Atomic processes relevant for high-temperature plasmas

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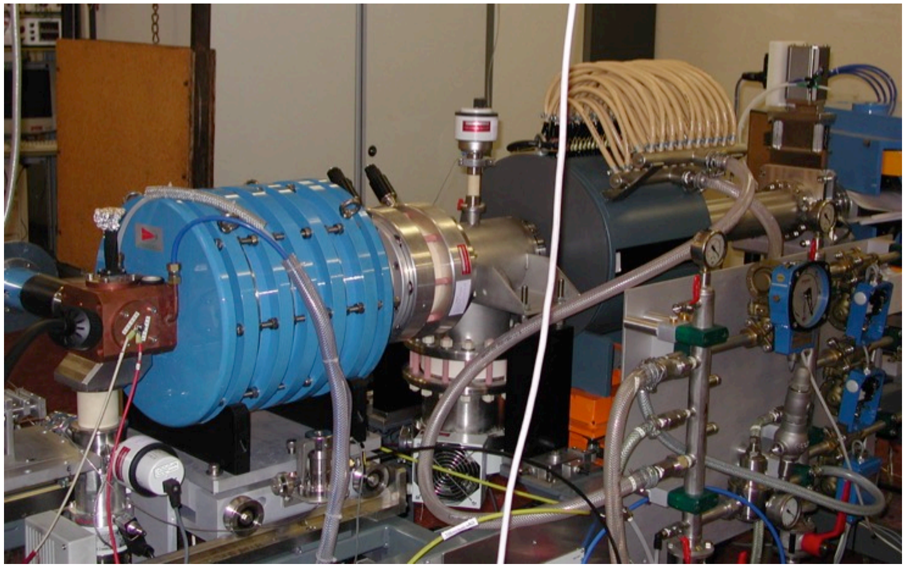
Outline of the talk

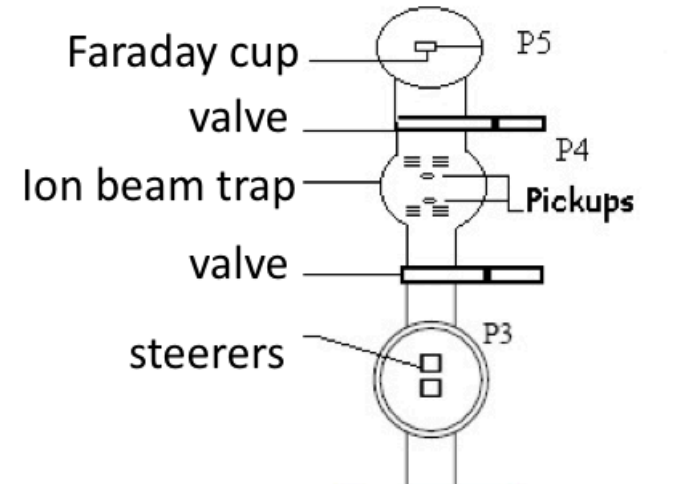
- High-precision reference-free measurements of x-ray transitions in ECRIS plasma
  - Probe and provide tests of BSQED and relativistic effects
  - x-ray standards.

- X-ray spectroscopy in EBIT plasma
  - Iron x-ray lines of astrophysical interest
  - Accurate measurement of electron collision cross sections
  - Preliminary measurements in tungsten

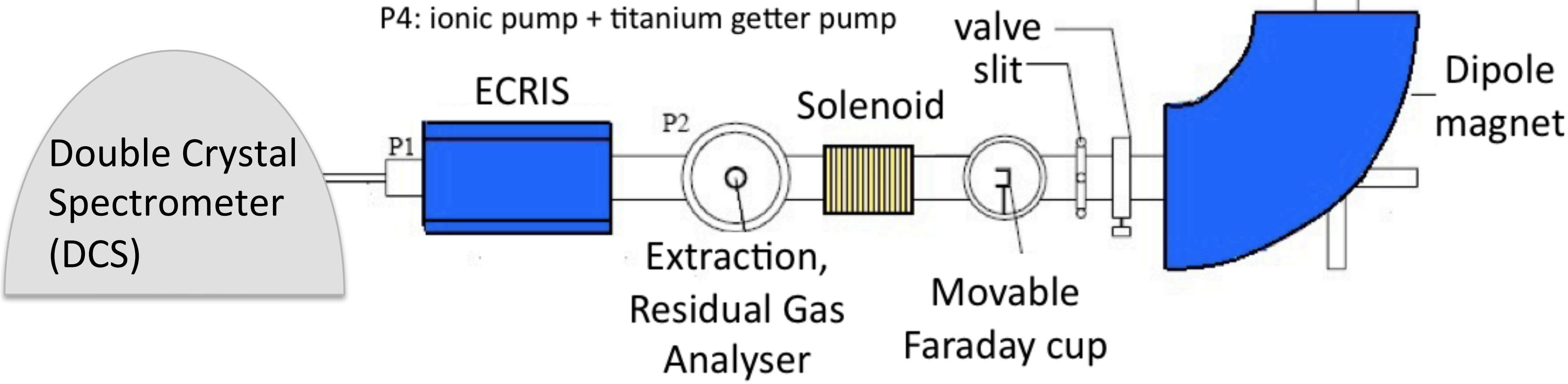
- Electron impact ionization cross section expression
  - Relativistic Binary Encounter Dipole model
  - Calculations for highly charged Kr and U

The SIMPA ECR Ion Source Laboratory





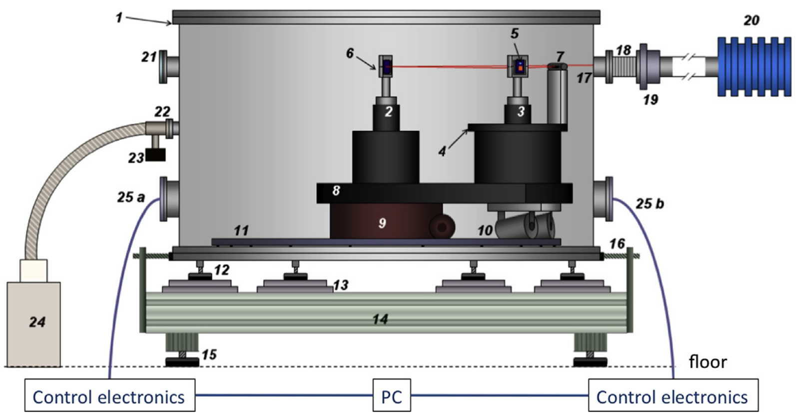
P1, P2, P5: turbo-molecular pump
P3: cryogenic pump
P4: ionic pump + titanium getter pump

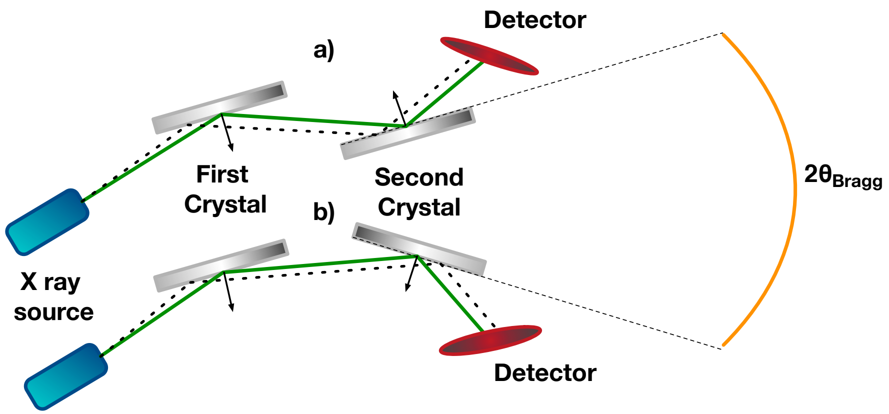


Double crystal spectrometer

The Bragg condition: $n\lambda = 2d\sin(\theta_B)$

can be satisfied in two orientations of the second crystal





The angle difference between the two peak positions is directly correlated to the Bragg angle of the transition in question according to

$$\theta B = [180 - (\theta disp - \theta\ nondis)]/2$$

High-accurate reference-free measurements

DCS simulations

Method:

***P. Amaro**, et. al, Phys. Rev. Lett.* ***109**, 043005(2012).*

Ar $1s2s\ ^3S_1 \rightarrow 1s^2\ ^1S_0$

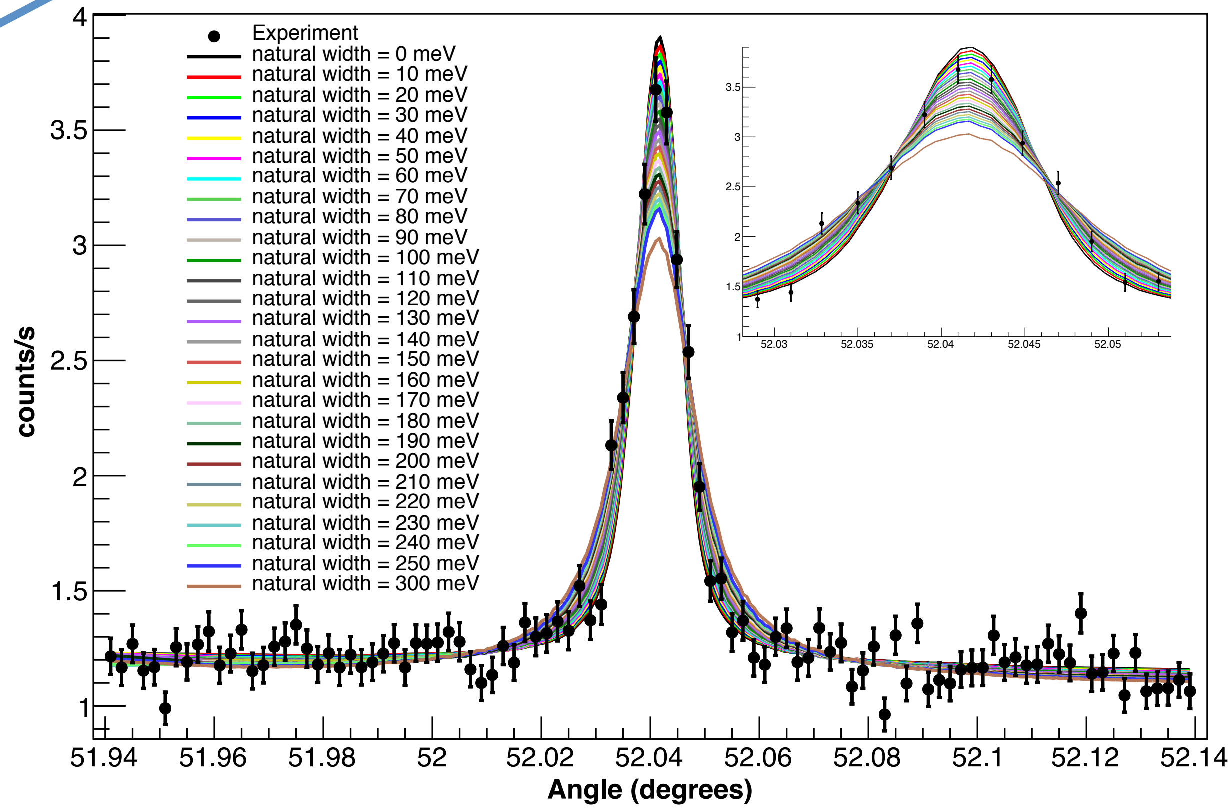
Natural Width < 10^{-6} eV

- Perform several simulations with the calculated theoretical energy ($\mathbf{E}_{th}$) and different Lorentzian width ($\boldsymbol{\Gamma}_L$);
- Exp. Gaussian Broadening ($\boldsymbol{\Gamma}_G$);
- Interpolate the simulated output spectra with splines;
- Fit the antiparallel spectra with the parametrized interpolated functions

$$I(\theta-\theta 0)=I\max S(\theta-\theta 0)+a+b\theta$$

- Get the χ^2 for each performed fit with the optimized fit coefficients by the the χ^2 minimization.

Doppler broadening (FWHM) of 80.5(4.6) meV



***P. Amaro**, et. al, Radia. Phys.s and Chems* ***98**, 132 (2014).*

Latest Measured transitions

- **4 x-ray transitions have been measured in 3 different argon charged states:**

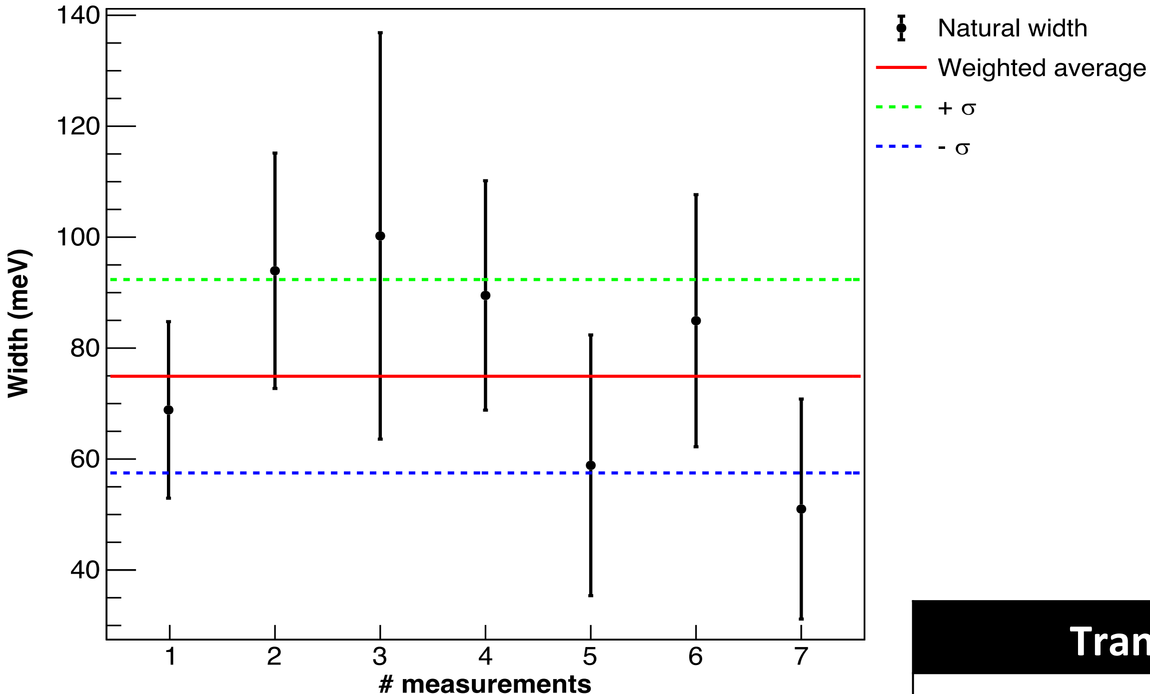
He-like Ar: $1s\,2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$

