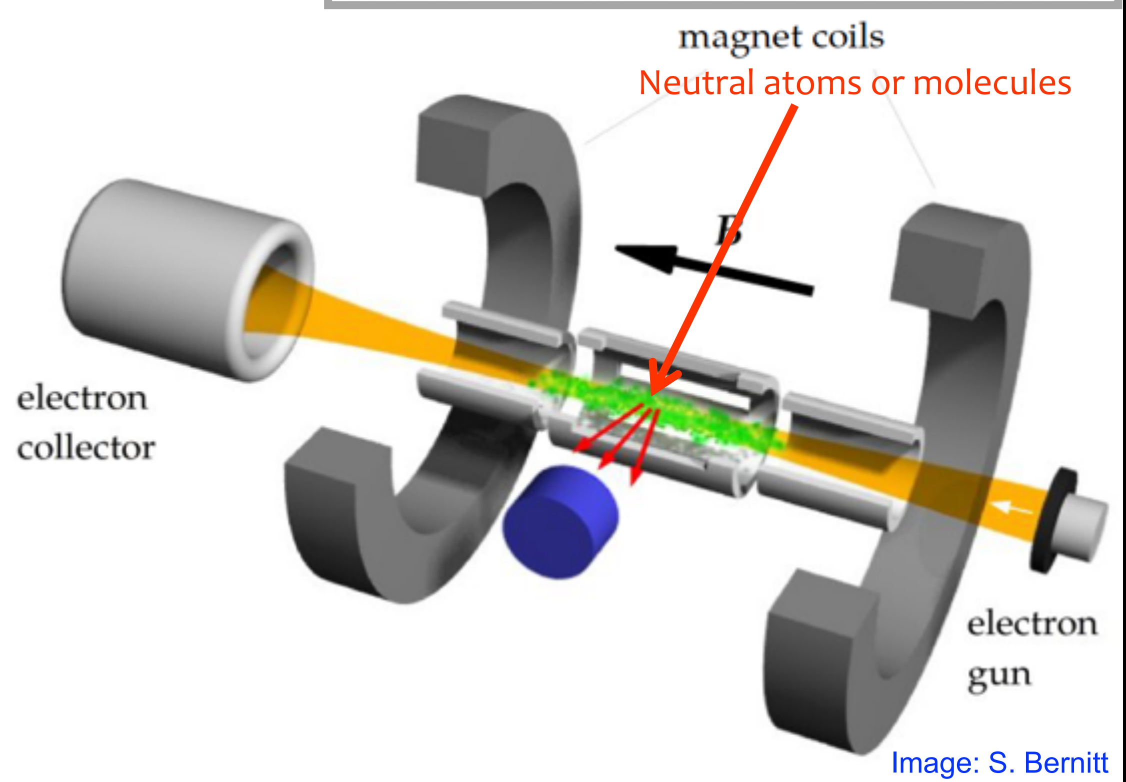
Beiersdorfer et al., ApJ (2002, 2004) Brown et al., ApJ (2001) de Plaa et al., A & A (2012) Bernitt et al., Nature (2012)

Classical Spectroscopy using EBITs

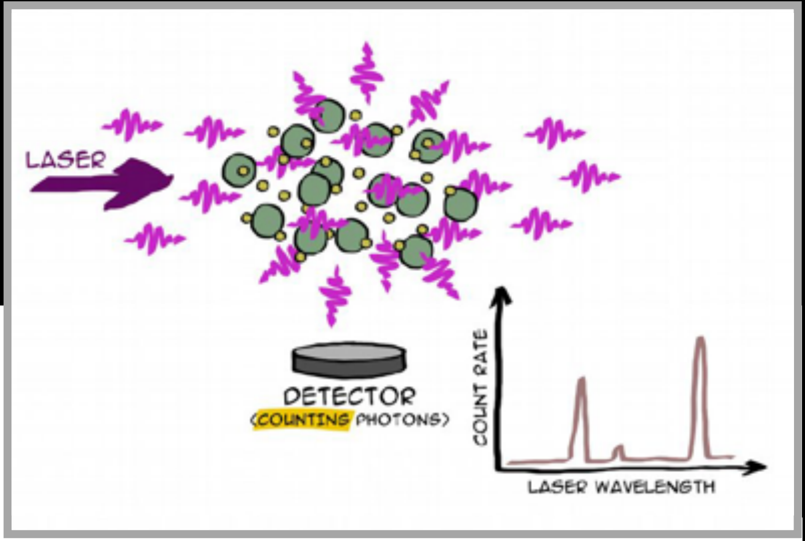
Electron beam drives ionization, excitation, recombination, and traps the ions



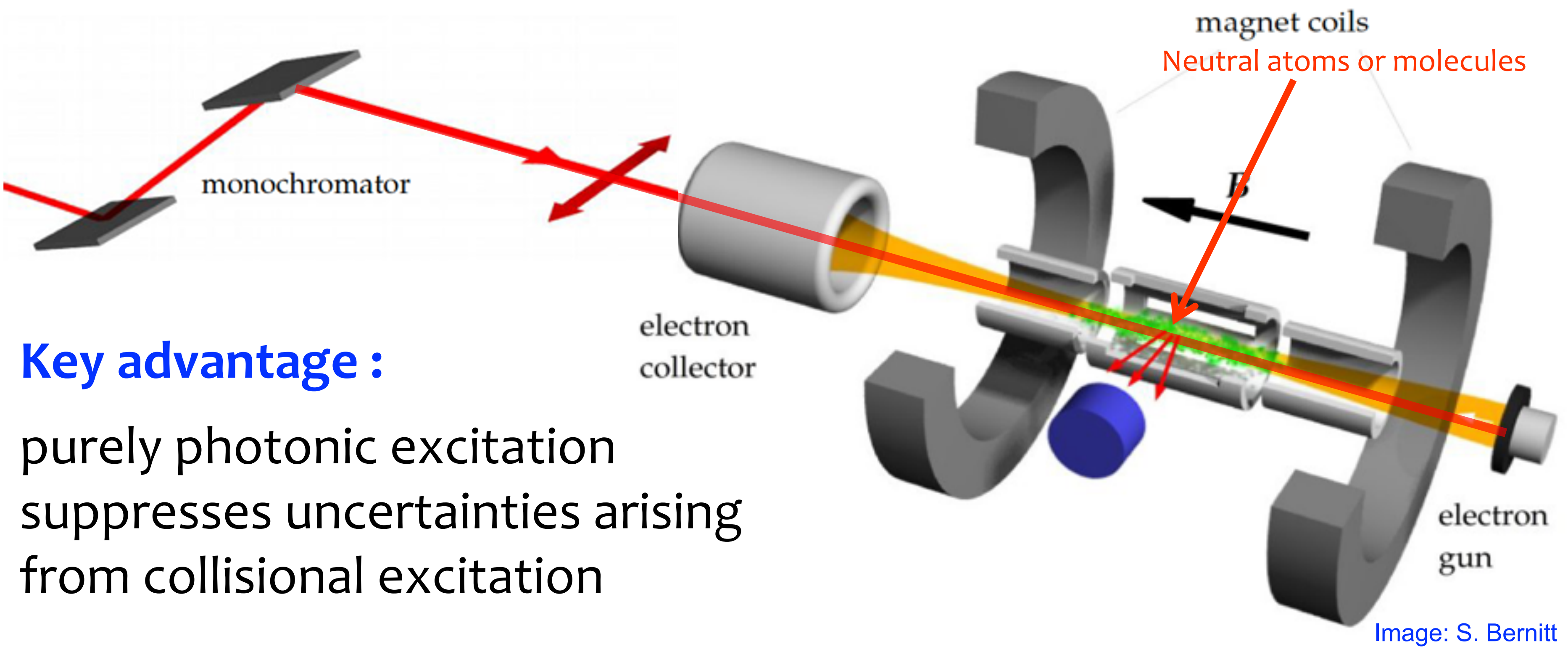




Laser Spectroscopy using EBITs



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



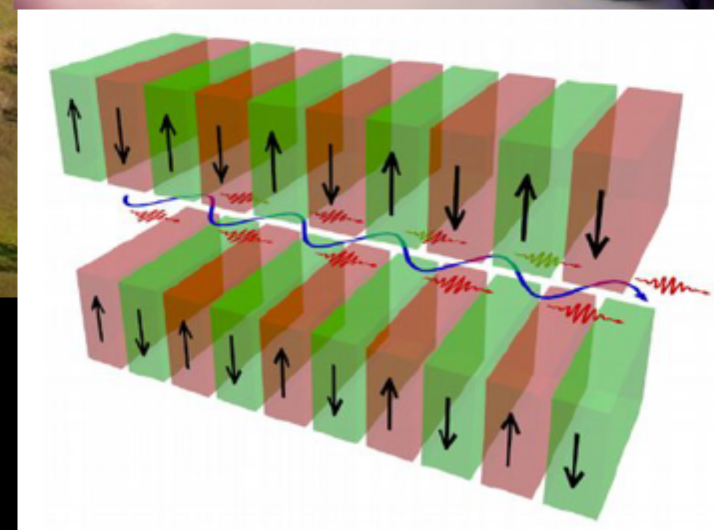
Key advantage :

purely photonic excitation suppresses uncertainties arising from collisional excitation

LCLS Stanford campaign

(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)

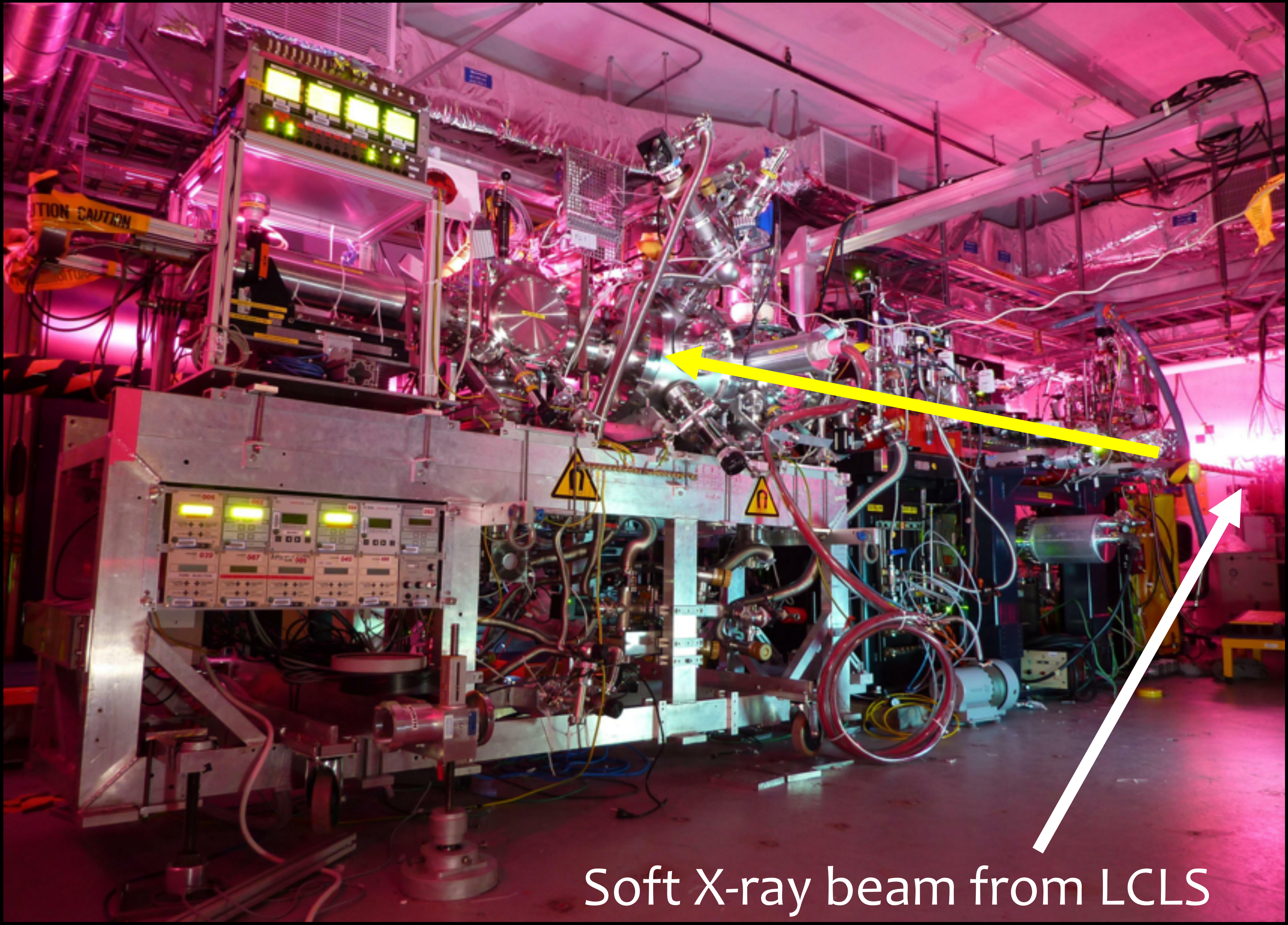
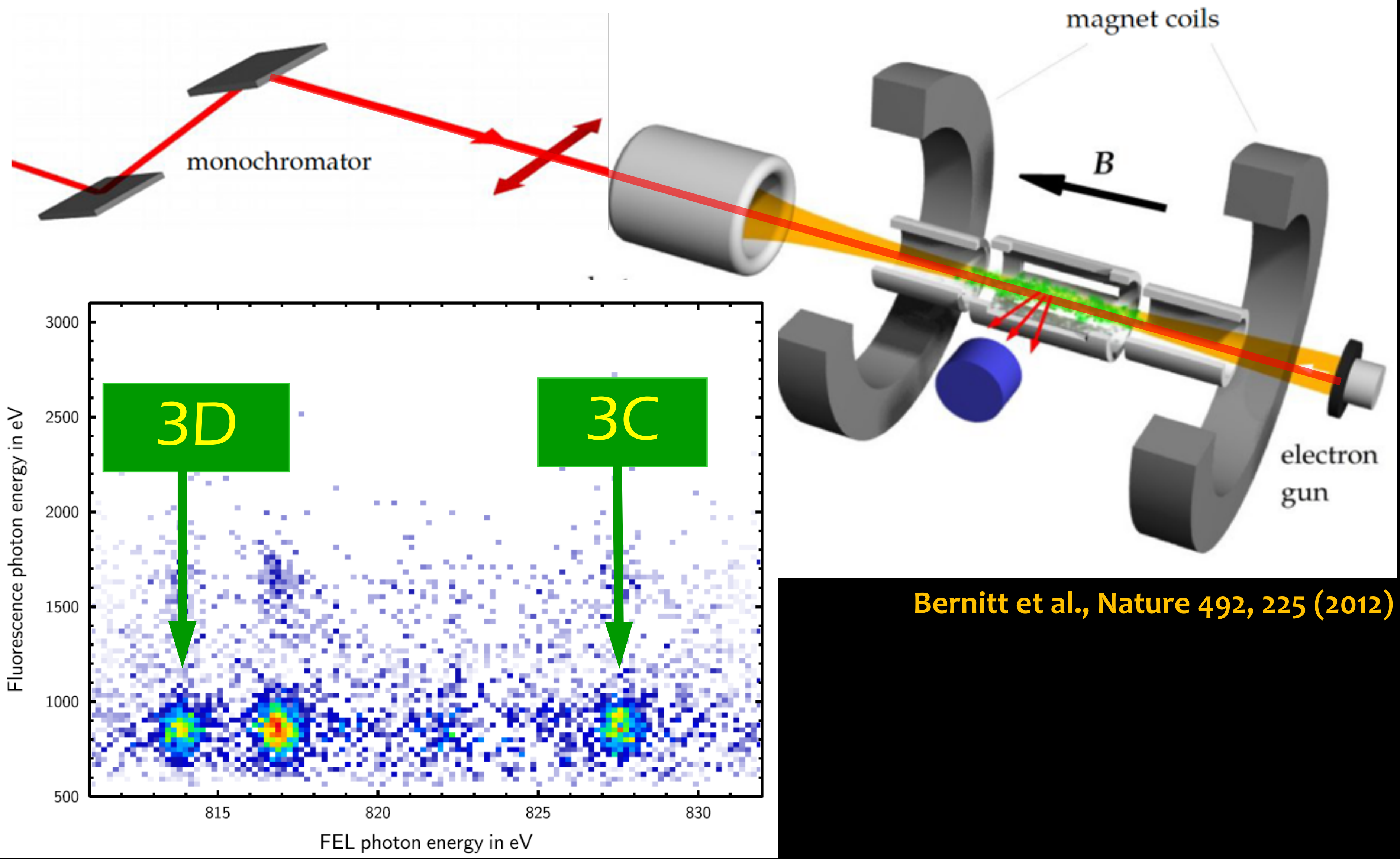