Be-like Ar: $1s\,2s^2\,2p\ ^1P_1 \rightarrow 1s^2\,2s^2\ ^1S_0$

J. Machado, *et. al, Phys. Rev. A* ***97****, 032517 (2018)*

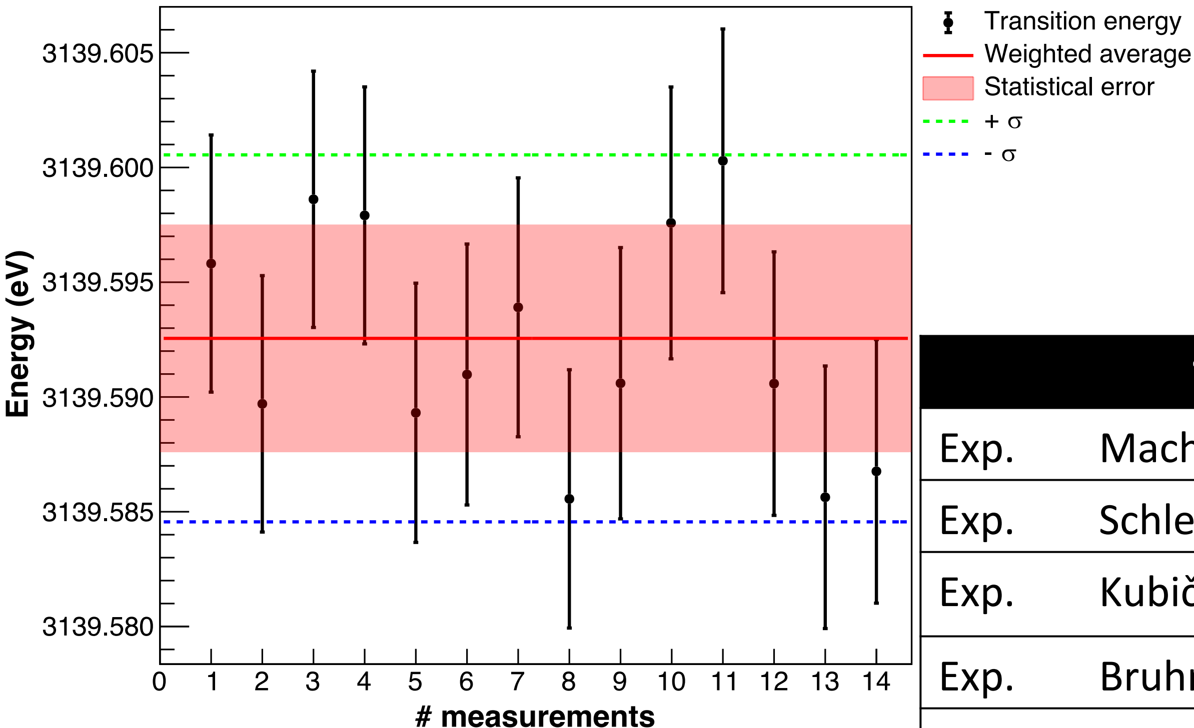
Li-like Ar: $1s\,2s\,2p\ ^2P_J \rightarrow 1s^2\,2s\ ^2S_{1/2}$, J = 1/2, 3/2

1s 2p 1P1 → 1s2 1S0 transition in He-like Ar



Transition Natural Width (meV)		
Exp.	Machado, et al.(2018)	75 (17)
Theo.	Johnson et al.(1995)	70.43
Theo.	Machado et al.(2018)	70.4778 (25)
Theo.	Drake (1979)	70.49 (14)

1s 2p 1P1 → 1s2 1S0 transition in He-like Ar

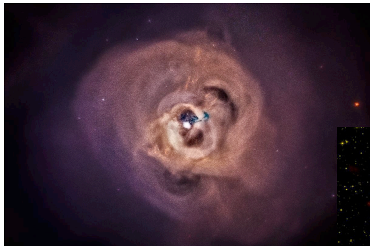


Transition Energy (eV)		
Exp.	Machado, et al.(2018)	3139.5927 (80)
Exp.	Schlesser et al.(2013)	3139.567 (11)
Exp.	Kubiček et al.(2012)	3139.581 (5)
Exp.	Bruhns et al.(2007)	3139.583 (63)
Theo.	Machado *et al.*(2018)	3139.584 (6)
Theo.	Artemyev *et al.*(2005)	3139.5821 (4)
Theo.	Plante *et al.*(1994)	3139.582
Theo.	Cheng *et al.*(1994)	3139.617

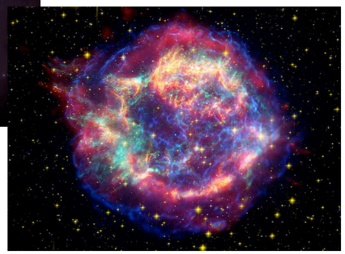
Summary of the goals

- ✓ Presented a high accurate spectrometer
  - ✓ Accuracies up to few ppm@keV
  - ✓ Reference-free
- ✓ Provide high-accurate energy and widths
  - ✓ He-like, Be-like and Li-like Ar
  - ✓ Data for S is currently being analyzed
- ✓ Can be highly profitable in spectra diagnostics based on special x-ray lines, specially metastable ones

X-ray spectroscopy in astrophysics



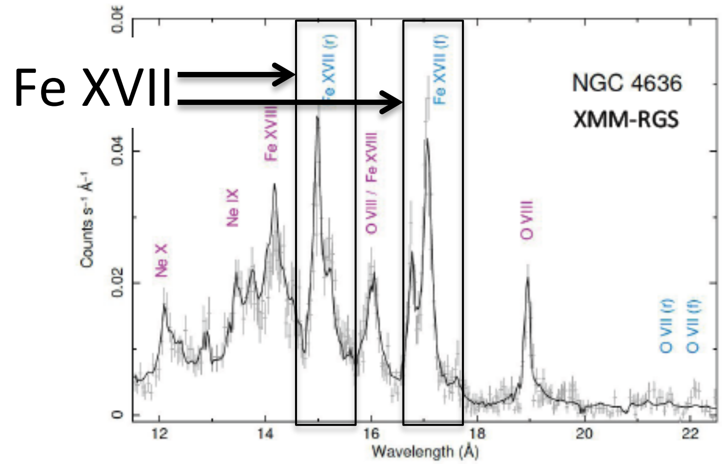
Perseus galaxy cluster



Cassiopeia A

ESA XMM-Newton
RGS - Reflection Grating Spectrometer (0.35-2.5 keV)
~2 eV@1keV

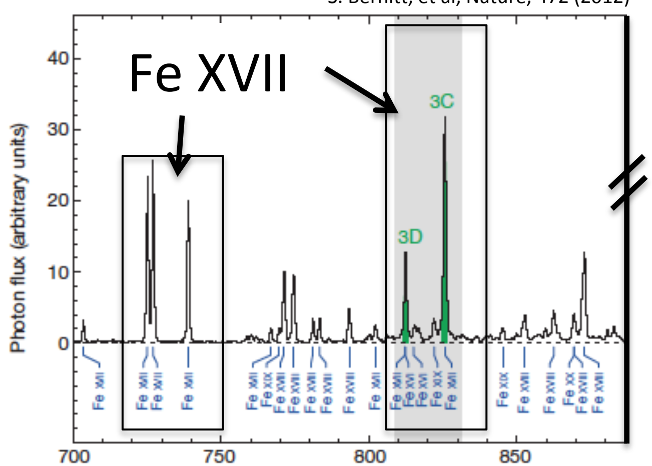
A. Ogorzalek, et al, Monthly Notices of the Royal Astronomical Society, 472 2017



NASA CHANDRA
HETG High Energy Transmission Grating Spectrometer (0.4-10 keV)
~1 eV@1 keV

JAXA ASTRO-H/Hitomi/XARM
SXS micro-calorimeter (0.3-10 keV)
~5 eV@6keV

S. Bernitt, et al, Nature, 472 (2012)

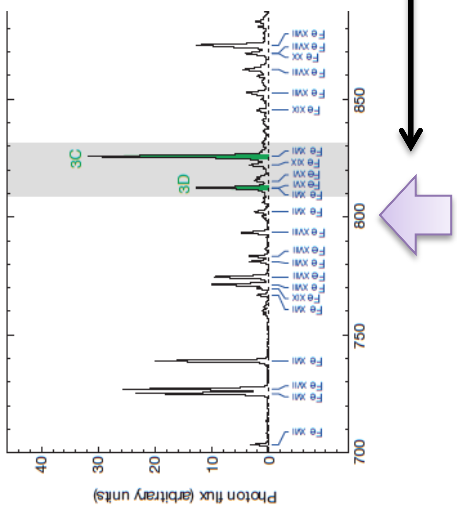


- Interpretation relies heavily on atomic data and plasma modeling and provides diagnostics of:
  - Ionic and electron temperatures
  - Densities and elemental abundances
  - X-ray opacities and velocity turbulences
  - Well-known codes: SPEX and AtomDB

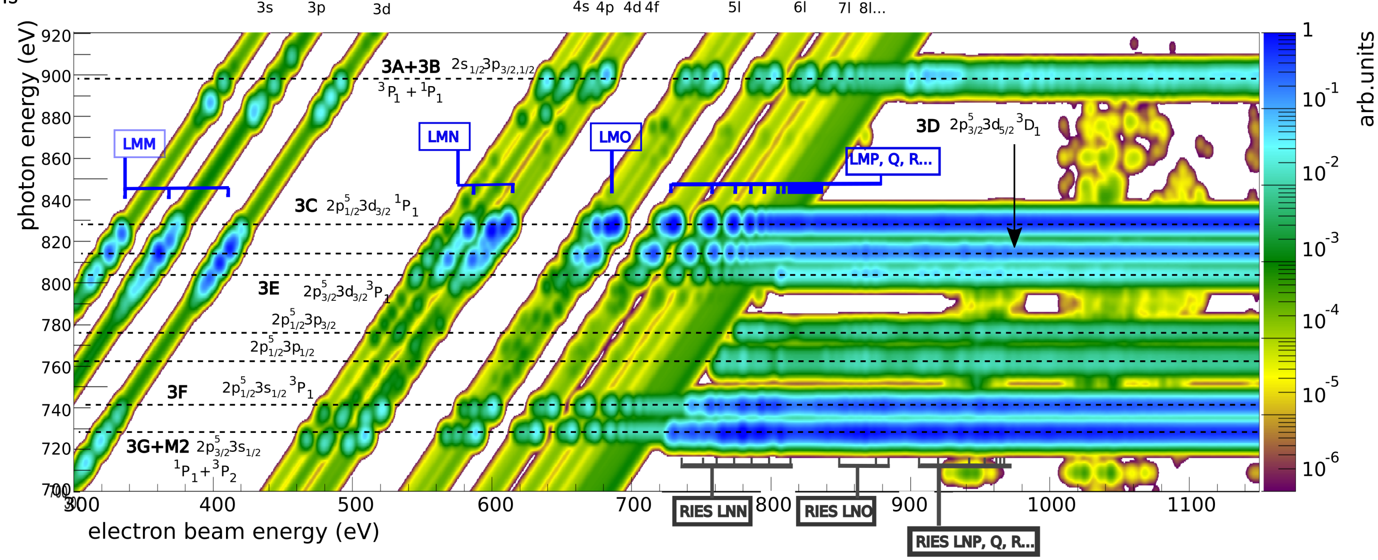
de Plaa, A&A, 539, 2012 and refs thererin

XVII Fe L-shell data

Electrons with Maxwell
or other thermal distributions



Fe XVII= Fe^{16+} (Ne-like Fe) ground state- $1s^2\ 2s^2 2p^6$

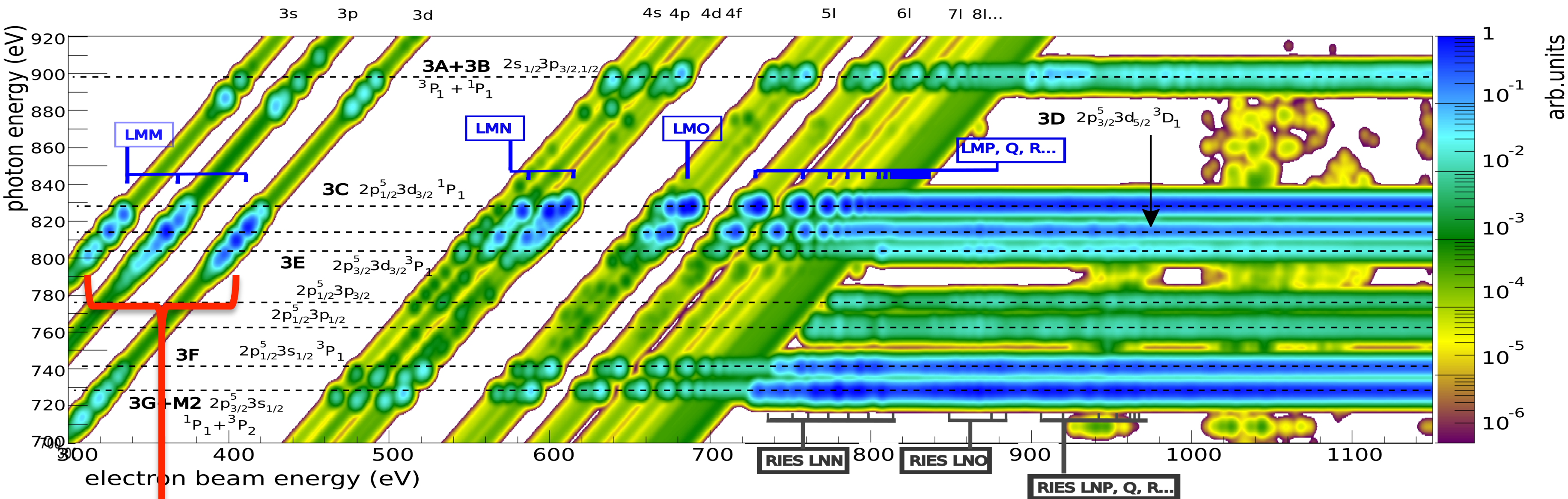


Important lines for x-ray opacity diagnostics based on photon resonant scattering

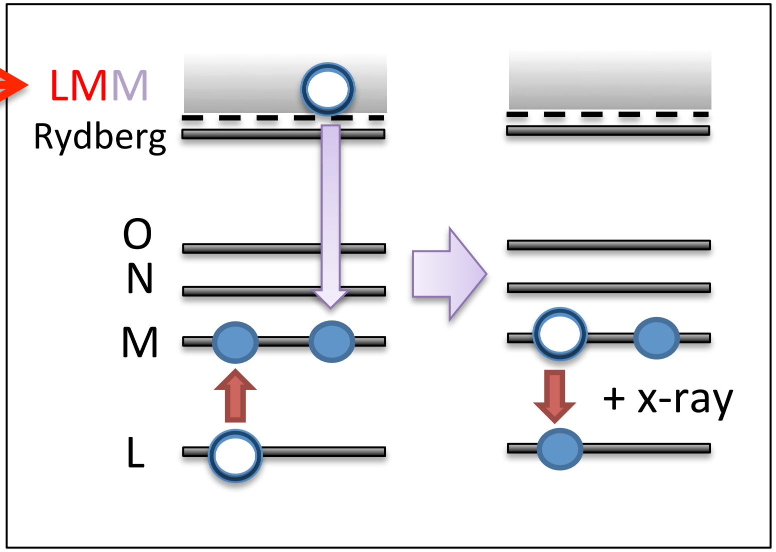
- **3C** $2p^5_{1/2}3d_{3/2}\ ^1P_1$
- **3D** $2p^5_{3/2}3d_{5/2}\ ^3D_1$
- 3C/3D ratio
  - Low cascade contributions
    - R. Mewe et al, A&A, 368, 888-900 (2001).
  - 3C collision strengths inconsistent with predictions
    - e.g. G. V. Brown, et al PRL, 96, 253201 (2006)
    - e.g. S. Bernitt, et al, Nature, 472, 225 (2012)

- **3F** $2p^5_{1/2}3s_{1/2}\ ^3P_1$
- **3G+M2** $2p^5_{3/2}3s_{1/2}\ ^1P_1 + ^3P_2$
- 3F/(3G+M2) ratio
  - M2 is optically thinner (M2 transition)
    - J. de Plaa, et al A&A, 539 (2012).
  - Complex cascade contributions
    - No experimental data available
    - Residual theoretical predictions

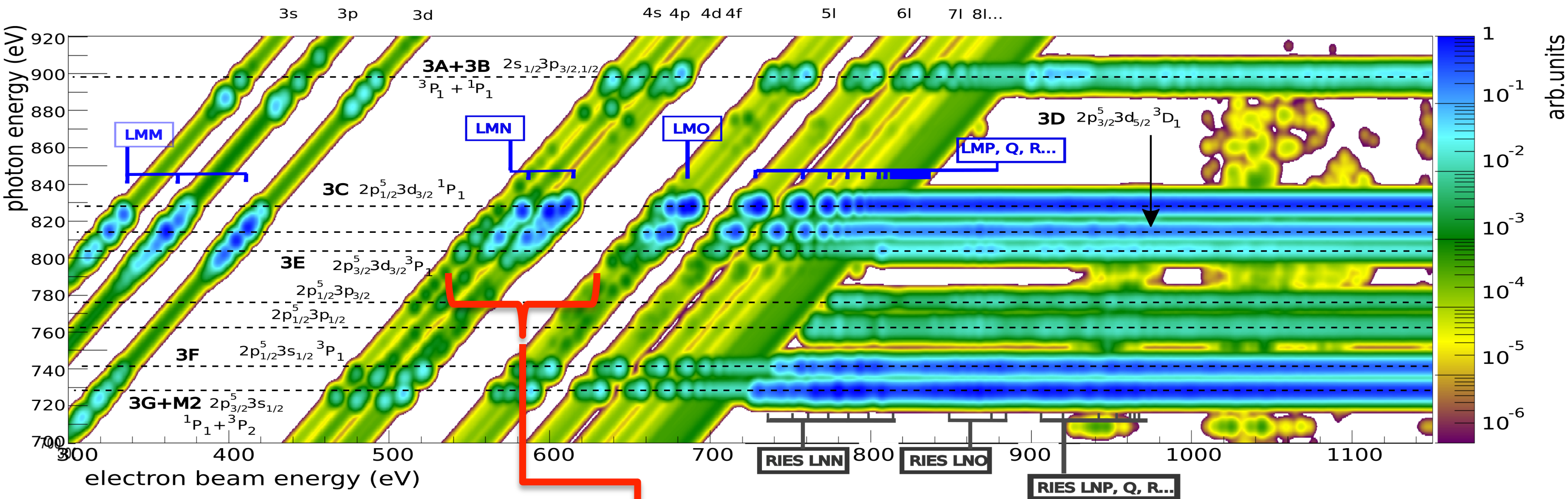
Atomic processes in Fe XVII



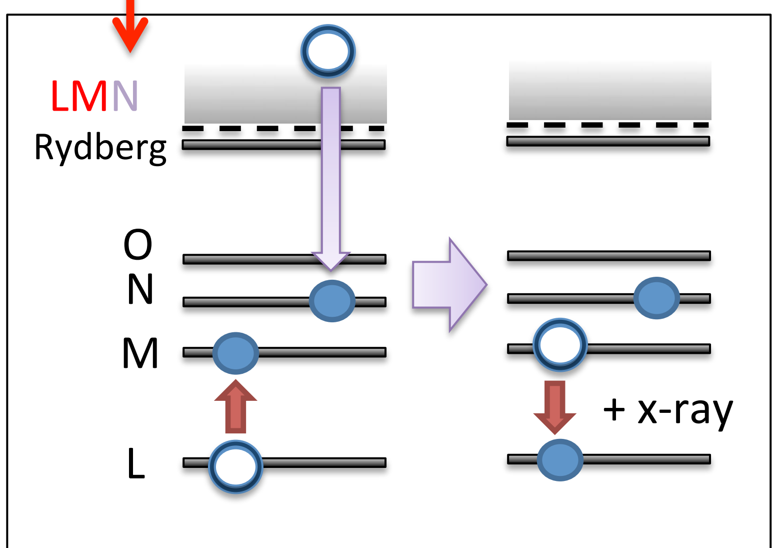
Dielectronic recombination (DR)



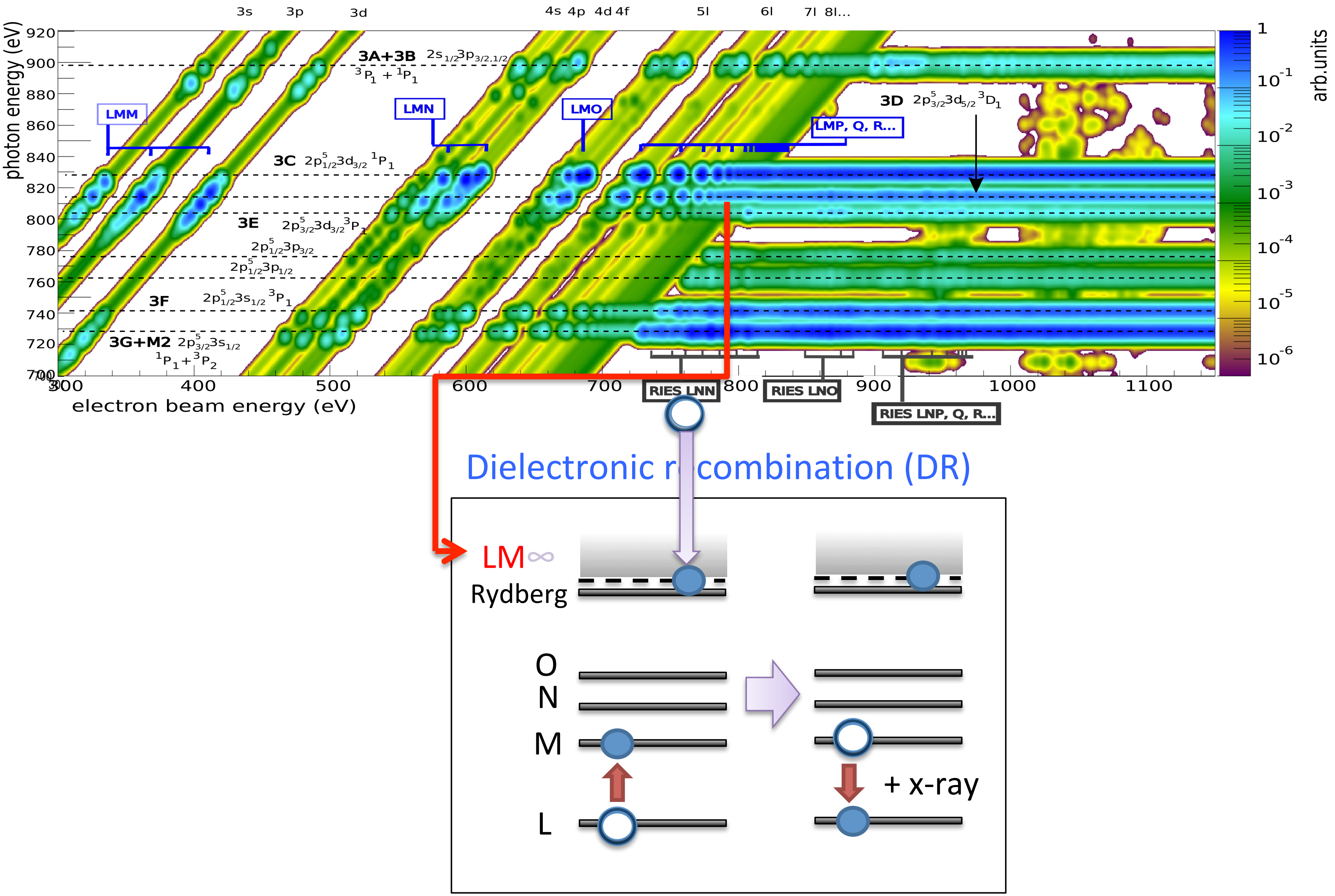
Atomic processes in Fe XVII



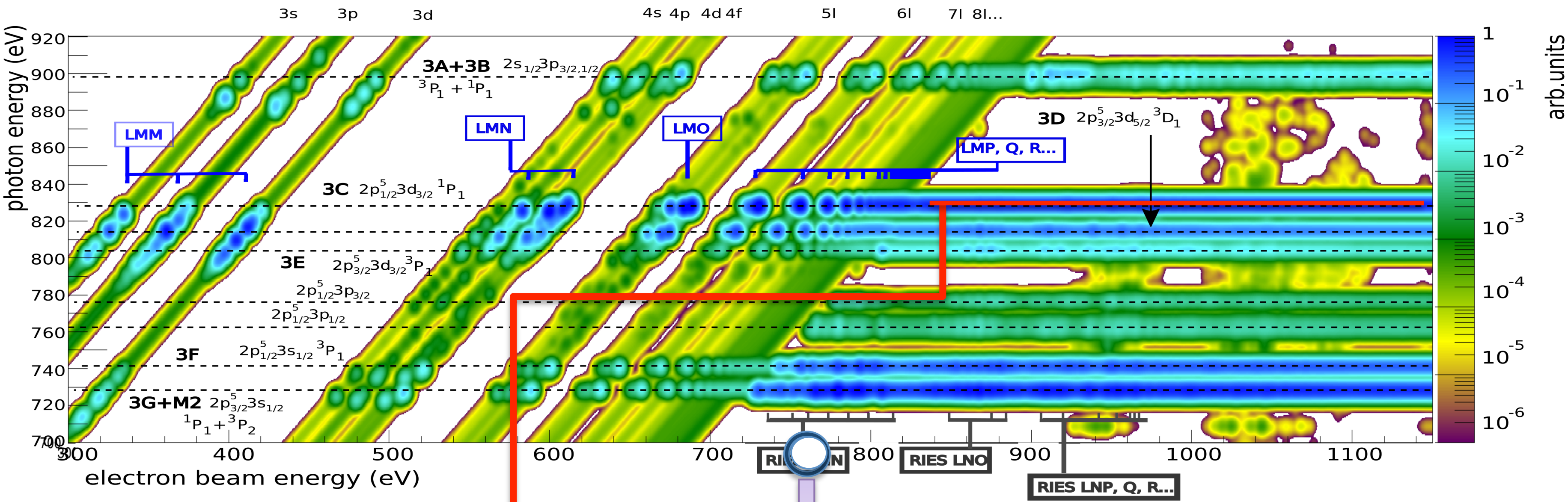
Dielectronic recombination (DR)