Image: J. Crespo

Measurement Technique

EBIT: production and trapping of highly charged ions

X-ray laser: photo-excited trapped highly charged ions

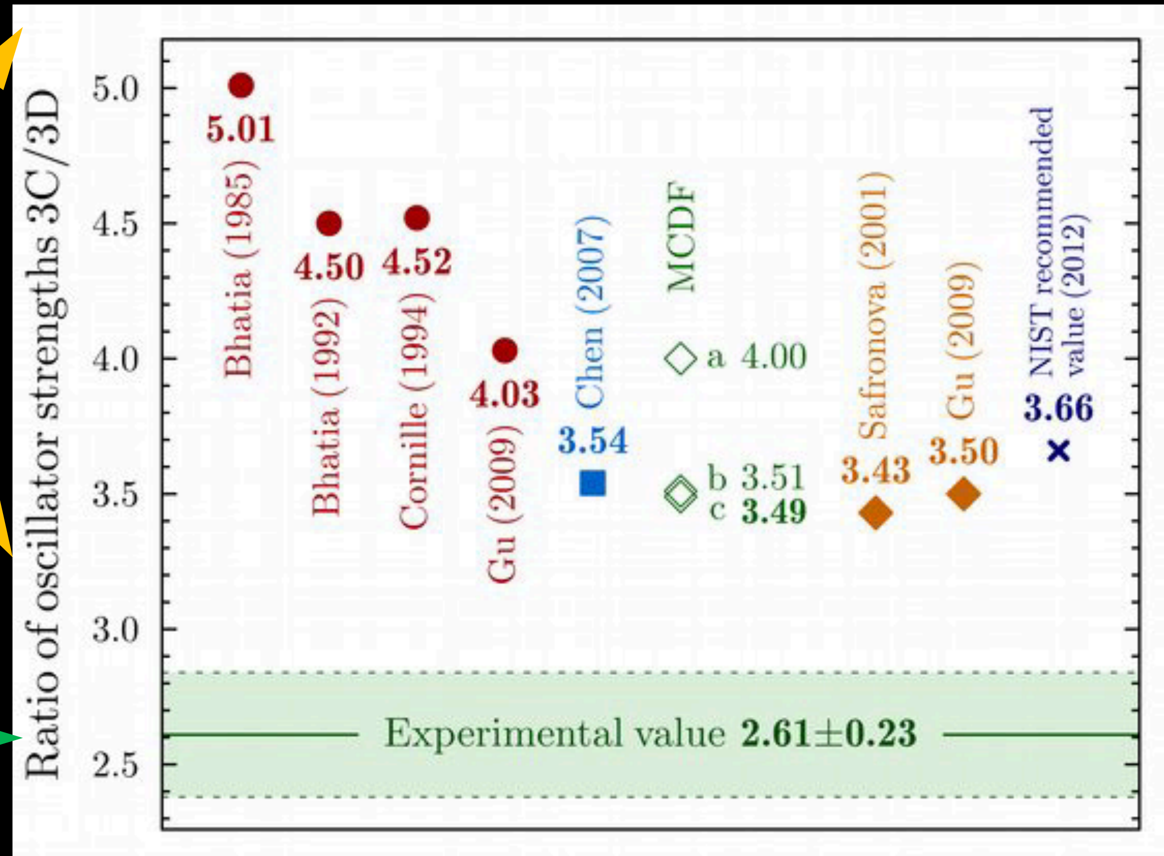


Bernitt et al., Nature 492, 225 (2012)

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 and astrophysical observation and laboratory measurements

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

PRL **113,** 143001 (2014) PHYSICAL REVIEW LETTERS week ending 3 OCTOBER 2014

Astrophysical Line Diagnosis Requires Nonlinear Dynamical Atomic Modeling

Natalia S. Oreshkina, Stefano M. Cavaletto, Christoph H. Keitel, and Zoltán Harman
Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany
(Received 3 July 2014; revised manuscript received 19 August 2014; published 29 September 2014)

THE ASTROPHYSICAL JOURNAL LETTERS, 801:L13 (5pp), 2015 March 1 doi:10.1088/2041-8205/801/1/L13

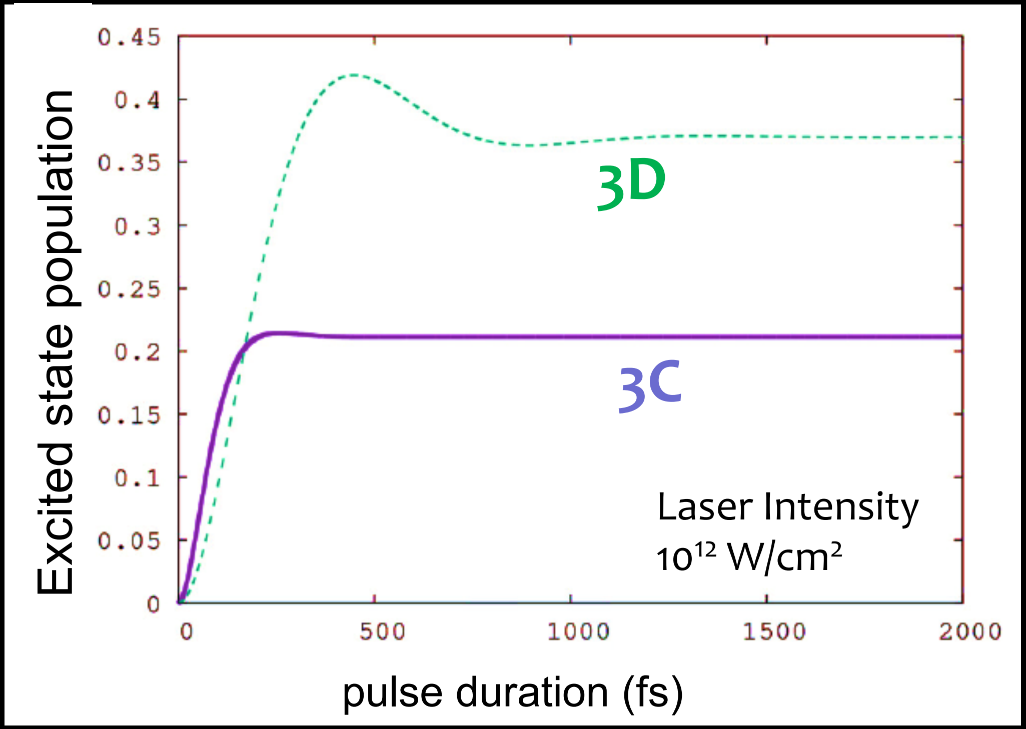
NON-EQUILIBRIUM MODELING OF THE FE XVII 3C/3D LINE RATIO IN AN INTENSE X-RAY FREE-ELECTRON LASER EXCITED PLASMA

S. D. LOCH[1], C. P. BALLANCE[1], Y. LI[1], M. FOGLE[1], AND C. J. FONTES[2]
[1] Auburn University, Auburn, AL 36849, USA; loch@physics.auburn.edu
[2] Los Alamos National Laboratory, MS F663, Los Alamos, NM 87545, USA
Received 2014 July 23; accepted 2015 February 9; published 2015 March 2

NRC Research Press ARTICLE

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

Y. Li, M. Fogle, S.D. Loch, C.P. Ballance, and C.J. Fontes



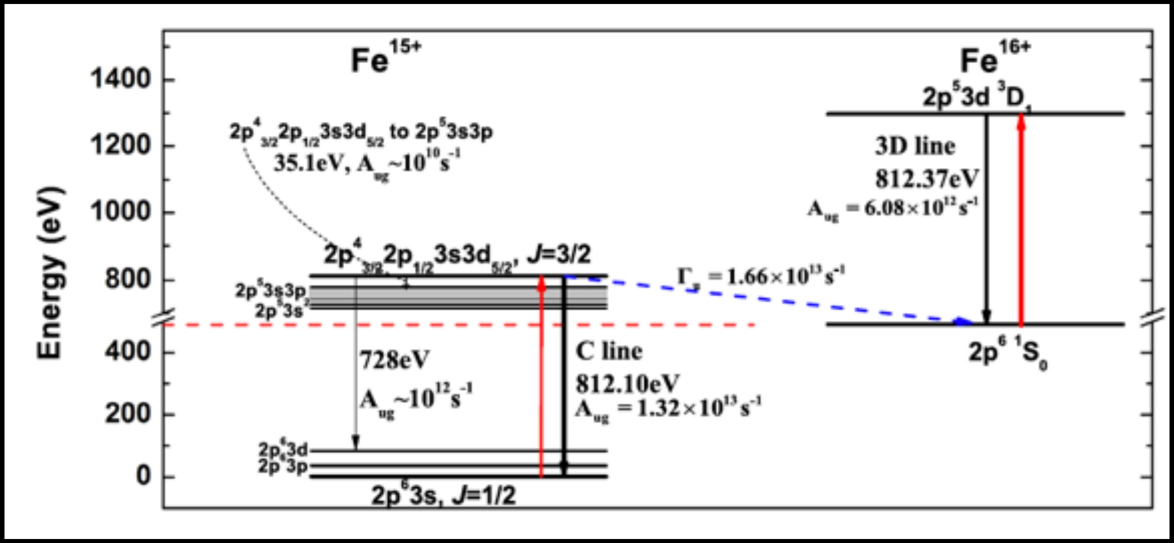
Reason 1: Non-linear Dynamics?

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

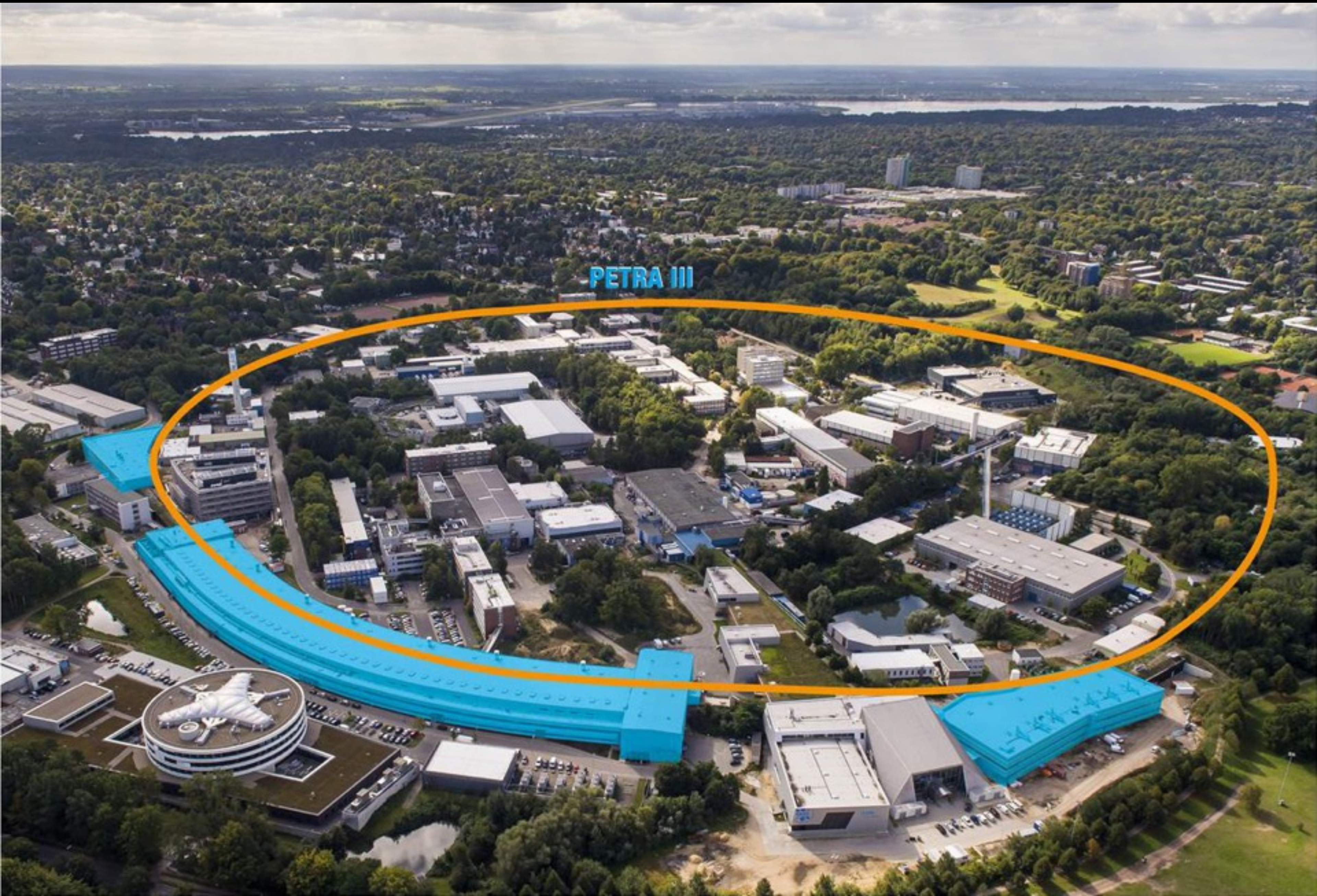
then upper state population of **(3C and 3D) states cannot reach equilibrium…**

Reason 2:
Population transfer?

between Fe15+ and Fe16+ due to strong autoionization channel, feeding the Fe15+ C-line **blended** with 3D