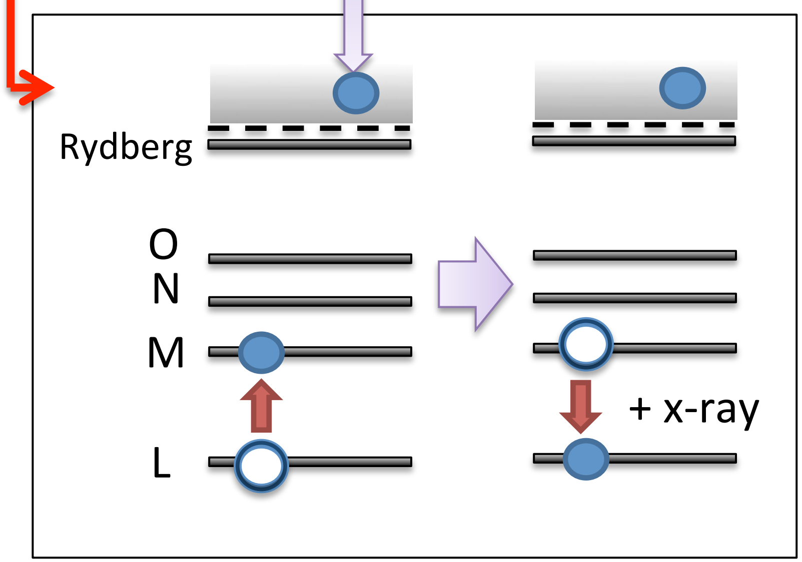
Atomic processes in Fe XVII



Atomic processes in Fe XVII



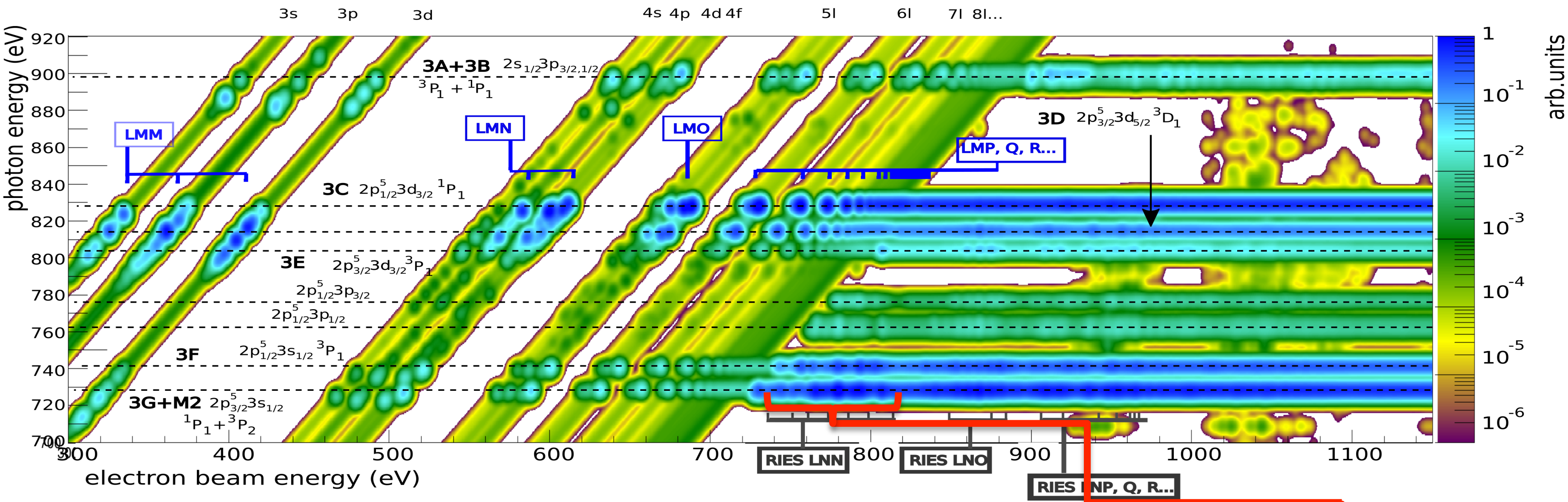
Collision excitation (CE)



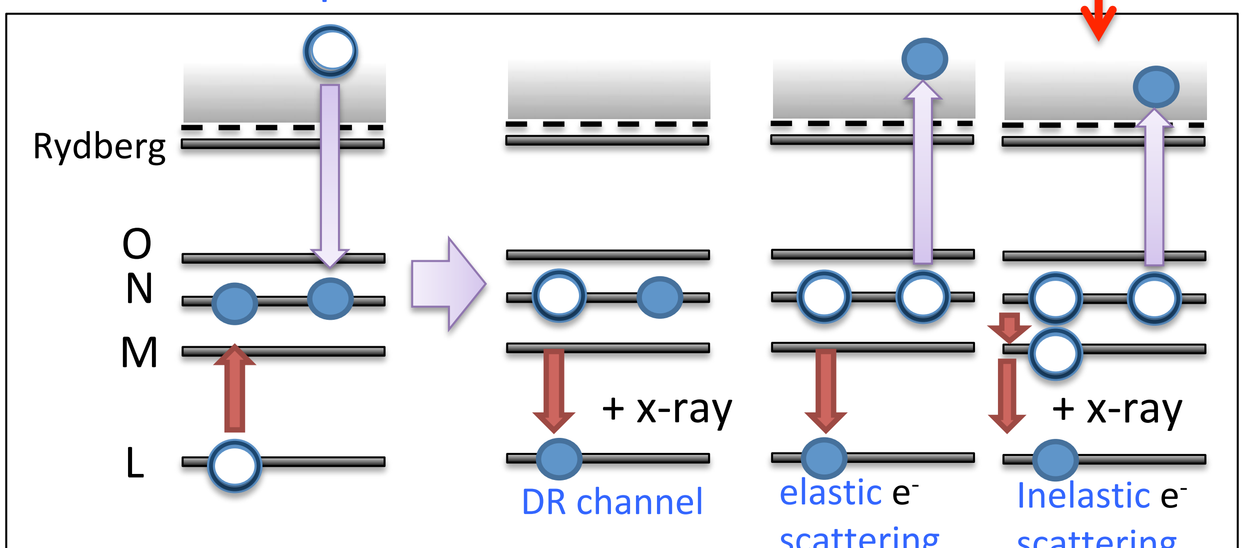
Goal of this work

- Investigate how the inclusion of the spectator electron after DR converge towards the 3C/3D CE

Atomic processes in Fe XVII



Dielectronic capture



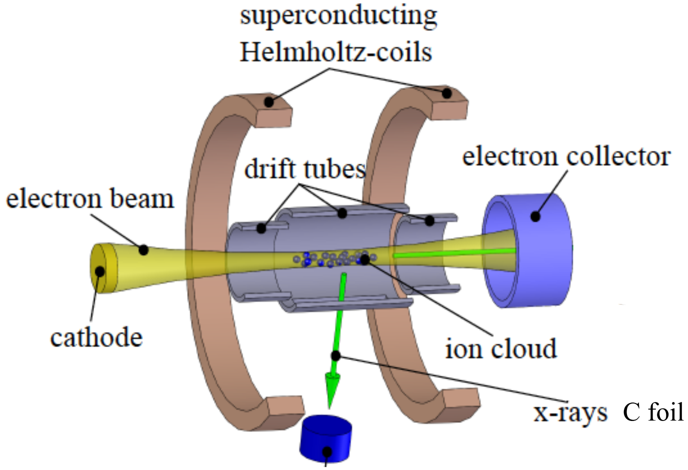
Resonant inelastic electron scattering (RIES)

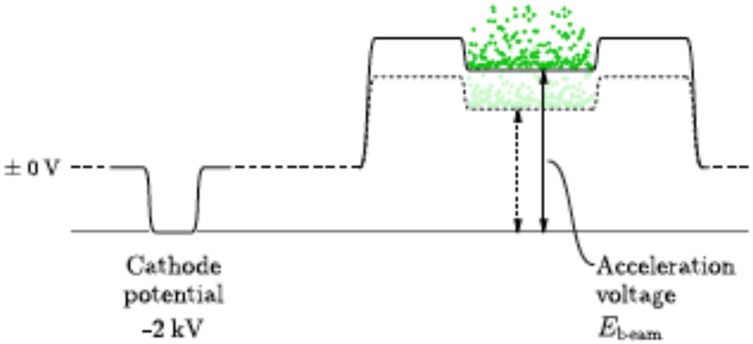
Goal of this work

- Provide data for the 3F+3G+M2 lines

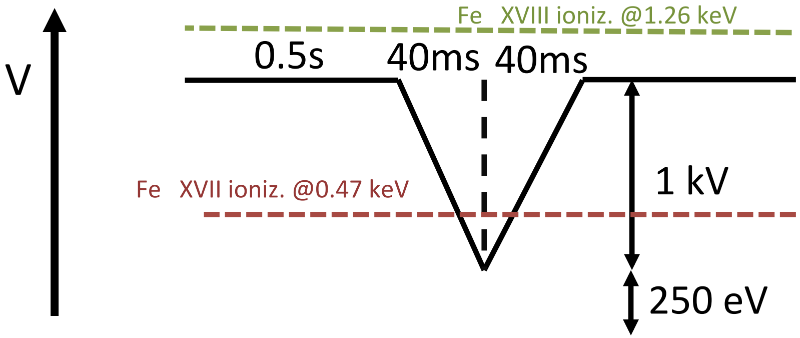
Experimental setup: electron beam ion trap

- FLASH-EBIT @Heidelberg





- Hot plasma with a monoenergetic electron beam
- Scan setup

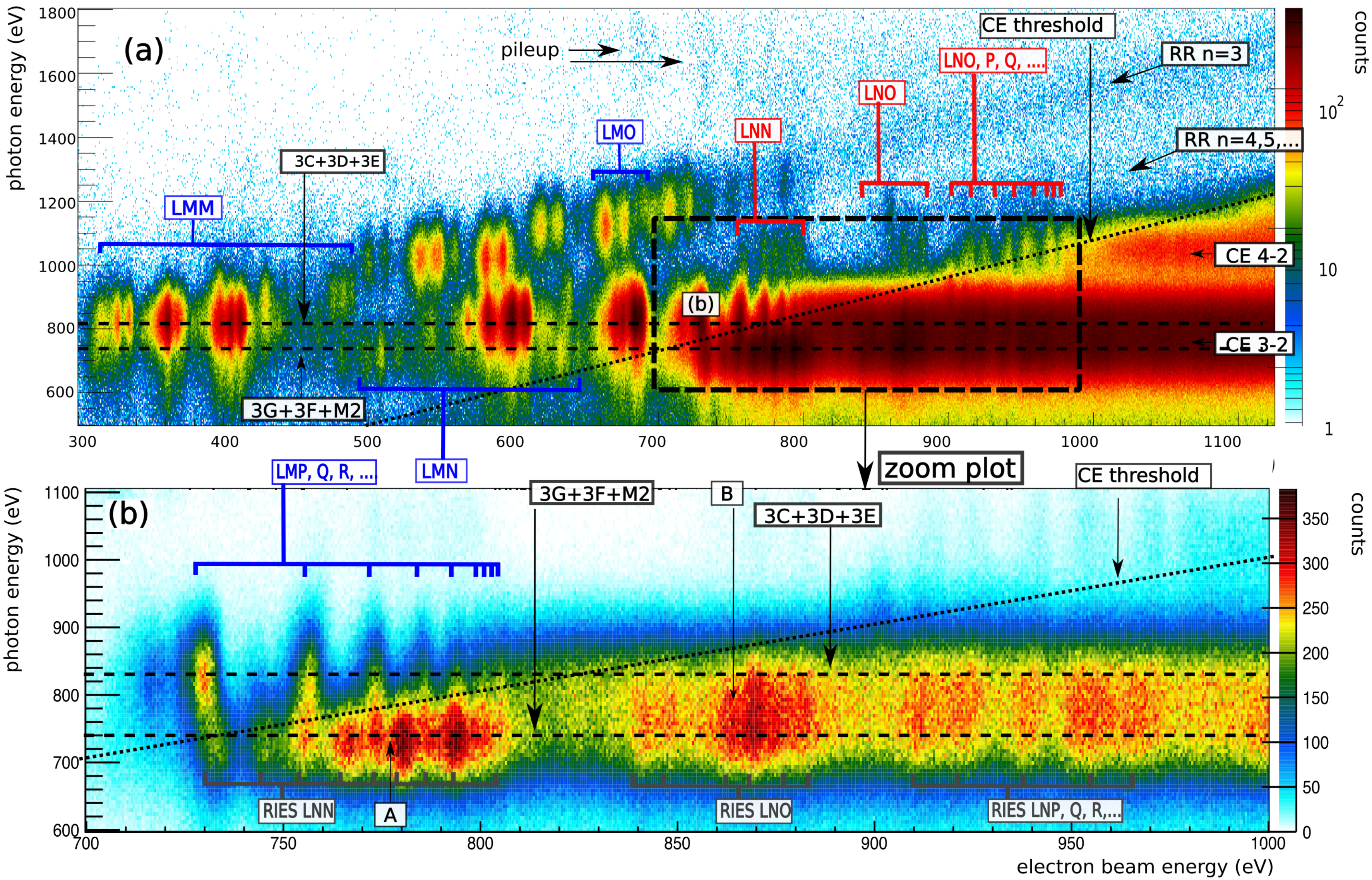


- Electron density current constant

$$n_e \propto I_e/\sqrt{E}$$

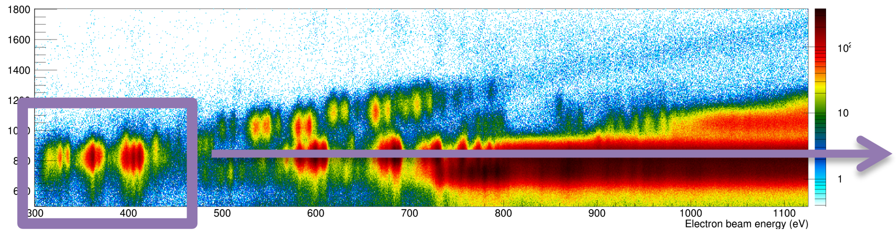
- Evaporative cooling for a electron energy resolution of 5 eV@900eV

Measurement example



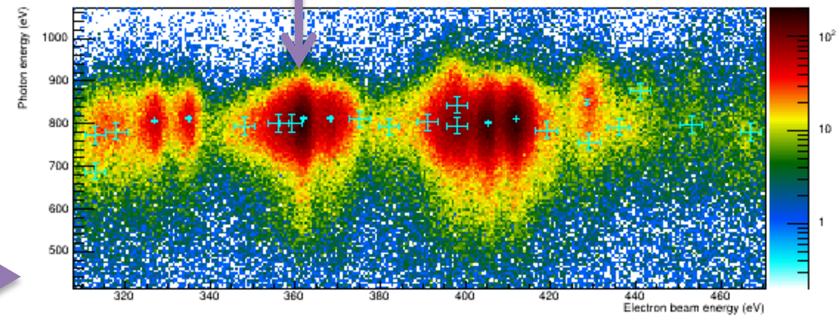
Data analyses

- 2D fit with detector response function
- Main LMM resonance used

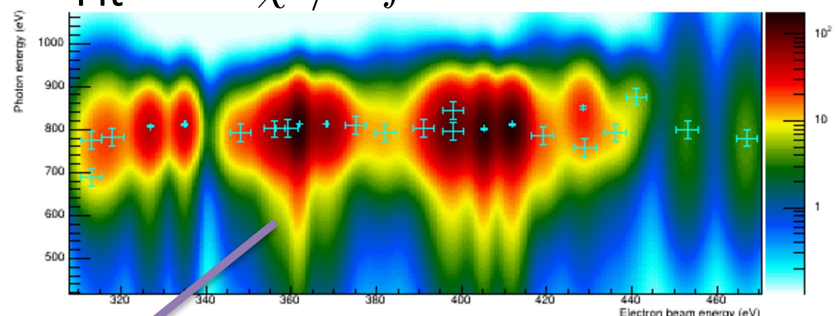


LI Zhe, *et al*, Nuclear Science and Techniques **24** (2013) 060206

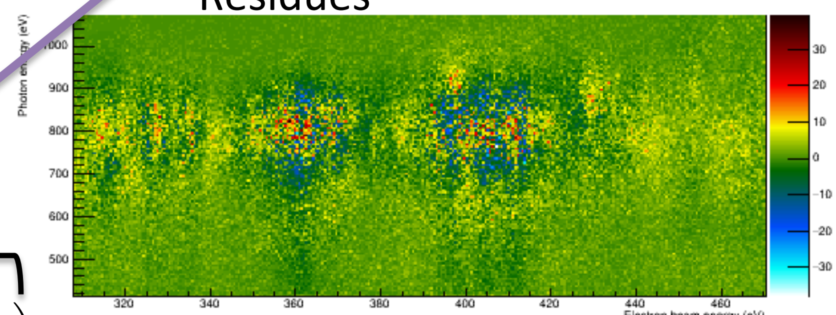
Data

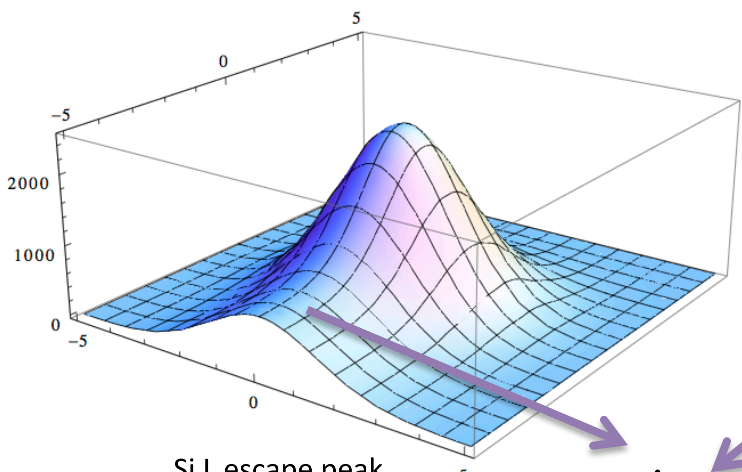


Fit $\chi^2/ndf = 1.6$



Residues

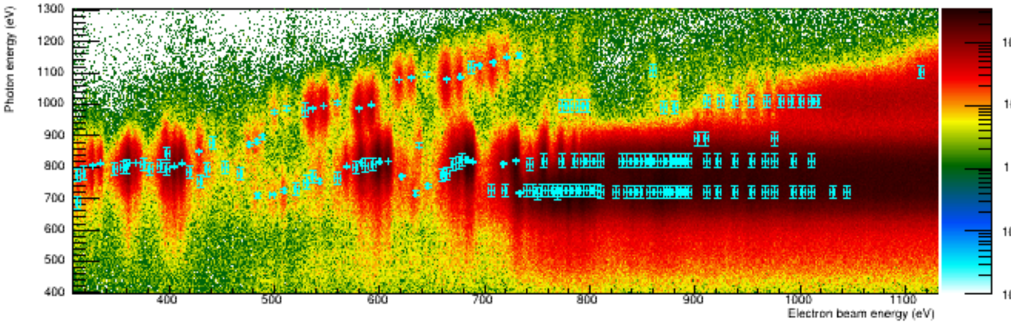




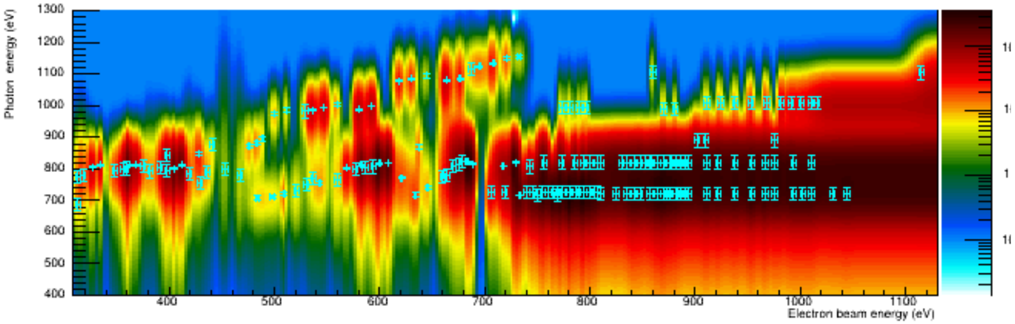
$$f(x,y) = C_1 e^{-\frac{(x-x_0)^2}{2\sigma_x^2}} \left(C_2 e^{-\frac{(y-y_0)^2}{2\sigma_y^2}} + \overbrace{C_3 e^{\frac{y-y_0}{\sigma'_y}} Erfc\left(\frac{y-y_0}{C_4\sigma_y} + \frac{\sigma_y}{C_4\sigma'_y}\right)}^{\text{Si L escape peak tail and compton}} \right)$$

Data analyses

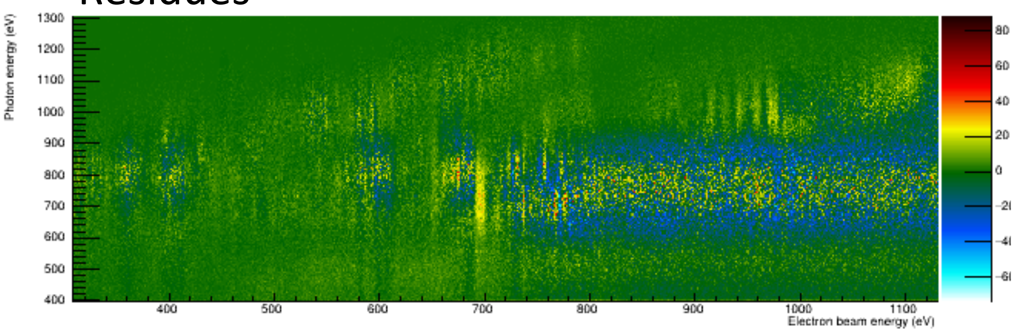
Data



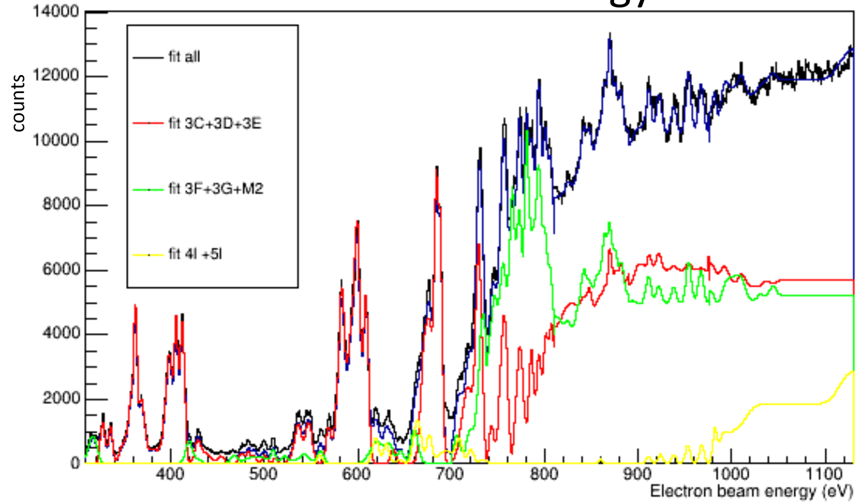
Fit

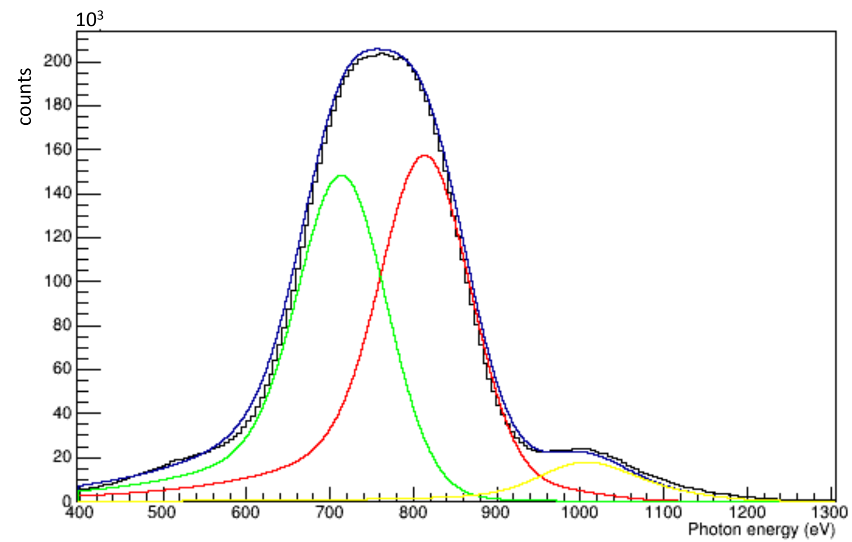


Residues



Sum over an electron energy



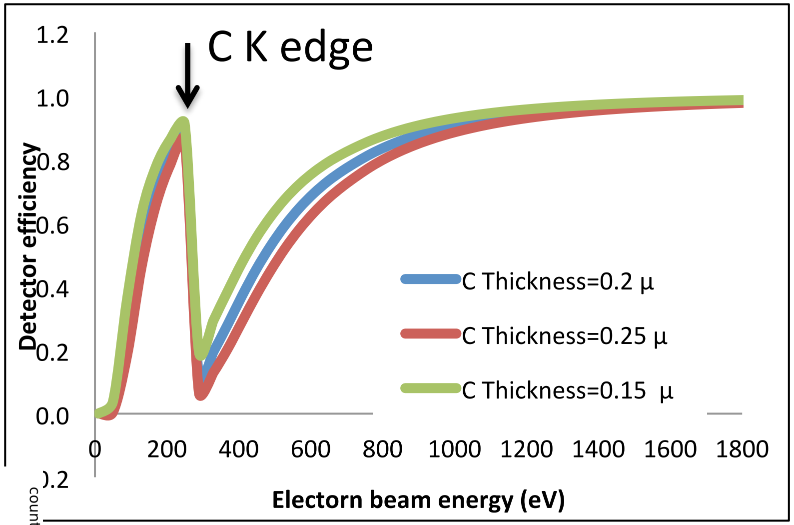


Sum for a photon energy

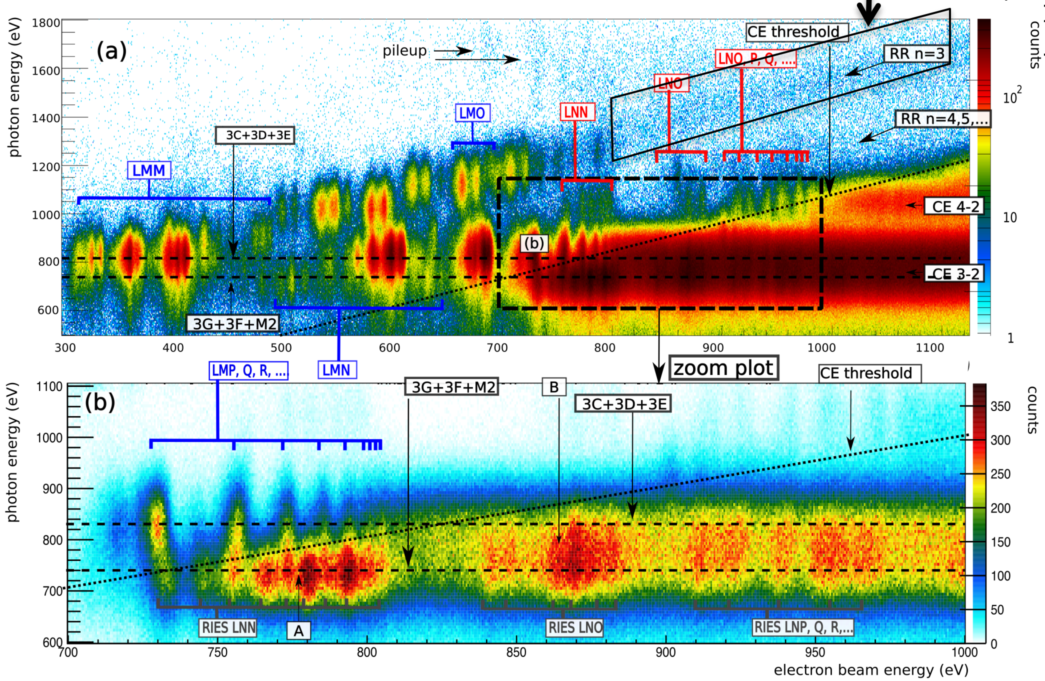
Cross section calibration based on RR

- RR cross sections calculated with 5% error
- Similar method of

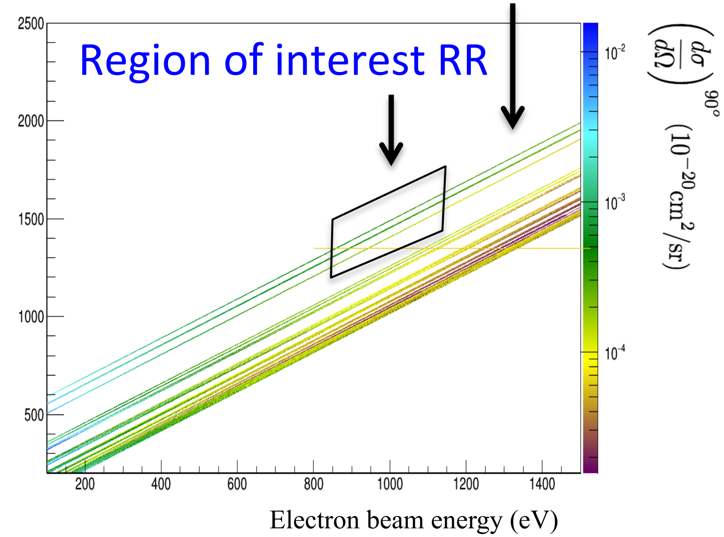
G. V. Brown, et al PRL, 96, 253201 (2006)