PETRA III Synchrotron at DESY, Hamburg



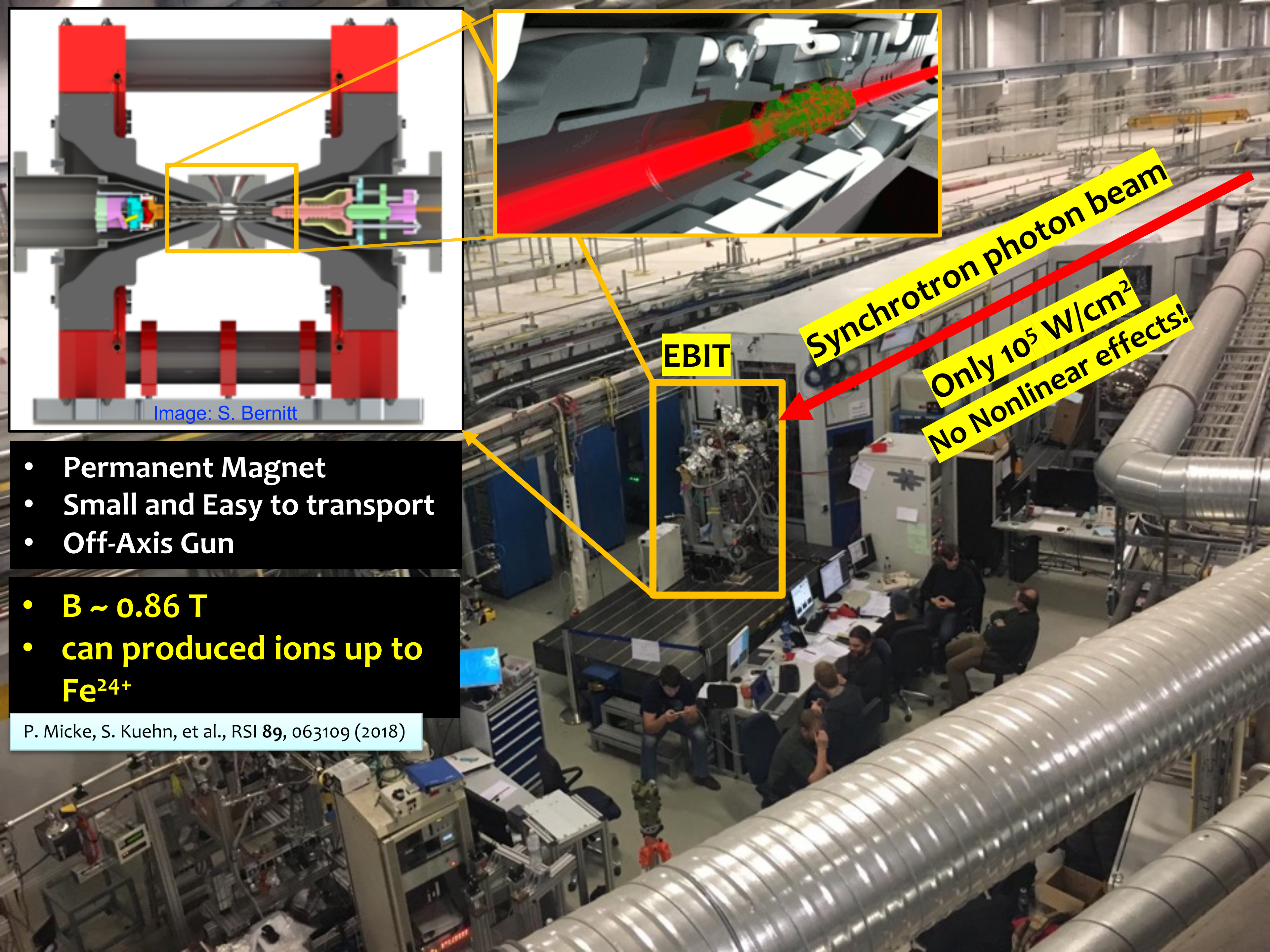
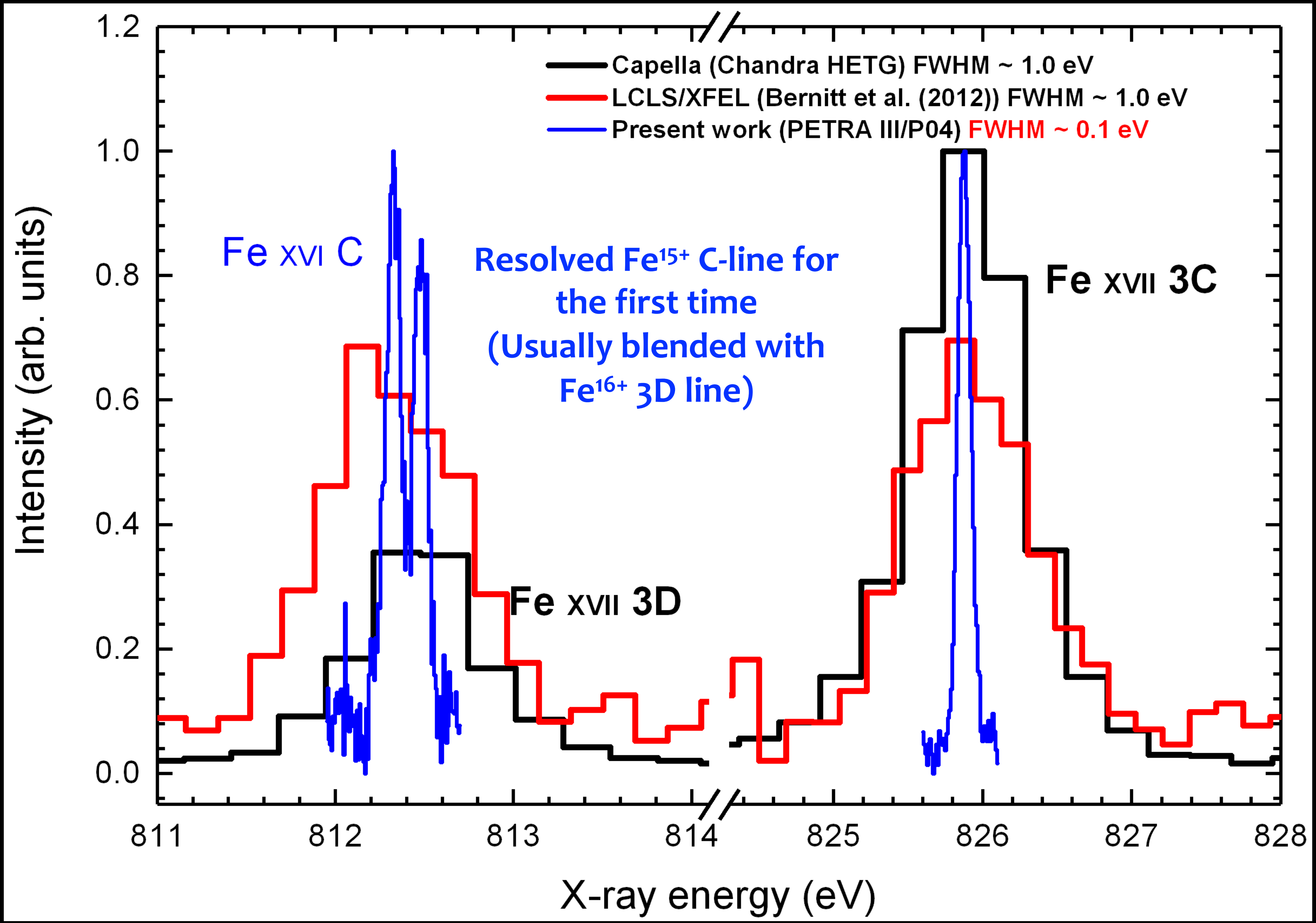
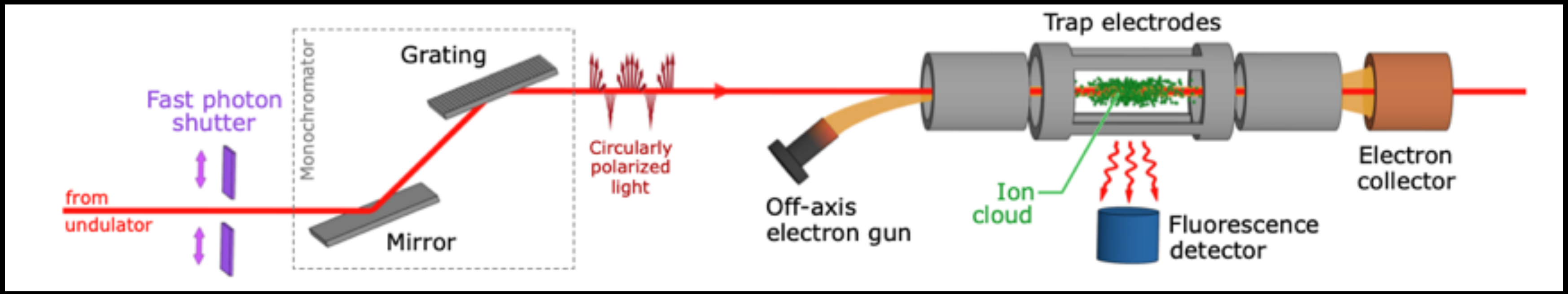


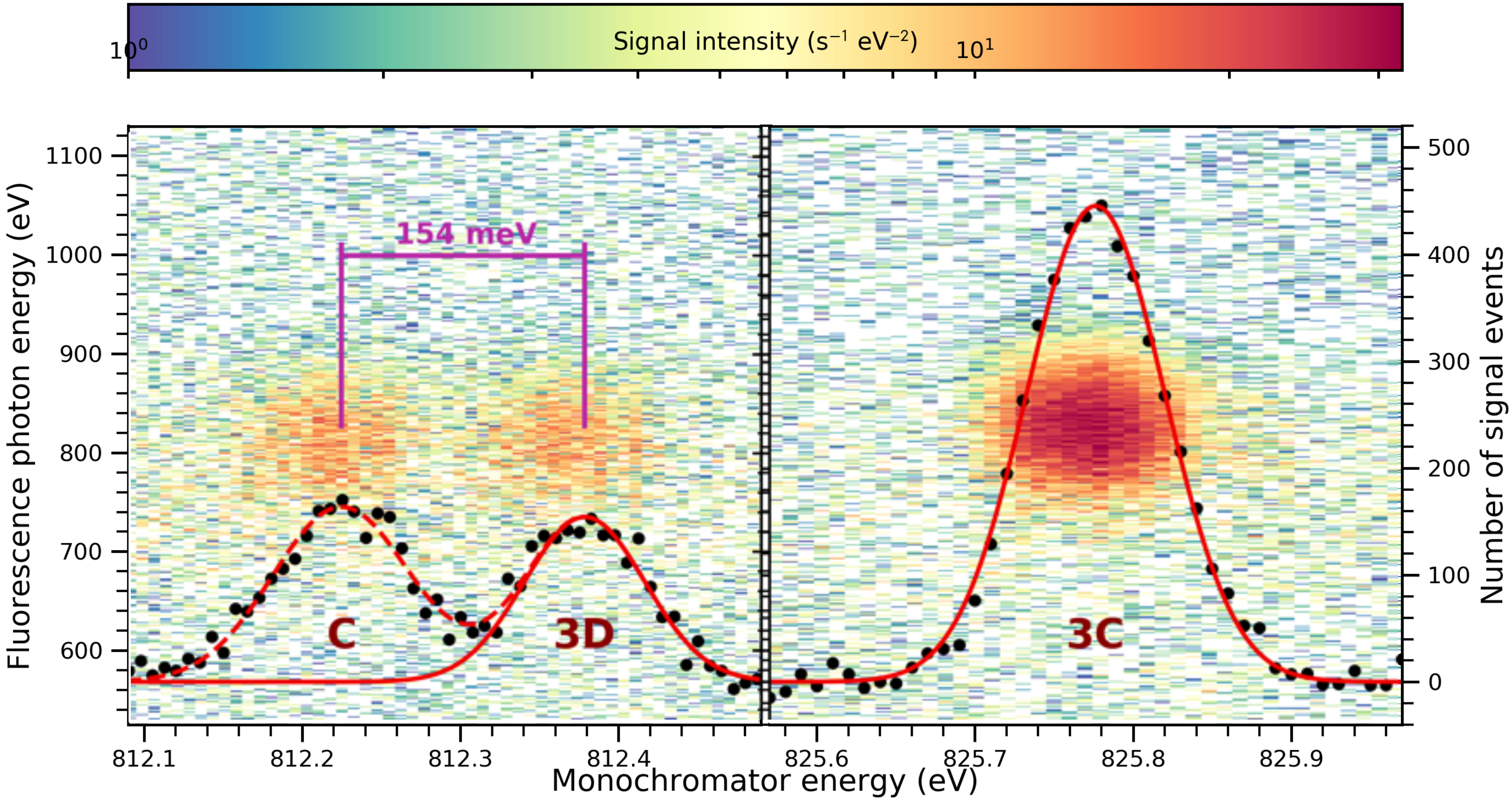
Image: S. Bernitt
EBIT
Synchrotron photon beam
Only 10⁵ W/cm²
No Nonlinear effects!
• Permanent Magnet
• Small and Easy to transport
• Off-Axis Gun
• B ~ 0.86 T
• can produced ions up to Fe^{24+}
P. Micke, S. Kuehn, et al., RSI **89**, 063109 (2018)