Region of interest RR

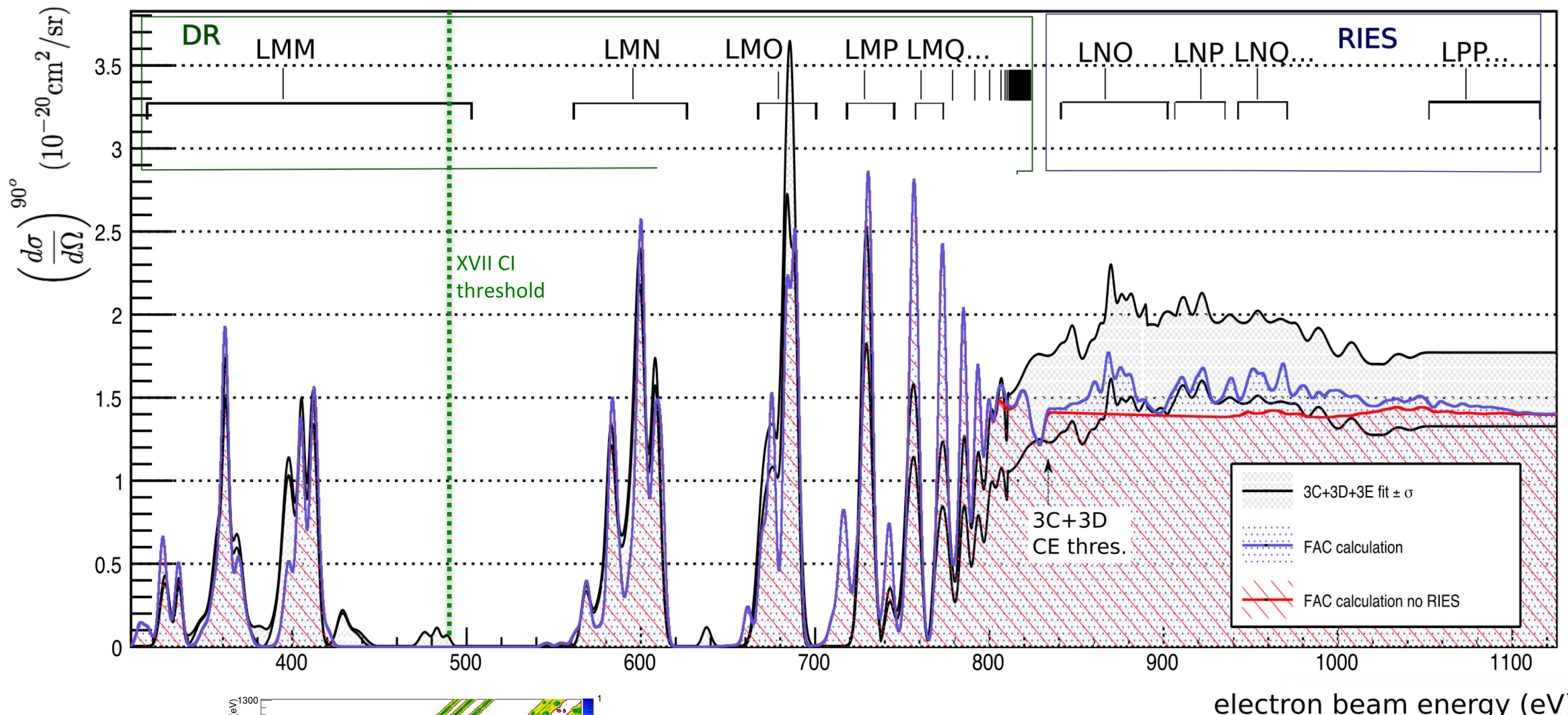


E. Saloman et al., At. Data Nucl. Data Tables 38, 1 (1988)

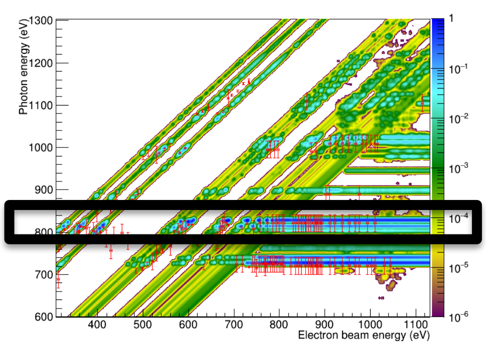


Results for 3C+3D+3E

- Region of interest of 3C+3D+3E for the entire scan



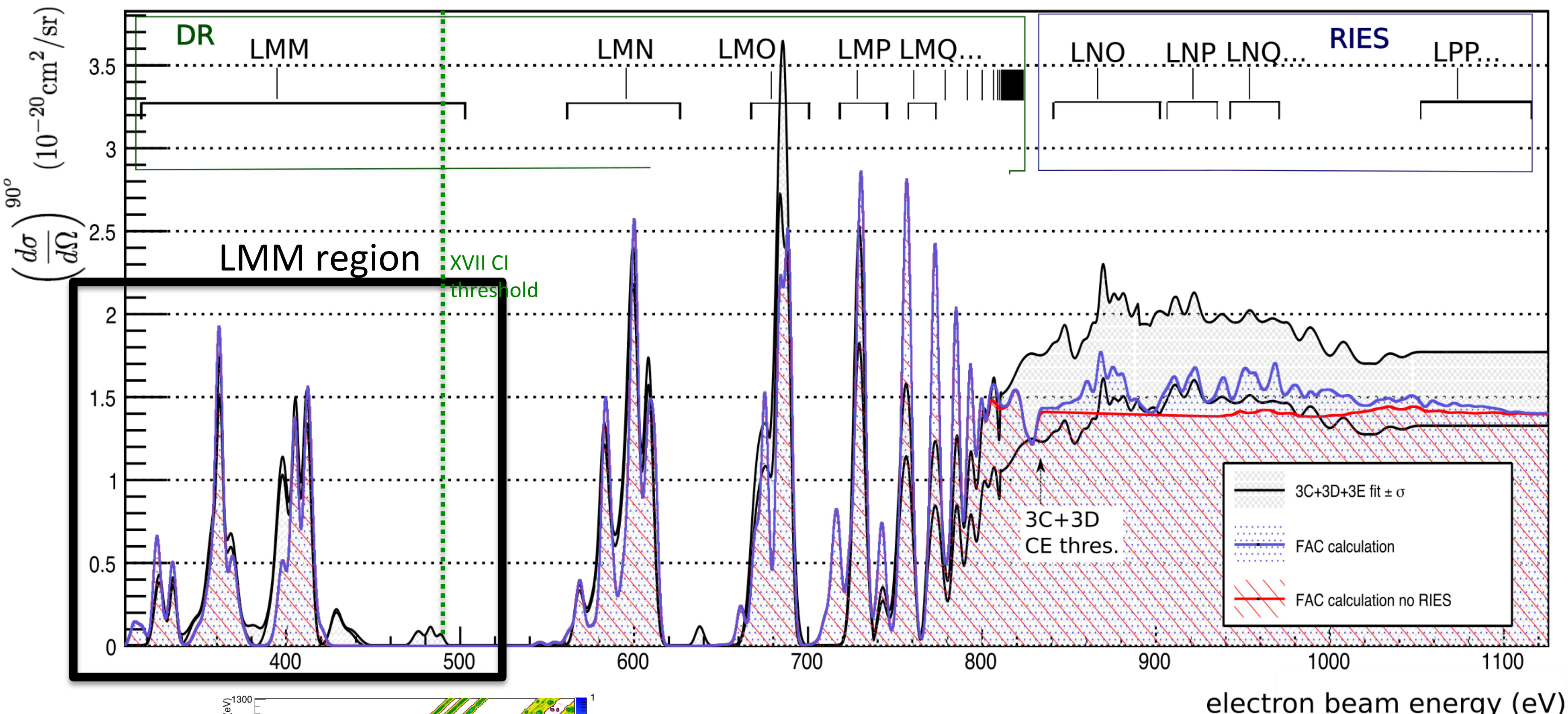
FAC-Flexible atomic code



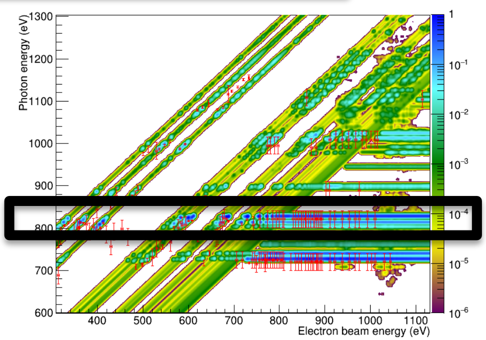
3C+3D+3E

Results for 3C+3D+3E

- Region of interest of 3C+3D+3E for the entire scan

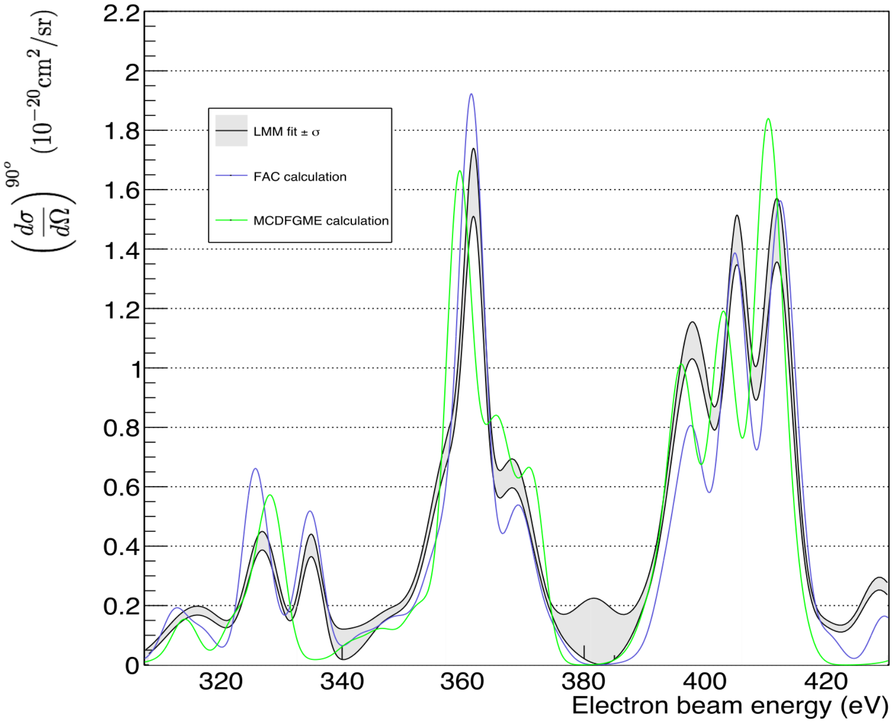


FAC-Flexible atomic code



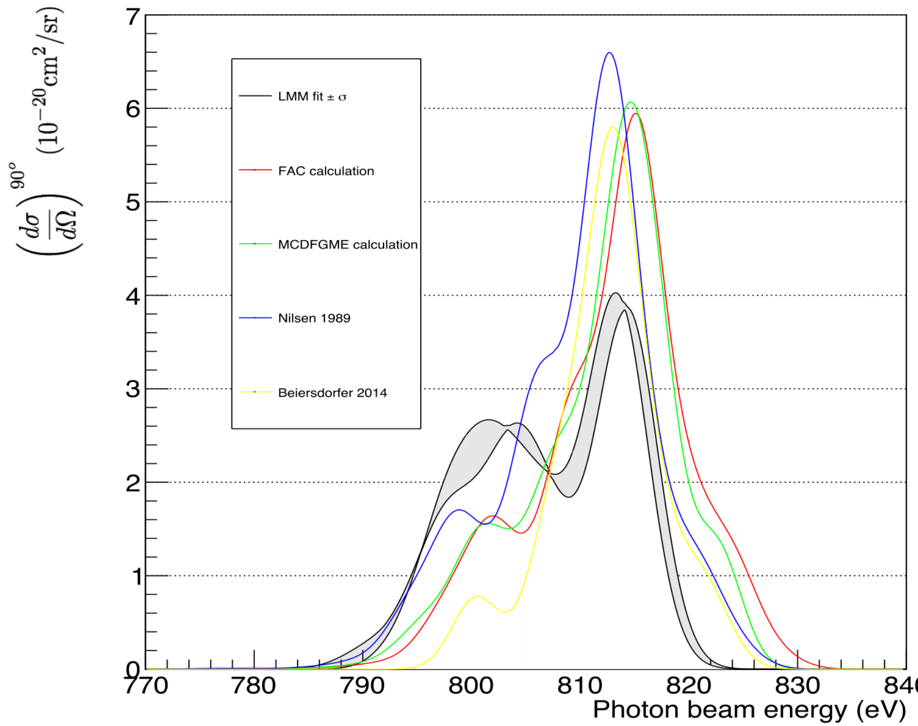
Results 3C+3D+3E LMM region

Sum over photon energy



- FAC-Flexible atomic code
- Multiconfiguration Dirac-Fock (MCDFGME) code of P. Indelicato and J.-P. Desclaux

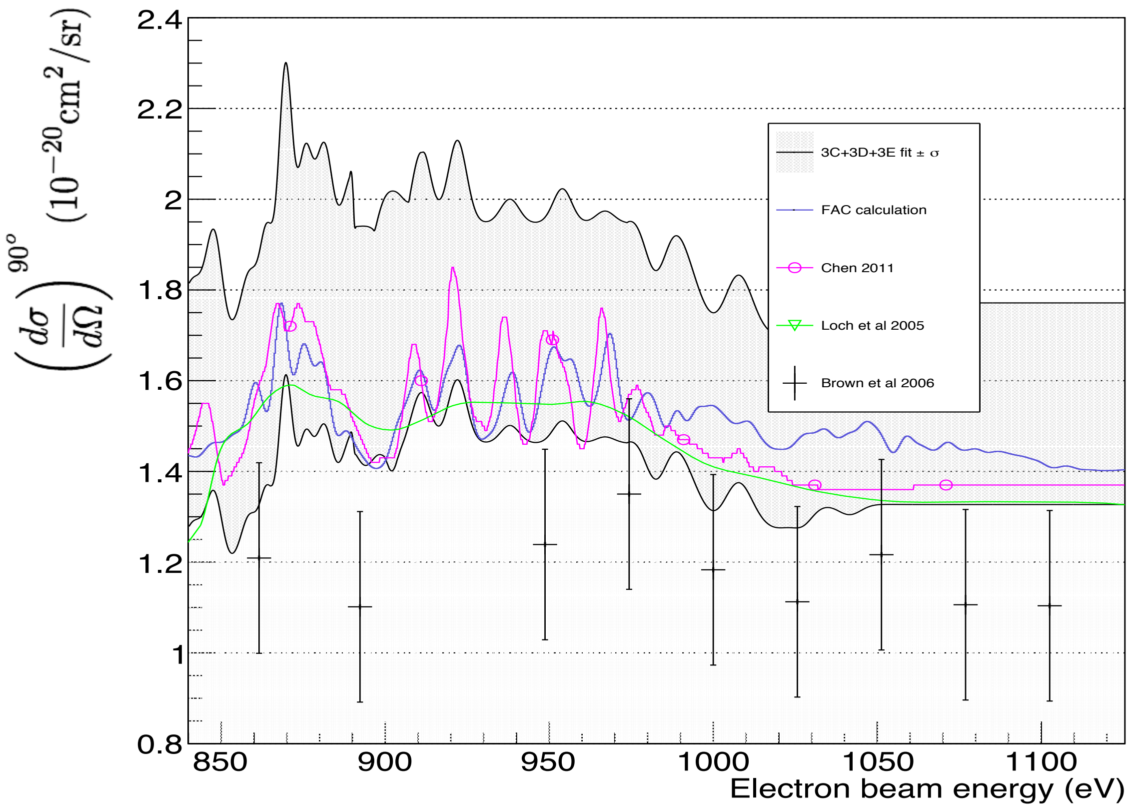
Sum over electron energy Preliminary



- J. Nilsen, Atomic Data and Nuclear Data Tables, 41, 131, (1989), multiconfiguration Dirac-Fock
- P. Beiersdorfer *et al*, ApJ, 793, 99, (2014) relativistic multi-reference Møller–Plesset perturbation theory

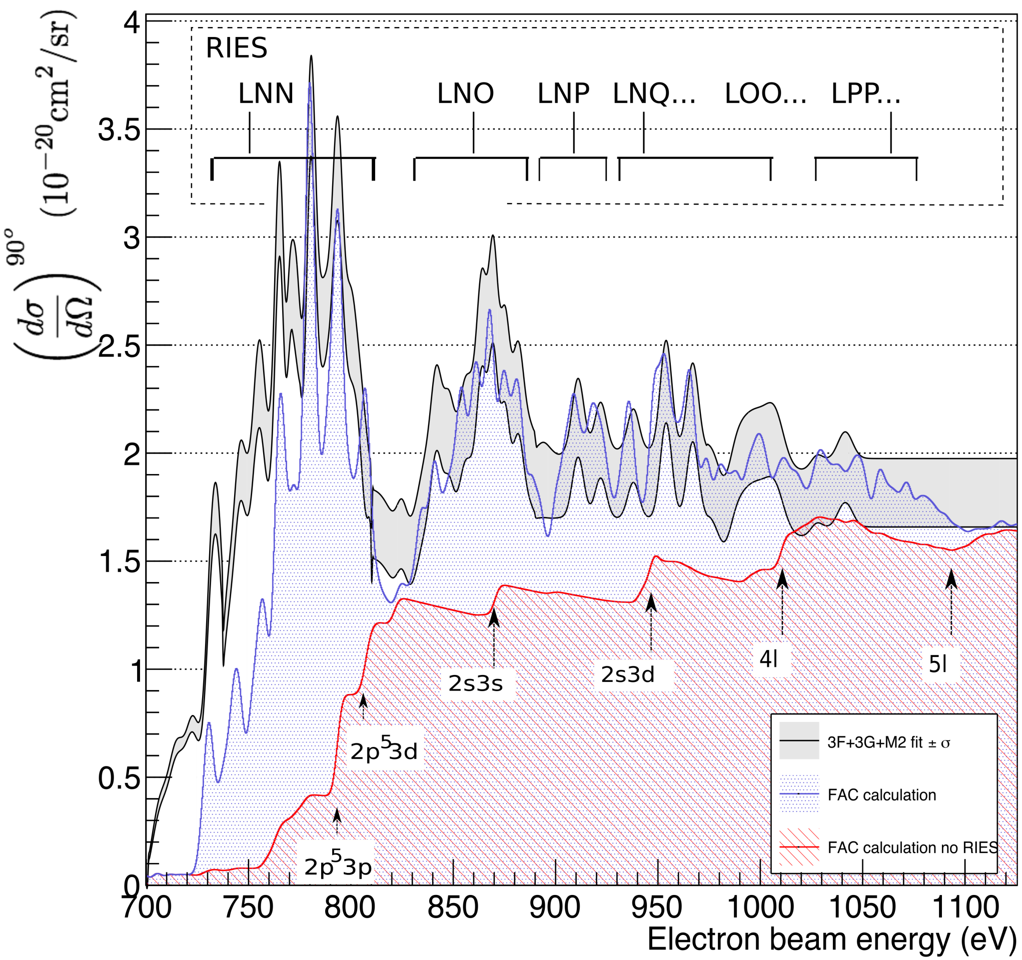
Results 3C+3D+3E CE region

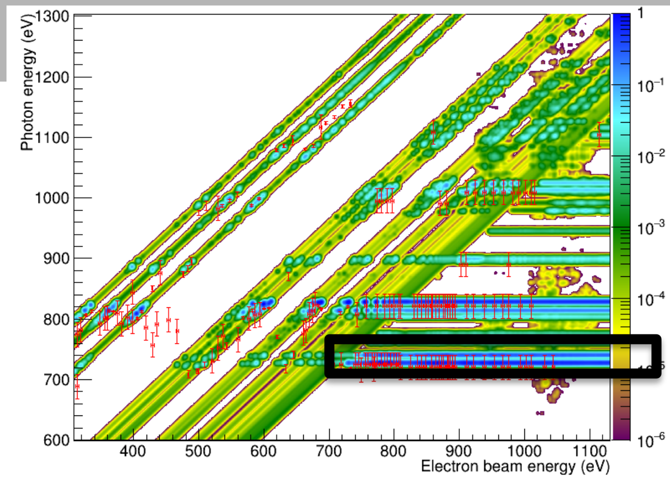
- G. X. Chen and A. K. Pradhan, PRL, 89, 013202 (2002) 30 eV broadening ; G. X. Chen PRA, 84, 012705 (2011) 5 eV broadening. Couple-cluster Breit-Pauli/Dirac R-matrix
- S. D. Loch, JPB 39, 85 (2005), 30 eV broadening, relativistic R-matrix calculation
- G. Brown *et al*, PRL, 96, 253201 (2006). Experimental calibrated with RR (E. Saloman et al., At. Data Nucl. Data Tables 38, 1 (1988).)



Results 3F+3G+M2

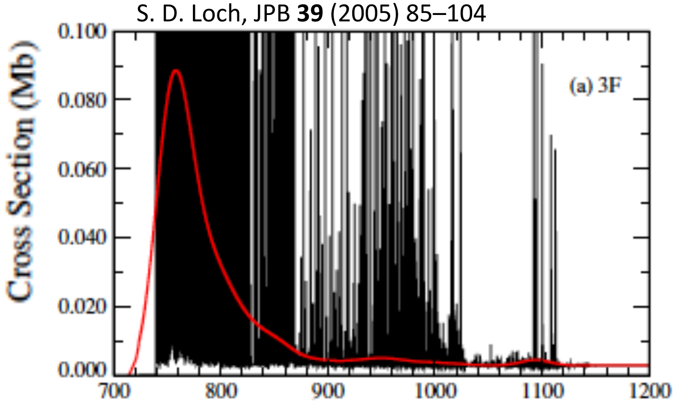
- Region of interest of 3F+3G+M2





- Complex cascade contribution from forbidden transitions into ground state
- Pronounced contribution of RIES

S. D. Loch, JPB **39** (2005) 85–104



Electron recombination in tungsten

- Energy region of MNN

MNN channel in Ag-like W

[Kr]$4f^1$ ⟶ [Ne] $3[s, p, d]^{17}$ $4[s, p, d]^{18}4f^3$

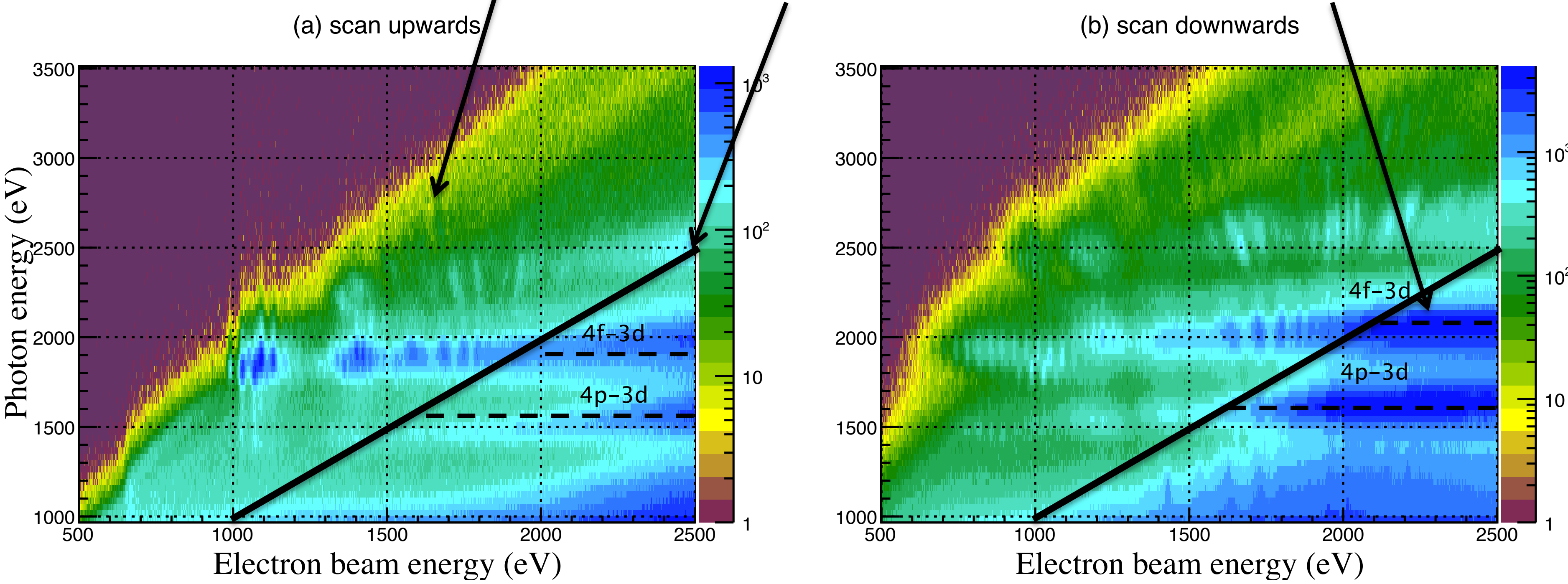
↓

[Ar] $3d^{10}$ $4[s, p, d]^{17}4f^3$

[Kr]$4f^2$

CE threshold

RIES contribution



Summary of the goals

- ✗ Investigate how the inclusion of the spectator electron after DR converge towards the 3C/3D CE
  - ❑ LMM structure predicated over the electron energy. Photon energies require further verification
  - ✓ No conclusion can be obtain for the 3C/3D conundrum in the **CE region** within the error bars
  - ✓ Pronounced discrepancy on DR after *n=4*
  - ✓ Synthetic maxwellian emission based on experimental centroids to be compared with satellite-mission spectra

- ✓ Provide data for the 3F+3G+M2 lines
  - ✓ Agreement with theory within error bars
  - ✓ RIES mechanism and the complex cascades are predicated

Ionization cross sections

Relativistic Version of Binary-enconter Model

PHYSICAL REVIEW A, VOLUME 62, 052710

Extension of the binary-encounter-dipole model to relativistic incident electrons

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$$t' = T/mc^2 \qquad \beta_t = v_t/c$$
$$b' = B/mc^2 \qquad \beta_b = v_b/c$$
$$u' = U/mc^2 \qquad \beta_u = v_u/c$$