Improvement in Resolution: *10x better than Chandra*

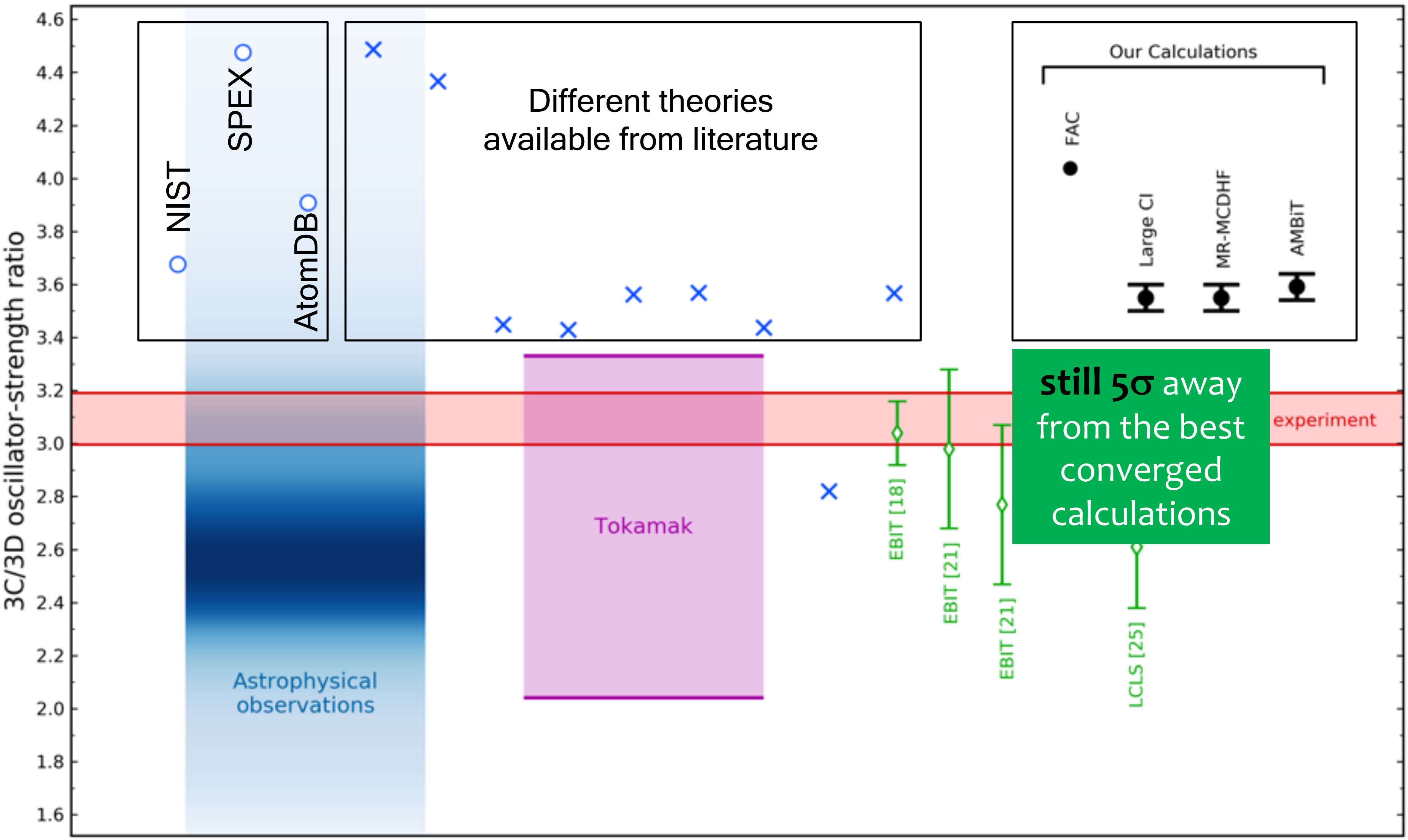


Measurement technique





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

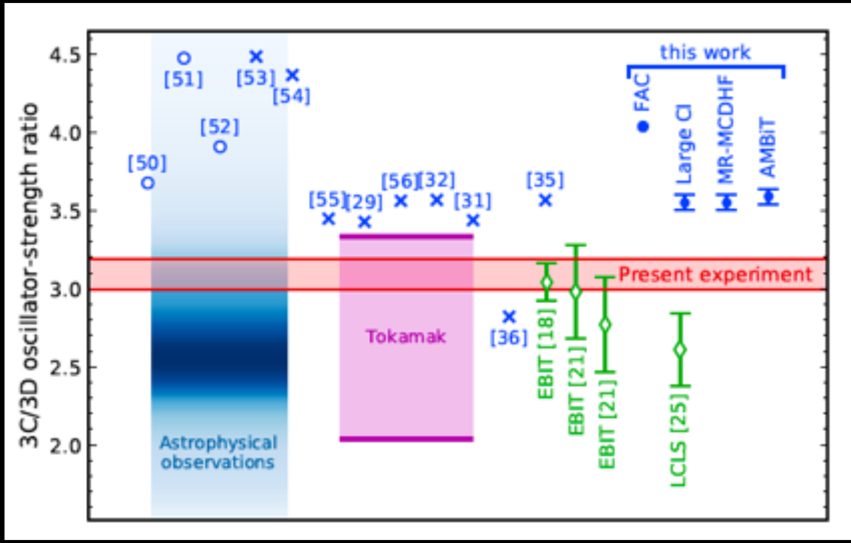


still 5σ away from the best converged calculations

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

Results on the Fe XVII problem

- ✓ This new experiment reinstate the 40-year problem with **5 sigma discrepancy** and **3 % uncertainty**
- ✓ **Low oscillator strengths are still a root cause** of this problem (as our previous experiment found).



PHYSICAL REVIEW LETTERS **124,** 225001 (2020)

Editors' Suggestion | Featured in Physics

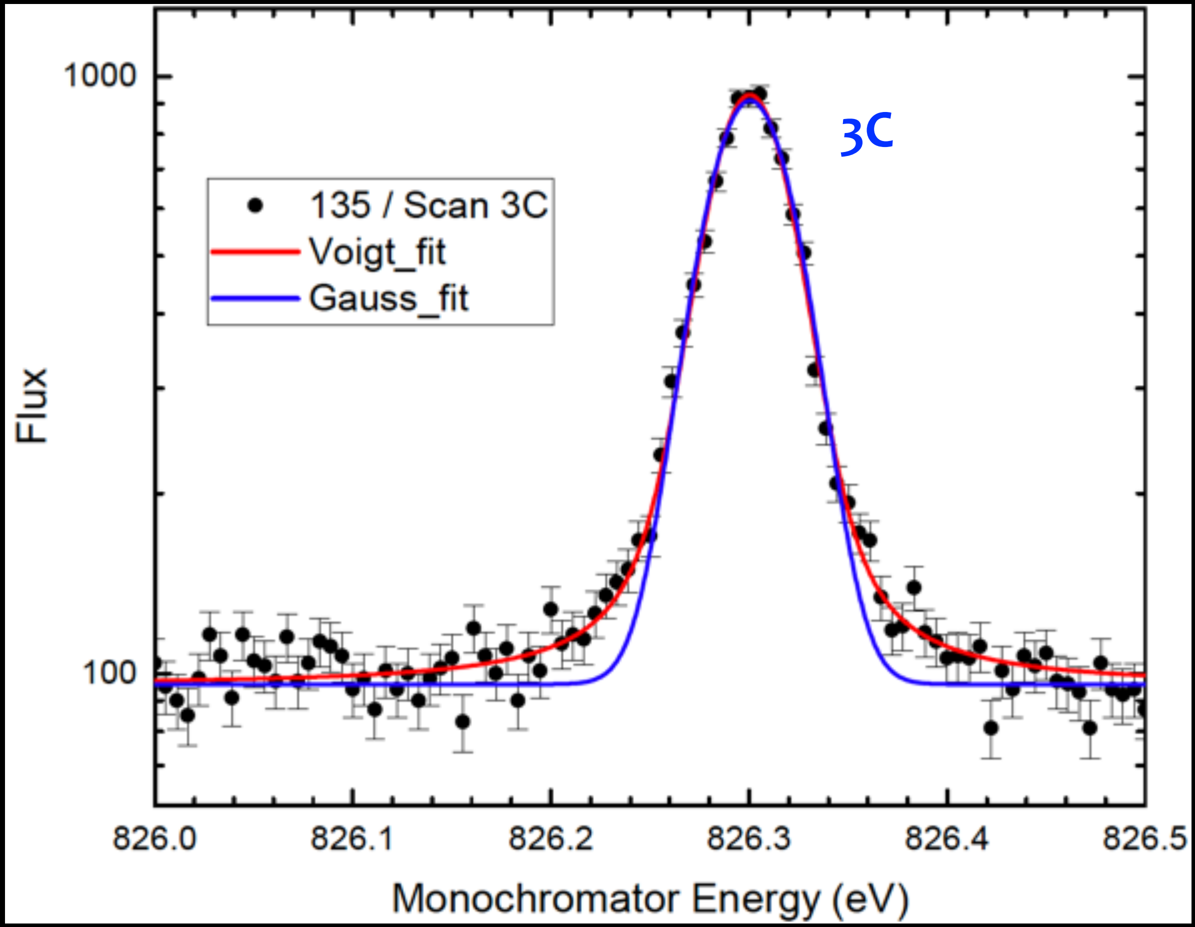
arXiv:1911.09707

High Resolution Photoexcitation Measurements Exacerbate the Long-Standing Fe XVII Oscillator Strength Problem

Steffen Kühn,[1,2,*] Chintan Shah,[3,1,†] José R. Crespo López-Urrutia,[1] Keisuke Fujii,[4] René Steinbrügge,[5] Jakob Stierhof,[6] Moto Togawa,[1] Zoltán Harman,[1] Natalia S. Oreshkina,[1] Charles Cheung,[7] Mikhail G. Kozlov,[8,9] Sergey G. Porsev,[8,7] Marianna S. Safronova,[7,10] Julian C. Berengut,[11,1] Michael Rosner,[1] Matthias Bissinger,[12,6] Ralf Ballhausen,[6] Natalie Hell,[13] SungNam Park,[14] Moses Chung,[14] Moritz Hoesch,[5] Jörn Seltmann,[5] Andrey S. Surzhykov,[15,16] Vladimir A. Yerokhin,[17] Jörn Wilms,[6] F. Scott Porter,[3] Thomas Stöhlker,[18,19,20] Christoph H. Keitel,[1] Thomas Pfeifer,[1] Gregory V. Brown,[13] Maurice A. Leutenegger,[3] and Sven Bernitt[1,18,19,20]

What's next for the Fe XVII problem?

Investigate individual oscillator strengths of 3C and 3D rather than their ratio.



Oct 2019 beamtime:

We improved resolution:
~18 000 Resolving power at line 3C

The instrumental profile (beamline) is still a problem at very high resolution…
~ 30 000 RP at O-w line

We plan to investigate this problem in the upcoming beamtime in November 2020 at PETRA III P04.

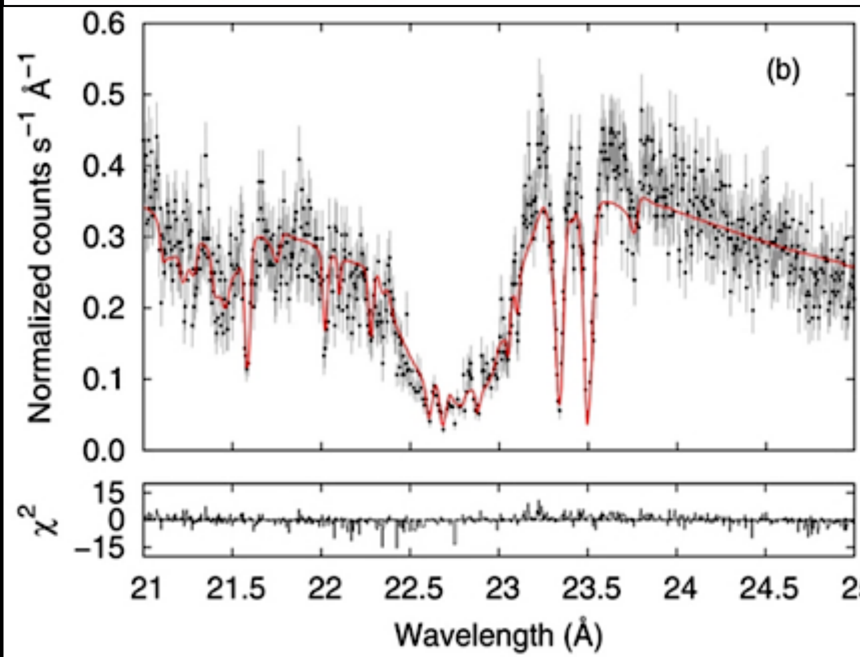
Issue with the atomic oxygen O I velocity in the interstellar medium

Chandra observations of atomic O I 2p-1s absorption in ISM – backlit by bright X-ray binaries

PHOTOIONIZATION MODELING OF OXYGEN K ABSORPTION IN THE INTERSTELLAR MEDIUM: THE *CHANDRA* GRATING SPECTRA OF XTE J1817-330

E. Gatuzz[1], J. García[2,3], C. Mendoza[1,4], T. R. Kallman[3], M. Witthoeft[3], A. Lohfink[2], M. A. Bautista[5], P. Palmeri[6], and P. Quinet[6,7]

The Astrophysical Journal, Volume 768, Number 1



A COMPREHENSIVE X-RAY ABSORPTION MODEL FOR ATOMIC OXYGEN

T. W. Gorczyca[1], M. A. Bautista[1], M. F. Hasoglu[2], J. García[3], E. Gatuzz[4], J. S. Kaastra[5,6], T. R. Kallman[7], S. T. Manson[8], C. Mendoza[1,4], A. J. J. Raassen[5,9] + Show full author list

The Astrophysical Journal, Volume 779, Number 1

Data Set	$1s \rightarrow 2p$
Astronomical observations	
Chandra, average of seven sources	527.44 ± 0.09
XMM-Newton, Mrk 421	527.30 ± 0.05
Juett et al. (2004), six sources	527.41 ± 0.18
Average	**527.37**
Chandra, Liao et al. (2013)	527.39 ± 0.02

O I (2p-1s): 23.502 ± 0.001 A

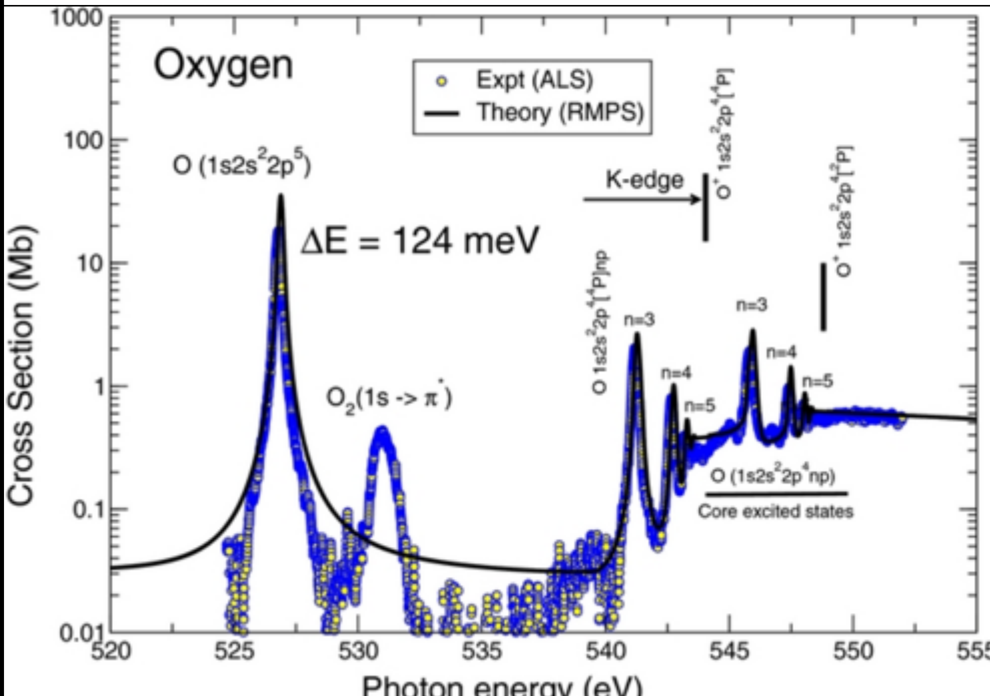
O I (2p-1s):
Chandra ~527.4 eV
XMM-Newton ~527.3 eV

High-resolution lab measurements at ALS (O I 1s → 2p)

HIGH PRECISION K-SHELL PHOTOABSORPTION CROSS SECTIONS FOR ATOMIC OXYGEN: EXPERIMENT AND THEORY

B. M. McLaughlin[1,2], C. P. Ballance[3], K. P. Bowen[4], D. J. Gardenghi[4], and W. C. Stolte[4,5,6]

The Astrophysical Journal Letters, Volume 771, Number 1



Laboratory rest energy O I

$\sim 526.79 \pm 0.04$ eV

Difference to line-of-sight average observed value from XMM and Chandra is

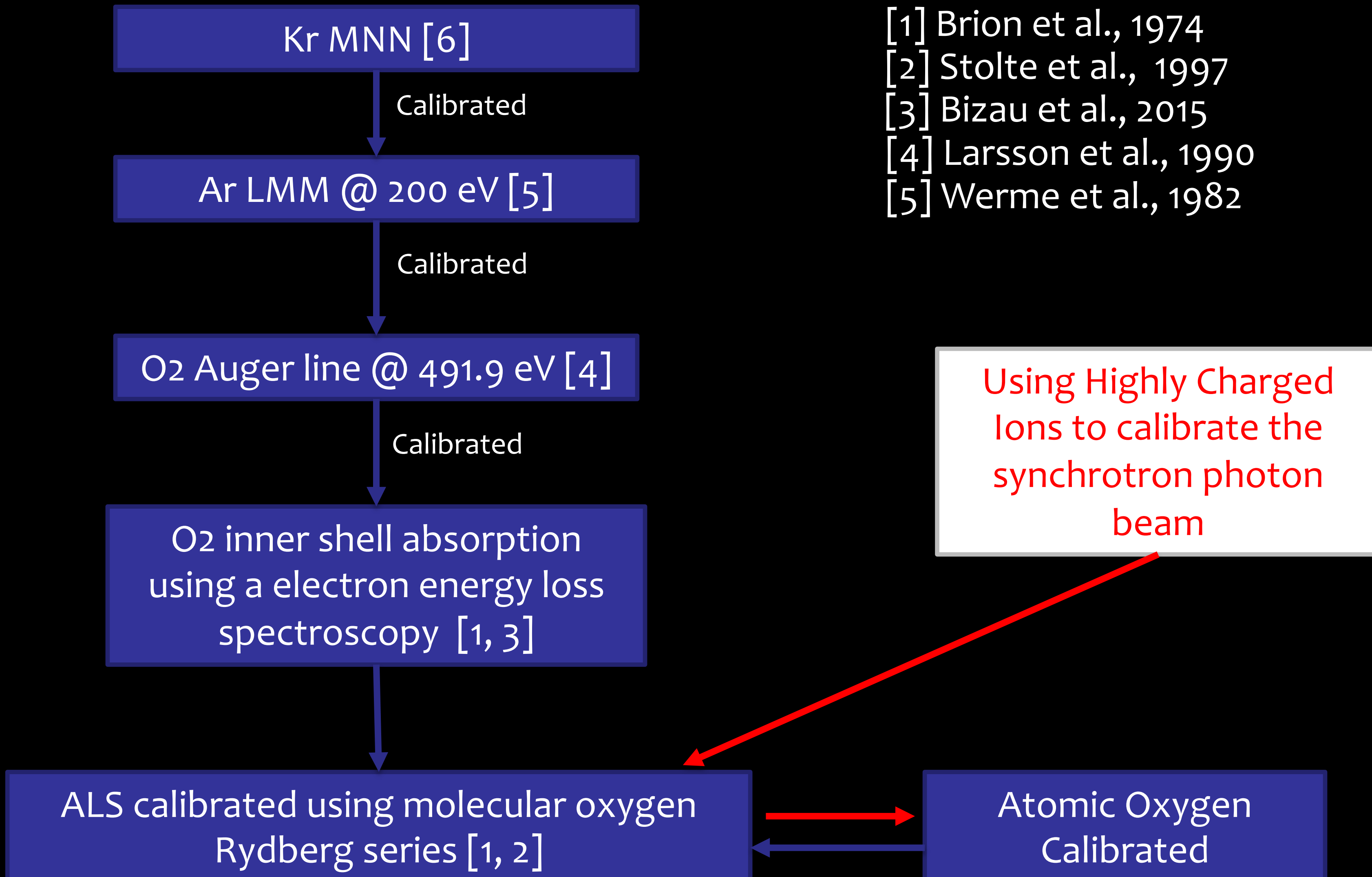
$\sim 500 - 600$ meV

If we treat this discrepancy as a real astrophysical Doppler shift,

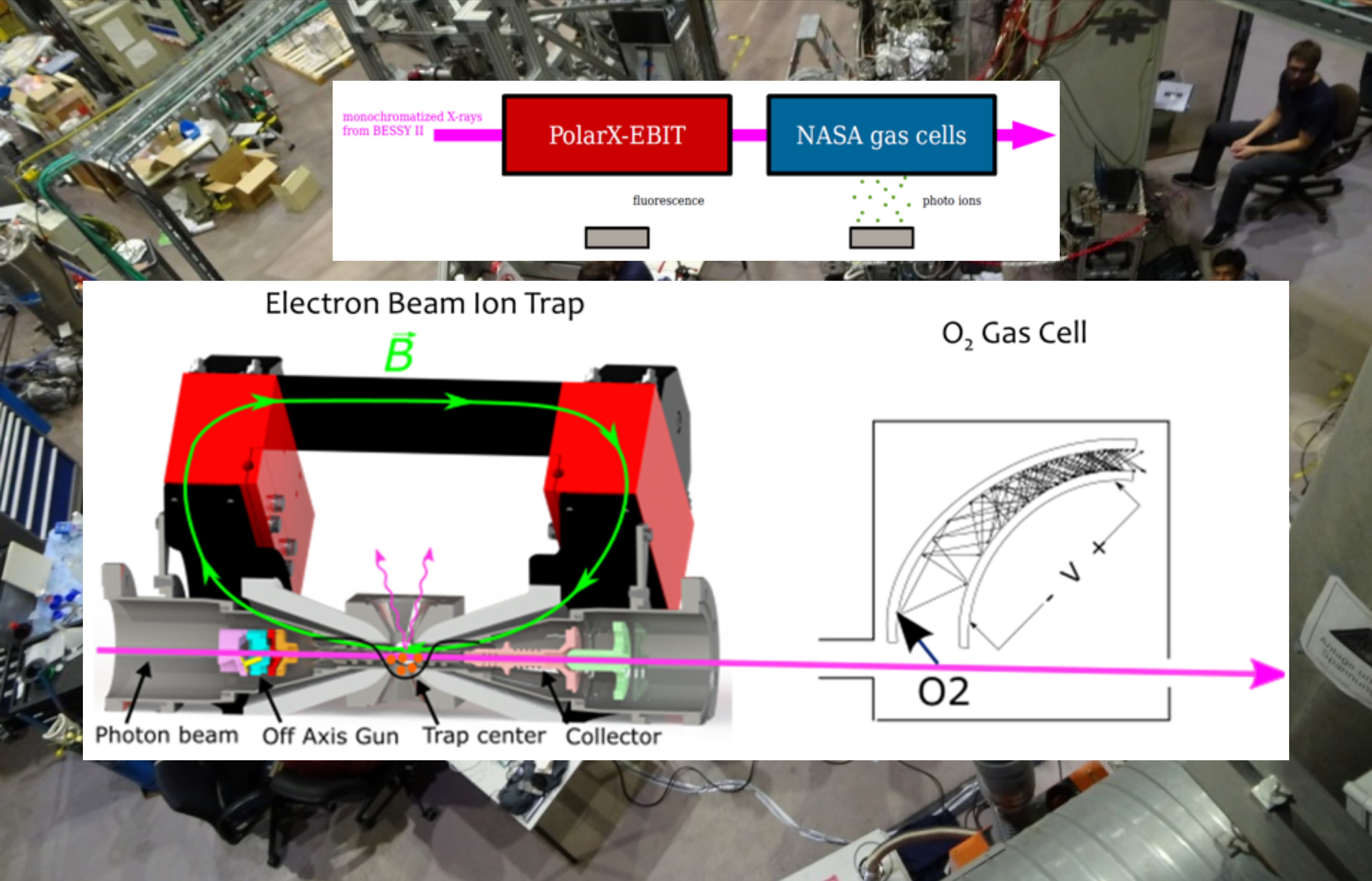
This would lead to a conclusion that the atomic oxygen along many line of sight is moving away from us at velocity of ~ $300 - 350$ km/s

High-resolution lab measurements at ALS (O I 1s → 2p)

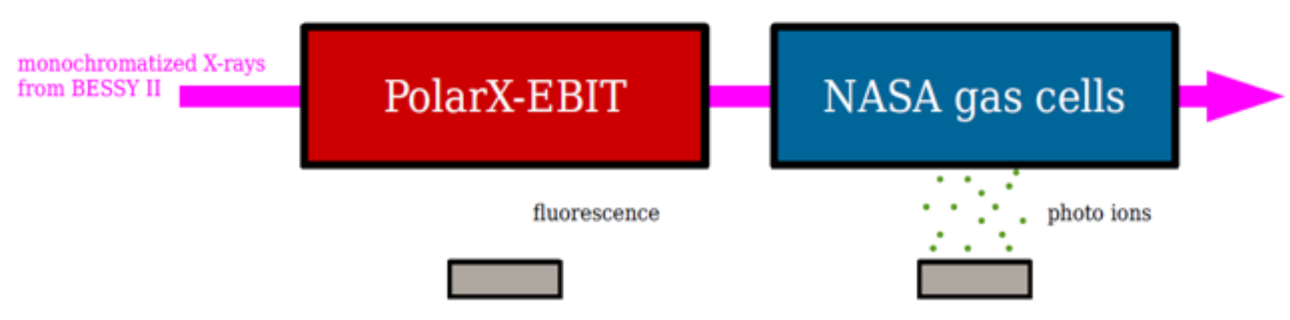
[1] Brion et al., 1974
[2] Stolte et al., 1997
[3] Bizau et al., 2015
[4] Larsson et al., 1990
[5] Werme et al., 1982



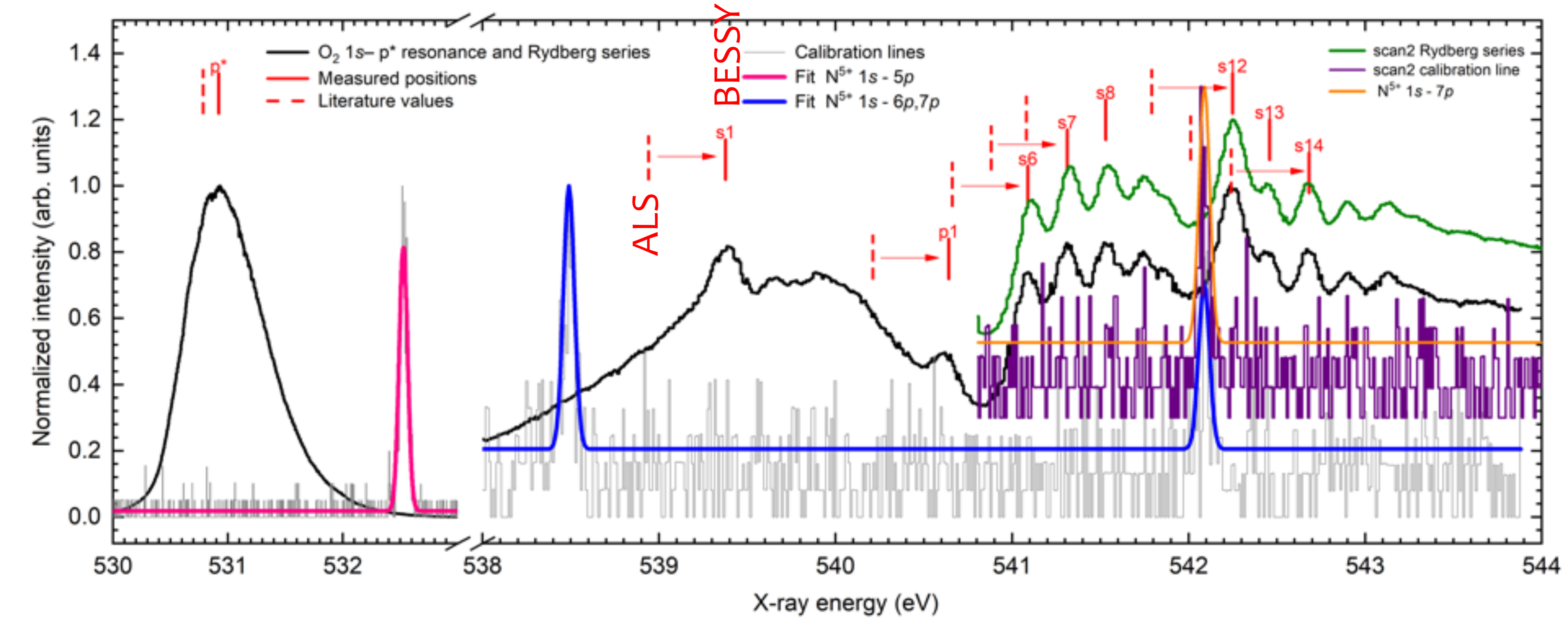
Experimental setup at BESSY Synchrotron in Berlin



Results

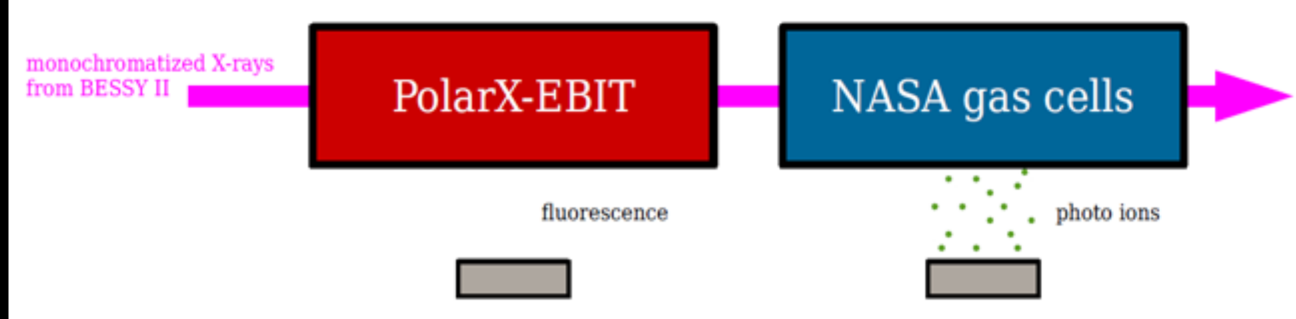


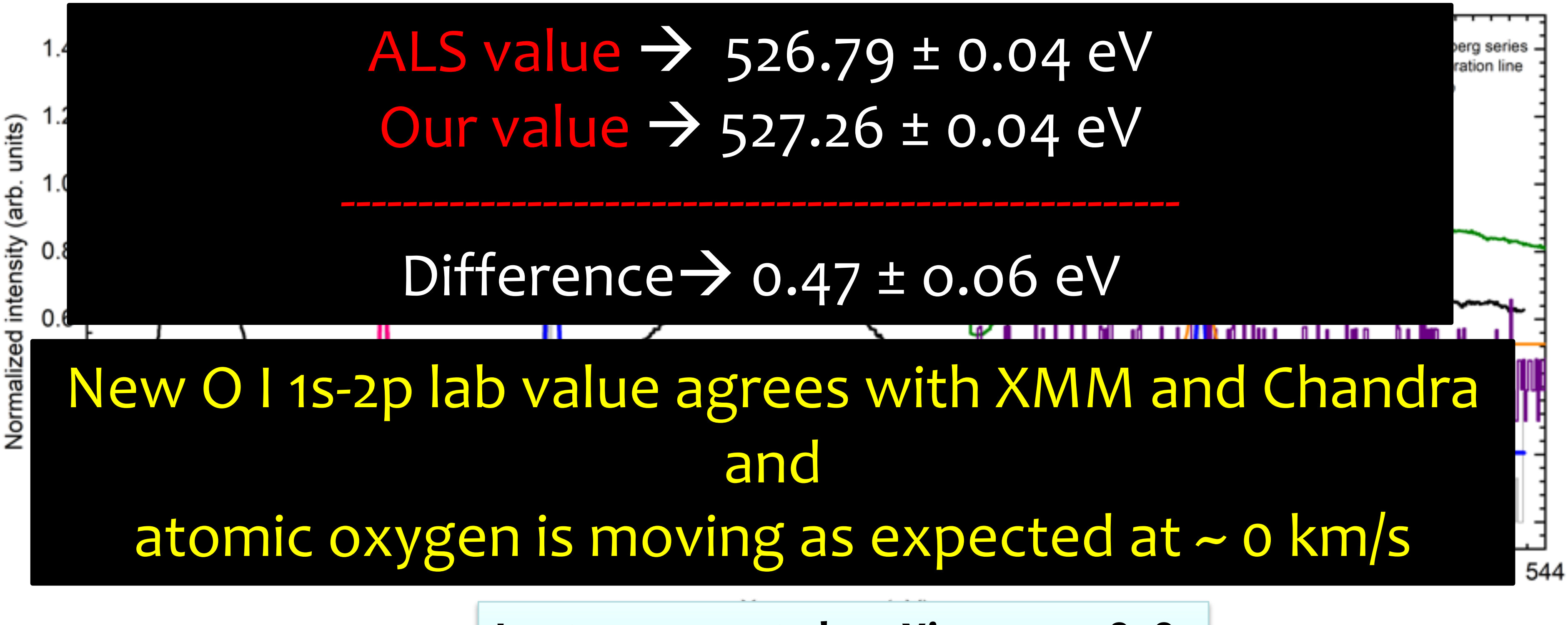
monochromatized X-rays from BESSY II
PolarX-EBIT
NASA gas cells
fluorescence
photo ions



O2 1s– p* resonance and Rydberg series
Measured positions
Literature values
Calibration lines
Fit N5+ 1s - 5p
Fit N5+ 1s - 6p,7p
scan2 Rydberg series
scan2 calibration line
N5+ 1s - 7p
BESSY
ALS
p*
s1
p1
s6
s7
s8
s12
s13
s14
Normalized intensity (arb. units)
X-ray energy (eV)

Results





ALS value → 526.79 ± 0.04 eV

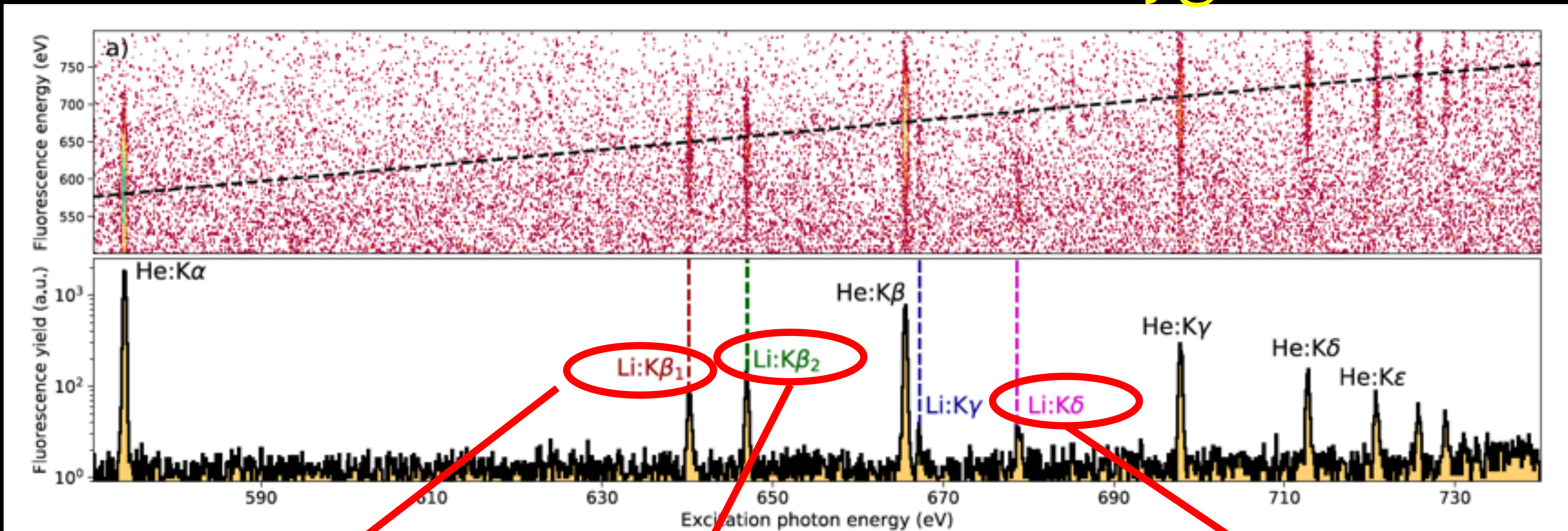
Our value → 527.26 ± 0.04 eV

Difference→ 0.47 ± 0.06 eV

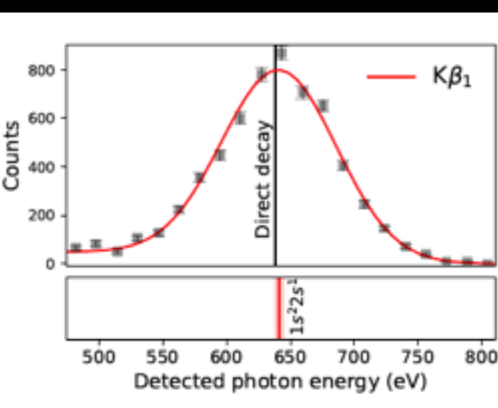
New O I 1s-2p lab value agrees with XMM and Chandra
and
atomic oxygen is moving as expected at ~ 0 km/s

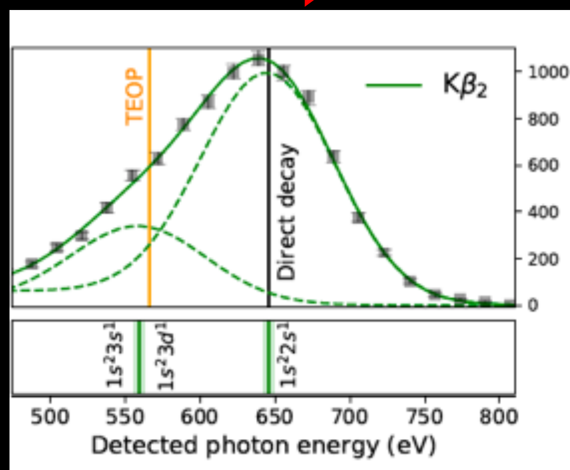
Leutenegger et al., arXiv:2003.13838

Photo-excitation in He- and Li-like Oxygen

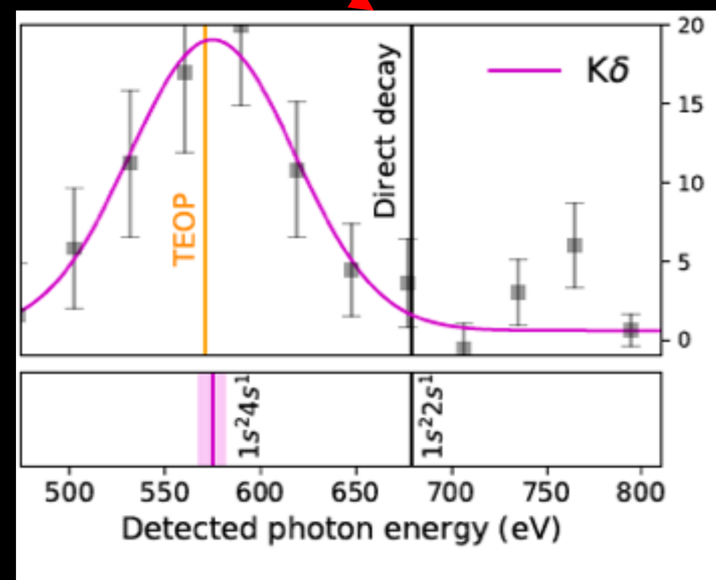


[1s² 2s] ⇆ [1s 2s 3p]*



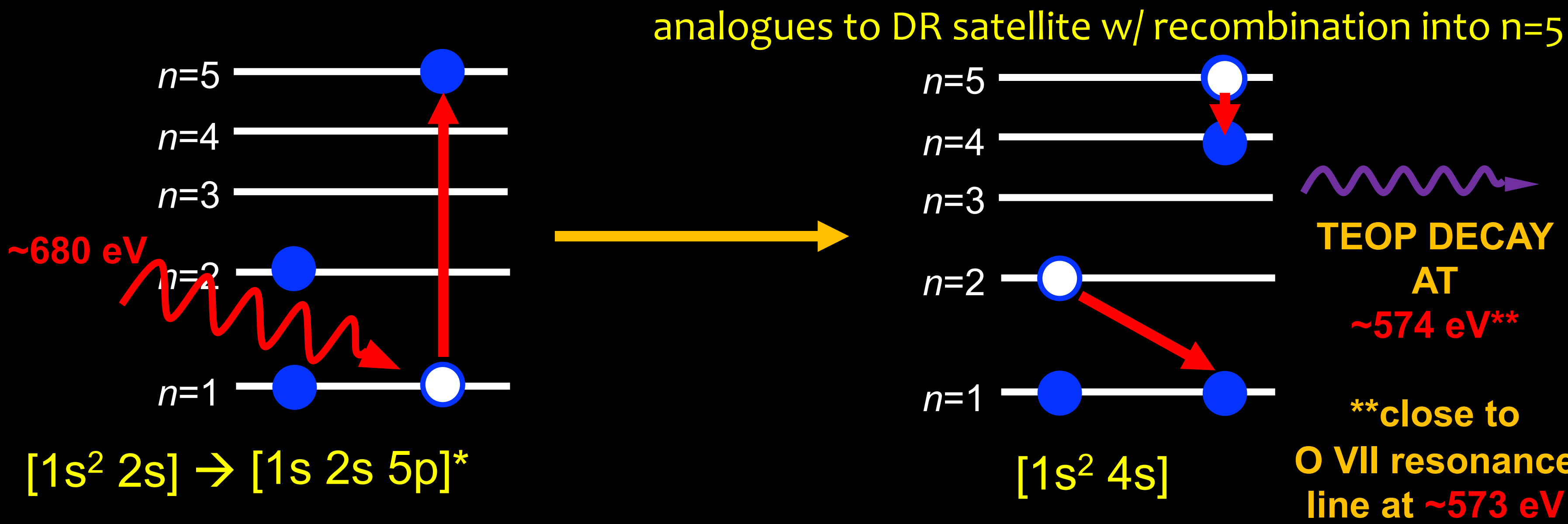


DD/TEOP
***Kβ$_2$* branching ratio**
= 1.73 +/- 0.19



Togawa et al., arXiv:2003.05965

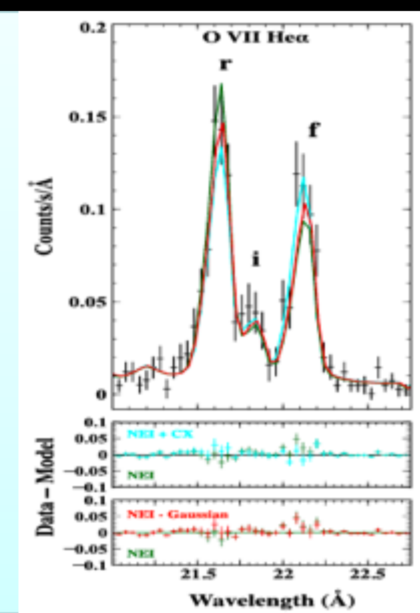
TEOP transitions are crucial for the plasma modeling



✓ TEOP processes dominate over allowed Auger and Radiative decay channels.

✓ TEOP contributions were only explained with the inclusion of the large set of configurations in our calculations.

✓ Blending with O VII resonance line may affect the resonance-to-forbidden line ratio.



arXiv:1911.09707

PHYSICAL REVIEW LETTERS 124, 225001 (2020)

Editors' Suggestion | Featured in Physics

High Resolution Photoexcitation Measurements Exacerbate the Long-Standing Fe XVII Oscillator Strength Problem

Steffen Kühn[1,2,*] Chintan Shah[3,1,†] José R. Crespo López-Urrutia[1] Keisuke Fujii[4] René Steinbrügge[5] Jakob Stierhof[6] Moto Togawa[1] Zoltán Harman[1] Natalia S. Oreshkina[1] Charles Cheung[7] Mikhail G. Kozlov[8,9] Sergey G. Porsev[8,7] Marianna S. Safronova[7,10] Julian C. Berengut[11,1] Michael Rosner[1] Matthias Bissinger[12,6] Ralf Ballhausen[6] Natalie Hell[13] SungNam Park[14] Moses Chung[14] Moritz Hoesch[5] Jörn Seltmann[5] Andrey S. Surzhykov[15,16] Vladimir A. Yerokhin[17] Jörn Wilms[6] F. Scott Porter[3] Thomas Stöhlker[18,19,20] Christoph H. Keitel[1] Thomas Pfeifer[1] Gregory V. Brown[13] Maurice A. Leutenegger[3] and Sven Bernitt[1,18,19,20]

arXiv: 2003.05965

Two-Electron-One-Photon Processes Can Dominate over Allowed Intershell Radiative and Auger Decay in Few-Electron Ions

M. Togawa[1,*] S. Kühn[1,2] C. Shah[1,3] P. Amaro[4] R. Steinbrügge[5] J. Stierhof[6] N. Hell[7] M. Rosner[1,2] K. Fujii[8] M. Bissinger[6] R. Ballhausen[6] M. Hoesch[5] J. Seltmann[5] S. Park[9] F. Grilo[4] F. S. Porter[3] J. P. Santos[4] M. Chung[9] T. Stöhlker[10,11,12] J. Wilms[6] T. Pfeifer[1] G. V. Brown[7] M. A. Leutenegger[3] S. Bernitt[1,11,10,12] and J. R. Crespo López-Urrutia[1,†]

arXiv: 2003.13838

High-Precision Determination of Oxygen-Kα Transition Energy Excludes Incongruent Motion of Interstellar Oxygen

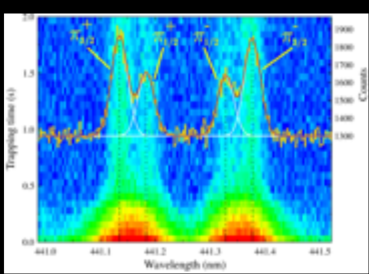
M. A. Leutenegger[1,*] S. Kühn[2] P. Micke[2,3] R. Steinbrügge[4] J. Stierhof[5] C. Shah[1,2] N. Hell[6] M. Bissinger[7] M. Hirsch[5] R. Ballhausen[5] M. Lang[5] C. Gräfe[5] S. Wipf[8] R. Cumbee[1,9] G. L. Betancourt-Martinez[10] S. Park[11] V. A. Yerokhin[12] A. Surzhykov[3,13] W. C. Stolte[14,†] J. Niskanen[15,16] M. Chung[11] F. S. Porter[1] T. Stöhlker[8,17,18] T. Pfeifer[2] J. Wilms[5] G. V. Brown[6] J. R. Crespo López-Urrutia[2] and S. Bernitt[8,18,17,2]

Extra Slides

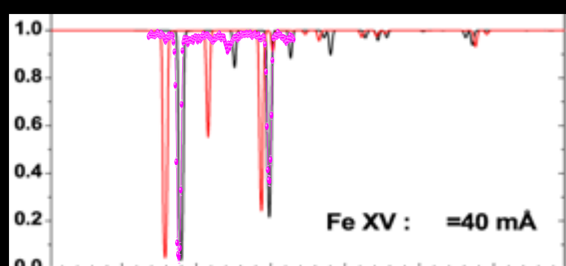
What else we have measured with EBITs and Synchrotrons?

- Photoionization studies from N^{3+} to Fe^{23+}
- $Fe^{15+...17+}$ resonance transitions
- Ly-series lines of H-like N, O, and F ions
- Fe Kα in $Fe^{17+...24+}$ ions excited at 6.7 keV
- Polarization-dependent X-ray fluorescence
- Oscillator strengths, line widths, and branching ratios

Visible M1
Ar^{13+}

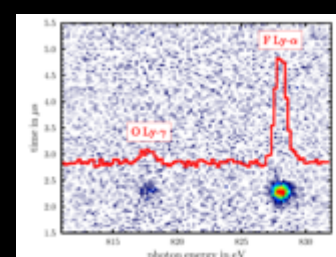


Soft X-ray photoionization
Fe^{14+}



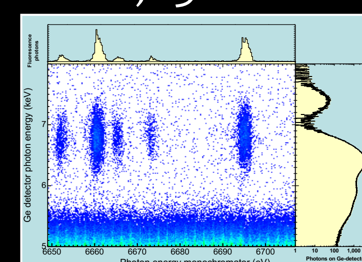
M. C. Simon et al.,
PRL **105** 183001 (2010)

FEL 800 eV
Fe^{16+}



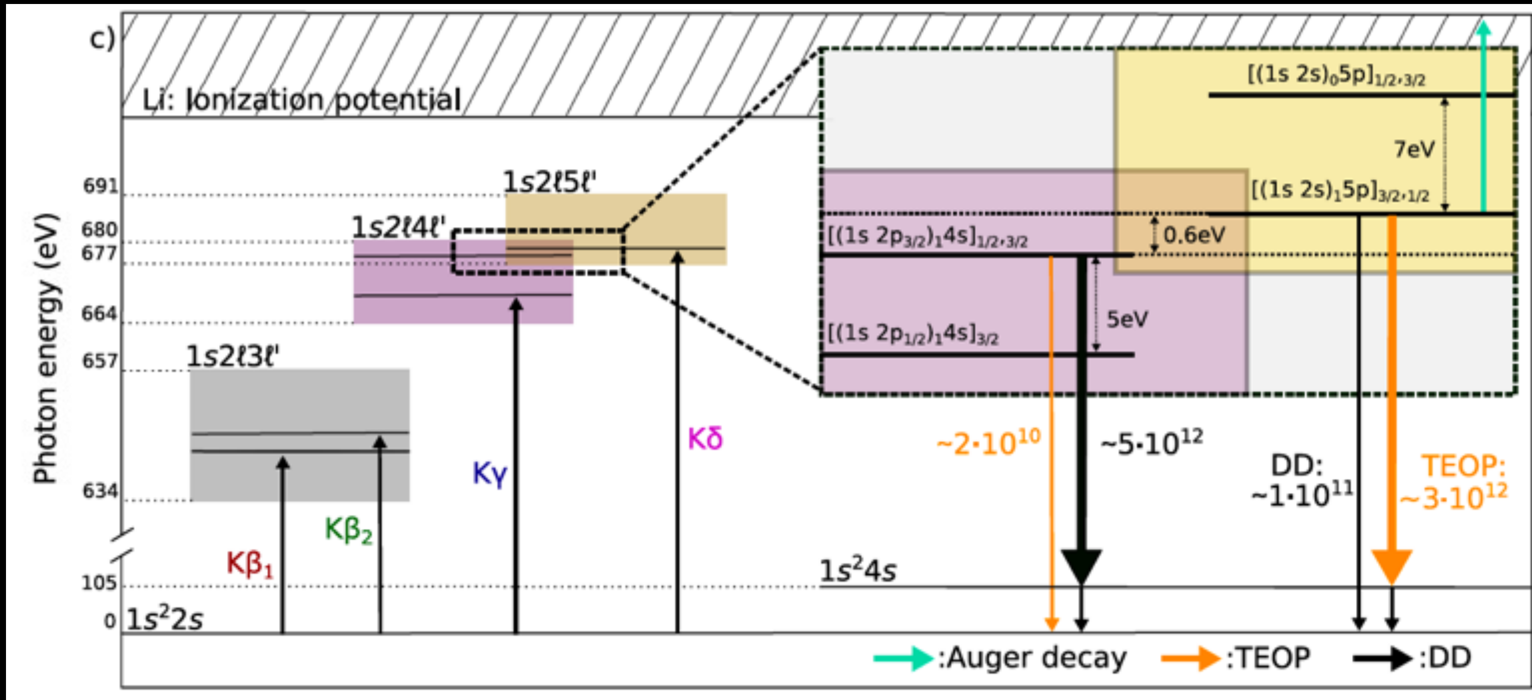
S. Bernitt et al.,
Nature **492**, 225 (2012)

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

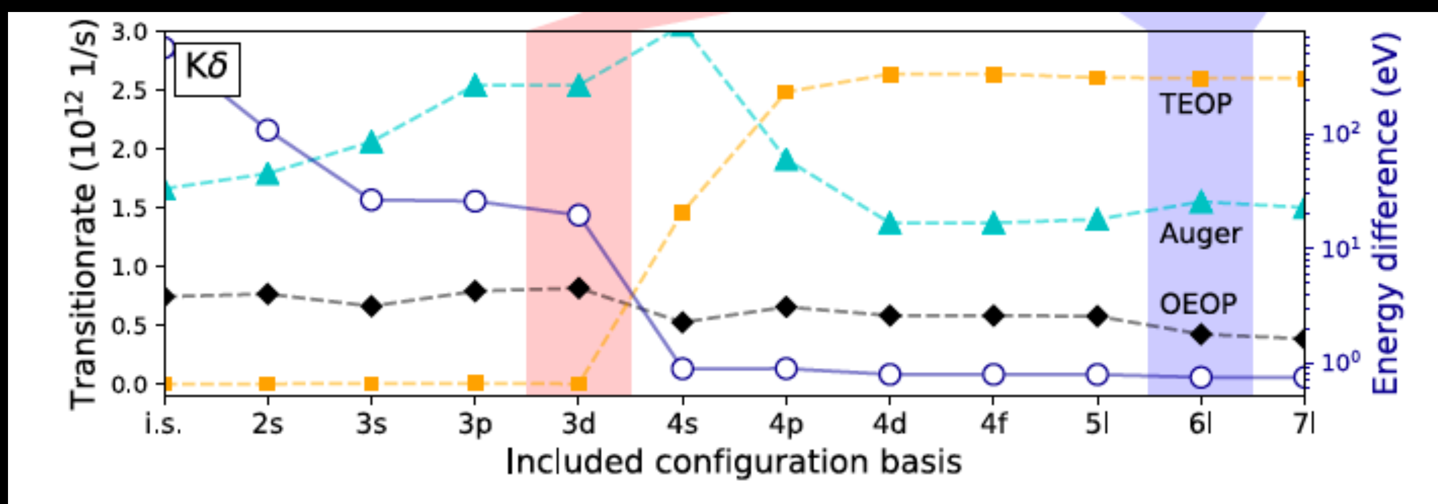


J. Rudolph et al.,
PRL **111**, 103002 (2013)

Two-Electron One-Photon Transitions in Li-like O^{5+}



CI label	Configuration set
initial set	$1s^22l$
	$1s^24l$
	$1s2s5l$
$2l$	$1s2l2l'$
$3s$	$1s^23s$
	$1s2l3s$
$3p$	$1s^23p$
	$1s2l3p$
$3d$	$1s^23d$
	$1s2l3d$
$4s$	$1s2l4s$
$4p$	$1s2l4p$
$4d$	$1s2l4d$
$4f$	$1s2l4f$
$5l$	$1s^25l$
$6l$	$1s^26l$
	$1s2l6l'$
$7l$	$1s^27l$
	$1s2l7l'$



Togawa et al., arXiv:2003.05965

Systematic Fe-L laboratory experiments

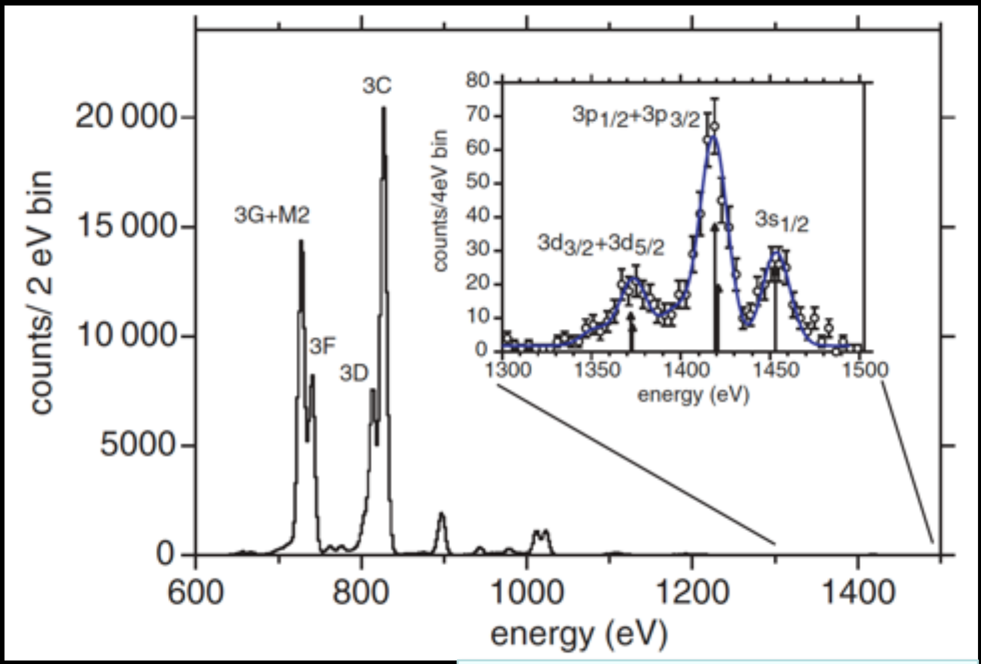
Checking of individual atomic components of 3s and 3d

- Electron impact direct excitation
- Dielectronic recombination satellites
- Resonant excitation
- Radiative cascades
- .....
-

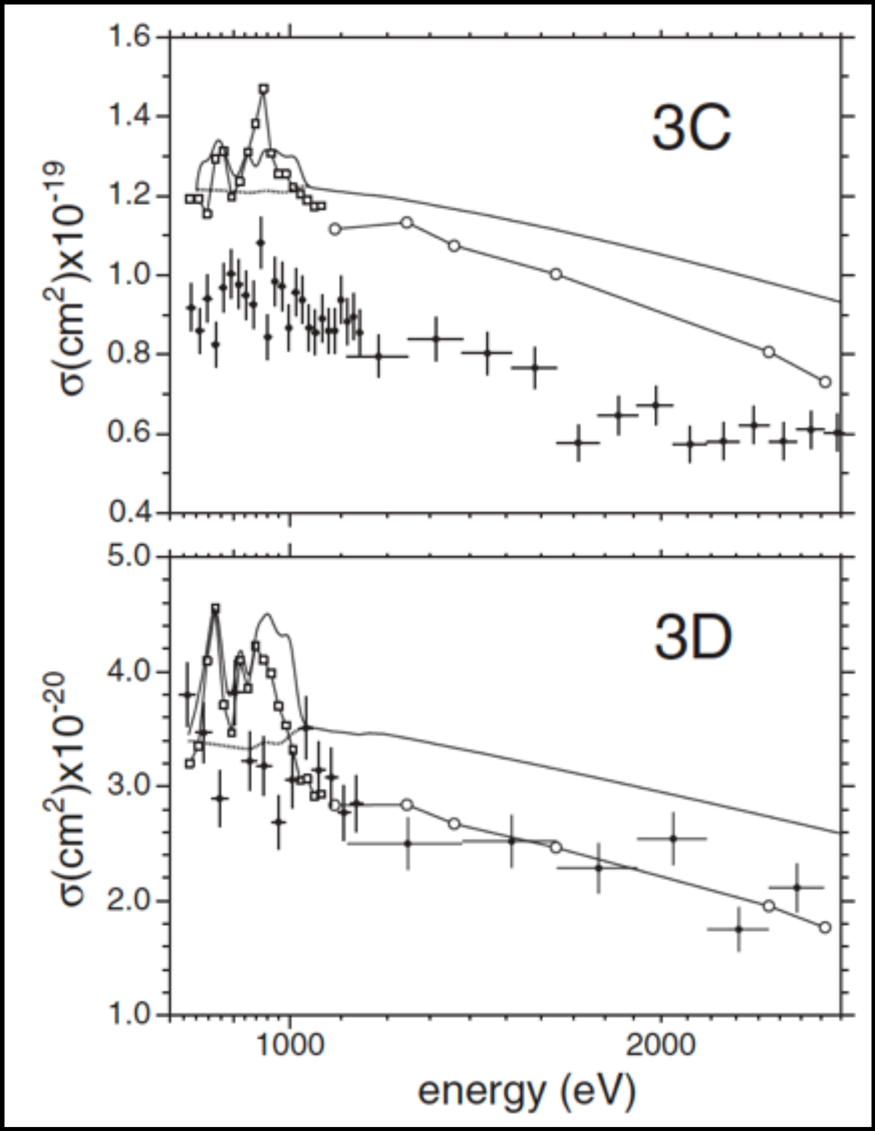
Electron impact excitation cross sections

Electron-impact excitation cross section

ECS *hitomi*-like microcalorimeter spectrum



G. Brown et al. PRL (2006)

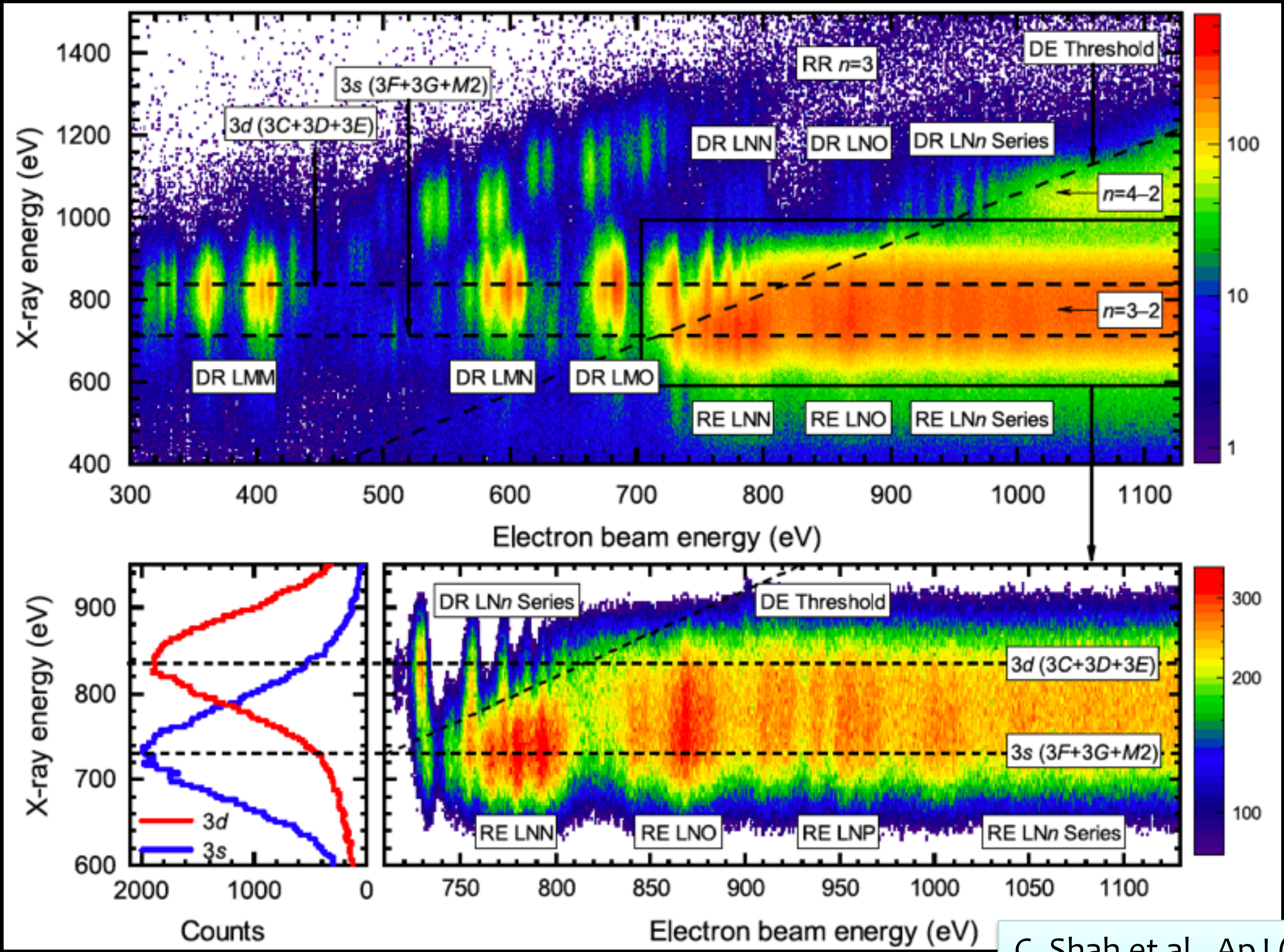


Theory overpredicts 3C cross sections by 20-30% ...

3D seems to be okay!

Optically thin cross sections – crucial for models

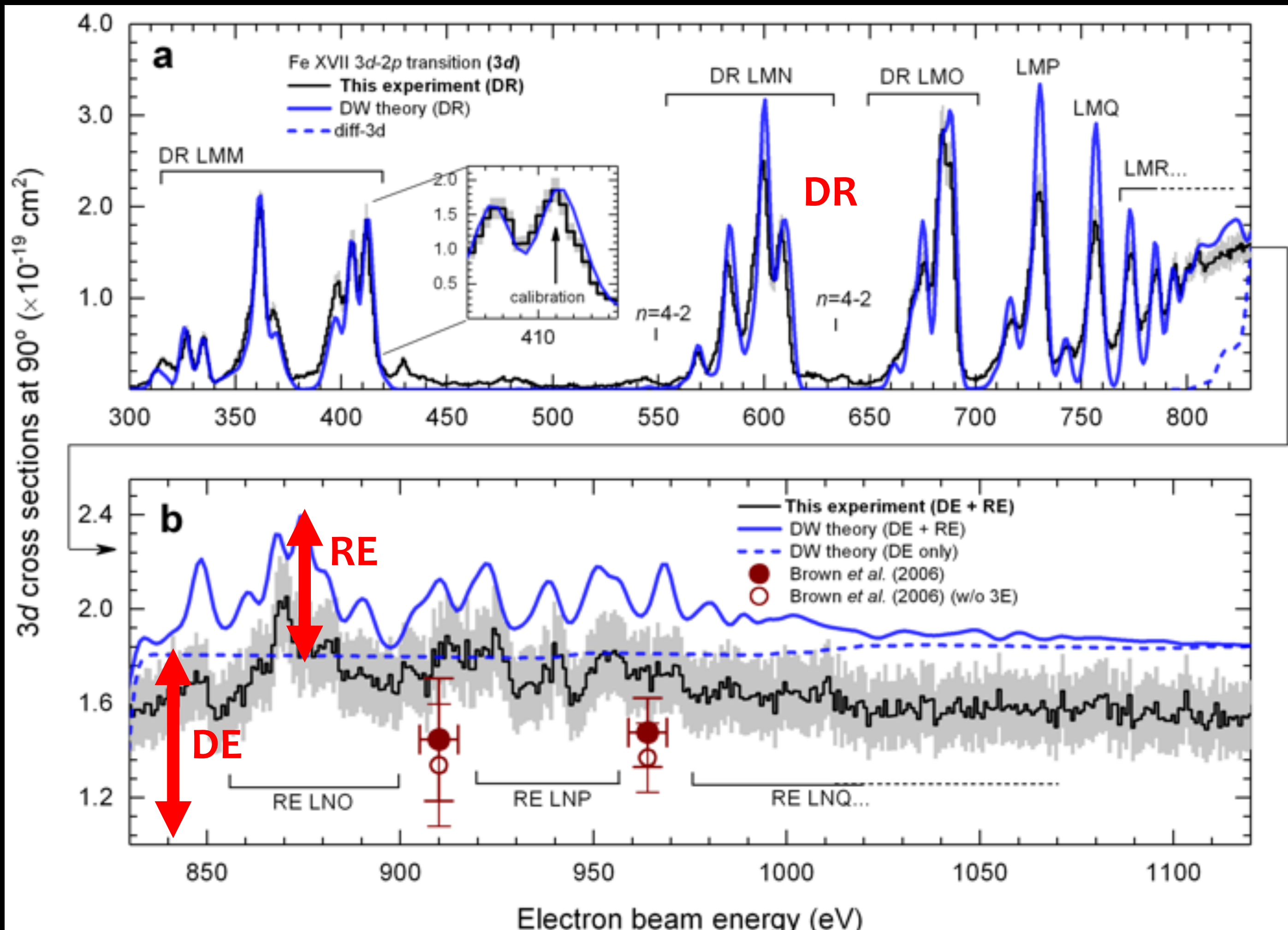
Dielectronic Recombination + Resonance Excitation cross sections



C. Shah et al., ApJ (2019)

Dielectronic Recombination and Resonance Exc.

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



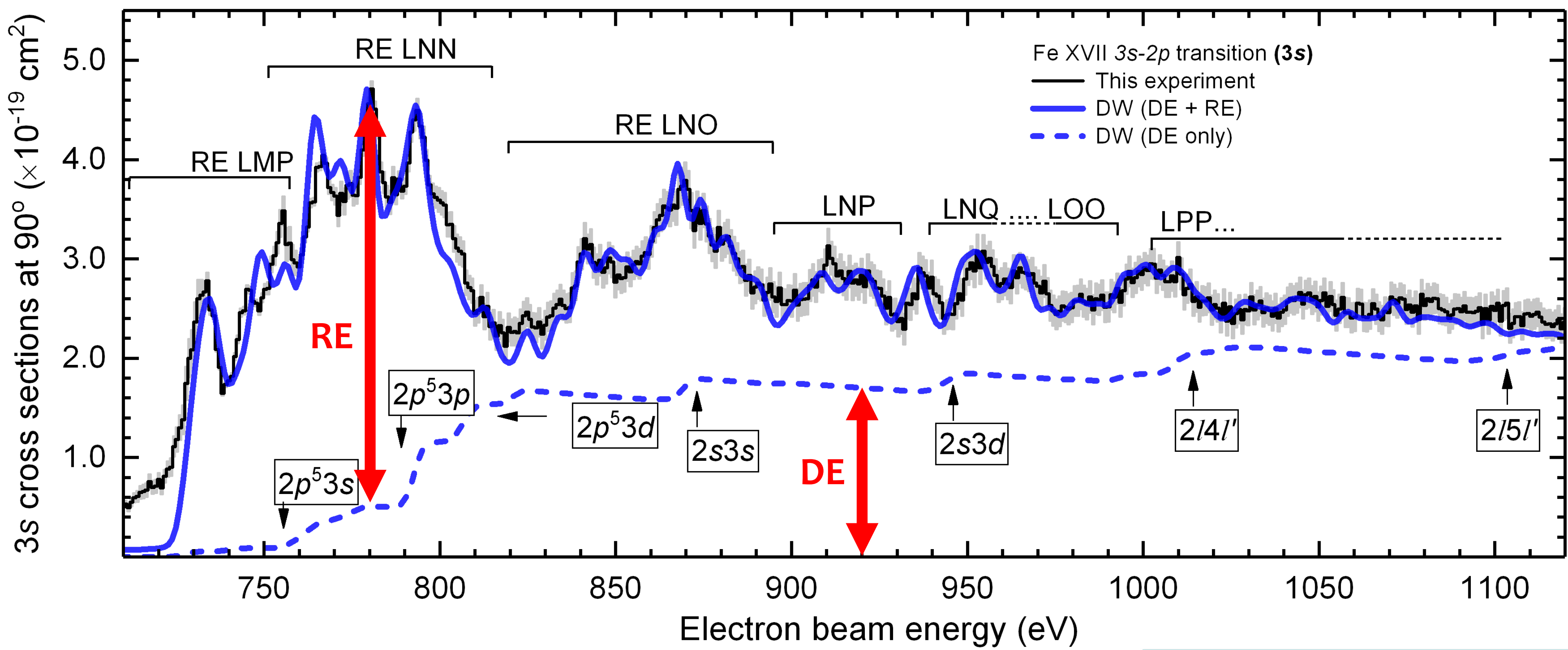
3d DW theory
overpredicts
high-*n* DR,
RE,
CE cross sections
by roughly ~20% ...

C. Shah et al., ApJ (2019)

Resonance Excitation and Cascades

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

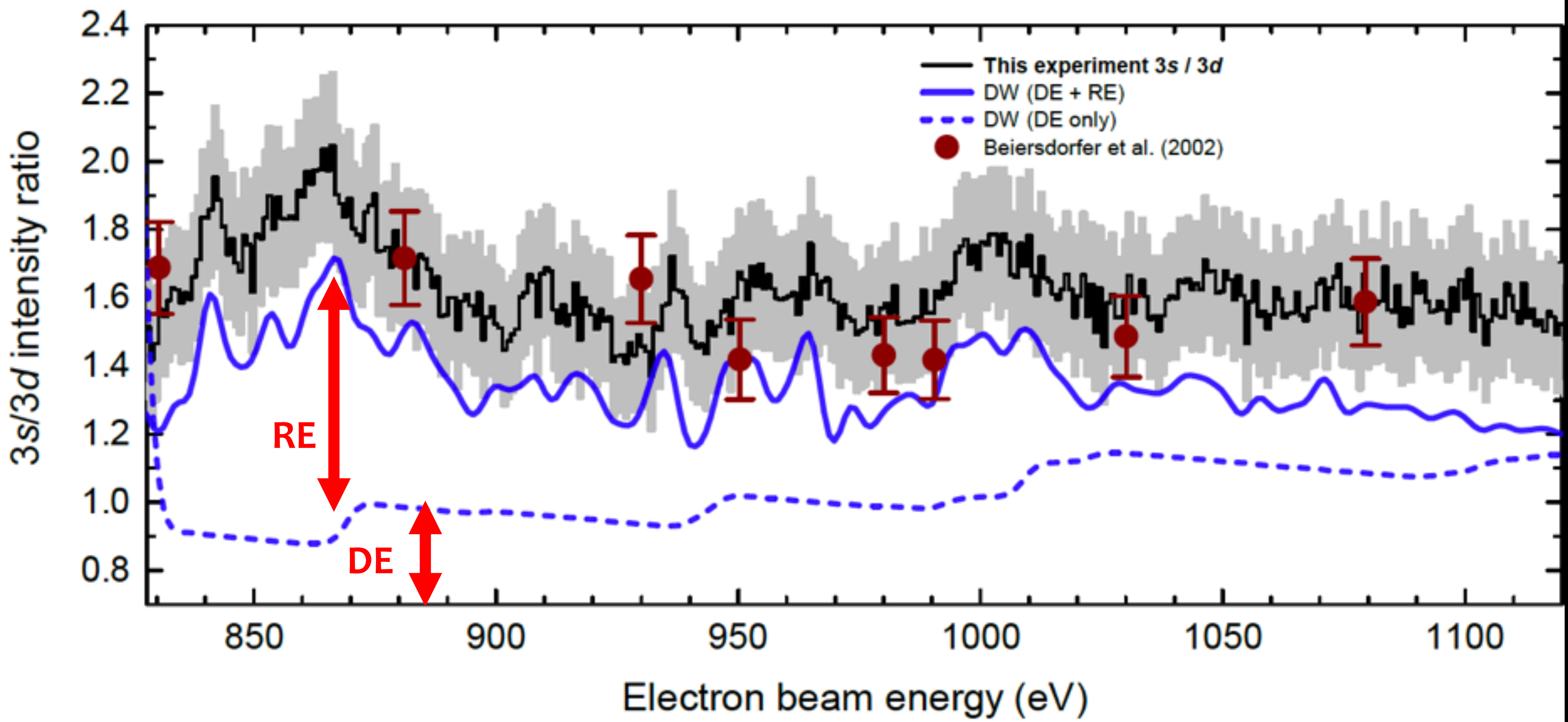
The 3s emission is fully dominated by Resonance Excitation and Cascades



C. Shah et al., ApJ (2019)

3s / 3d line ratio

Still disagree w/ theory (3C can be a culprit behind)



C. Shah et al., ApJ (2019)

Systematic laboratory experiments

Checking of individual atomic components of 3s and 3d

- ~~Electron impact direct excitation~~
- ~~Dielectronic recombination satellites~~
- ~~Resonant excitation~~
- ~~Radiative cascades~~

Checking the most fundamental quantity of any electronic transition

Oscillator strengths (or Einstein Coefficients *A*)