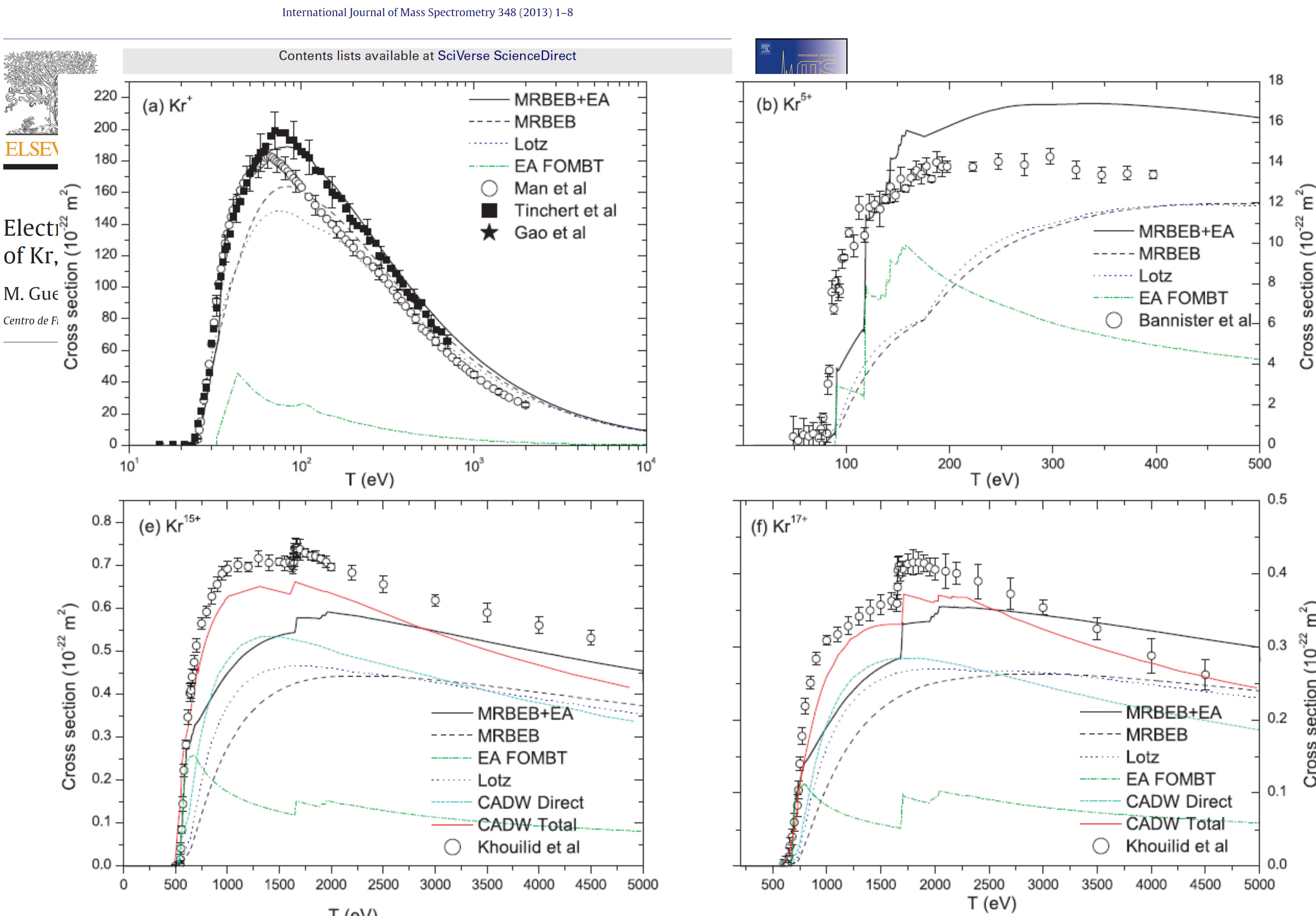
- T → Kinetic energy of the incident electron
- W → Kinetic energy of the ejected electron
- a_0 → Bohr's radius
- R → Rydberg's constant
- T-W → Kinetic energy of the scattered electron

$$\beta_t^2 = 1 - \frac{1}{(1+t')^2}$$
$$\beta_b^2 = 1 - \frac{1}{(1+b')^2}$$
$$\beta_u^2 = 1 - \frac{1}{(1+u')^2}$$

$$\sigma_{RBEB}(t) = \frac{4\pi a_0^2 \alpha^4 N}{\boxed{\left(\beta_t^2 + \beta_u^2 + \beta_b^2\right)} 2b'} \left[\frac{1}{2}\left[\ln\left(\frac{\beta_t^2}{1-\beta_t^2}\right) - \beta_t^2 - \ln(2b') \right]\left(1 - \frac{1}{t^2}\right) + 1 - \frac{1}{t} - \frac{\ln t}{t+1}\frac{1+2t'}{(1+t'/2)^2} + \frac{b'^2}{(1+t'/2)^2}\frac{t-1}{2} \right]$$

Total Ionization of Highly Charged Ions

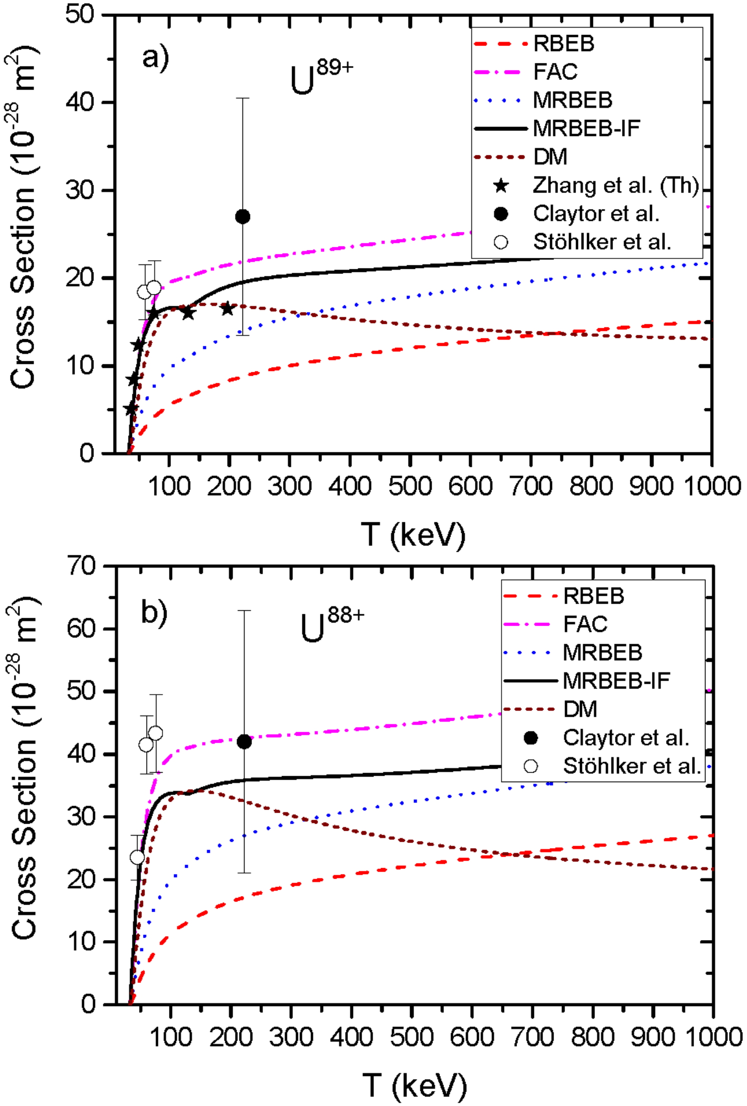
Modified Binary Encounter Bethe Model

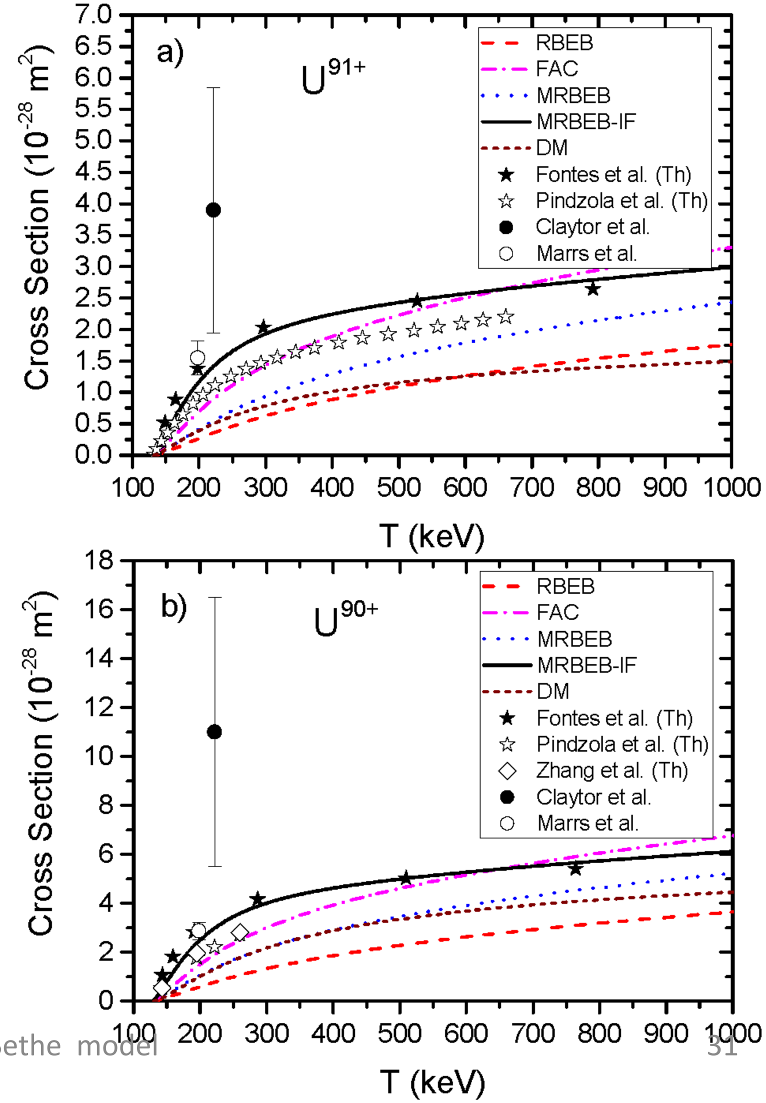


Total Ionization of Highly Charged Ions

IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics
J. Phys. B: At. Mol. Opt. Phys. **48** (2015) 144027 (5pp) doi:10.1088/0953-4075/48/14/144027

Electron impact ionization cross sections for





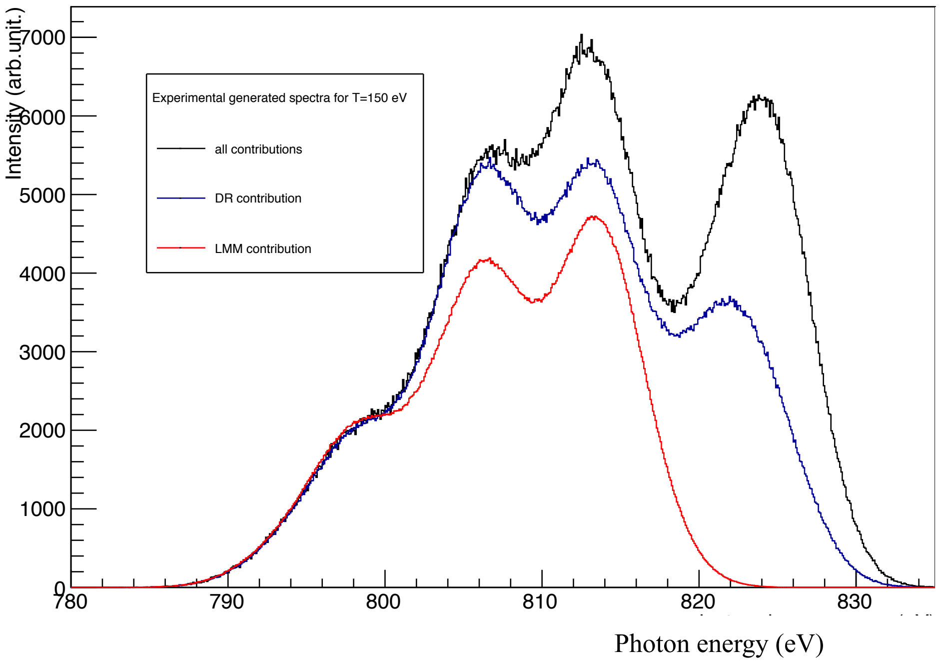
Summary of the goals

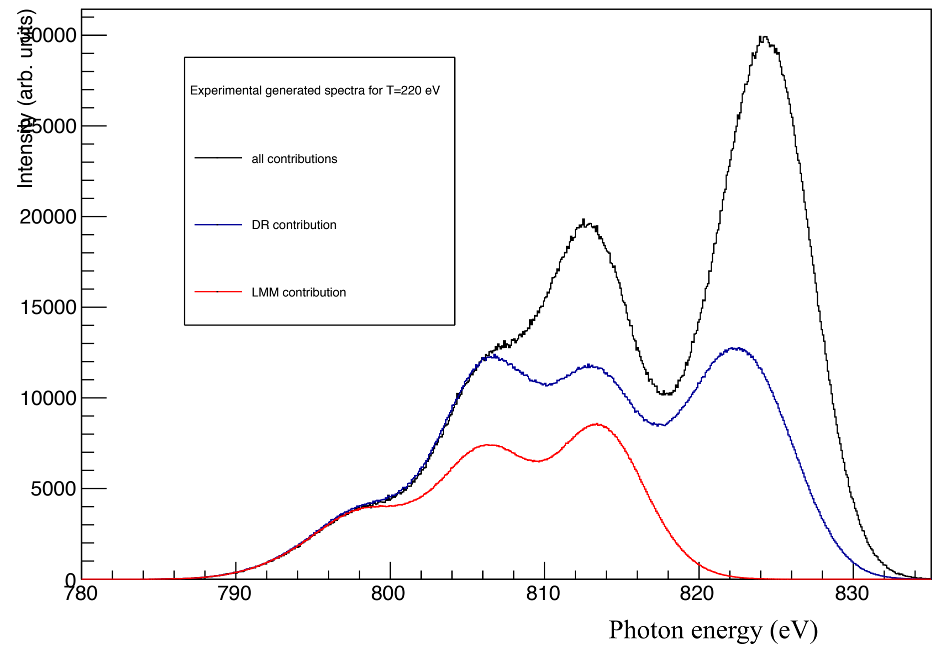
- ✓ Provided cross sections based in the MRBEB
  - ✓ Several ionization states of Kr
  - ✓ H- and He-like U

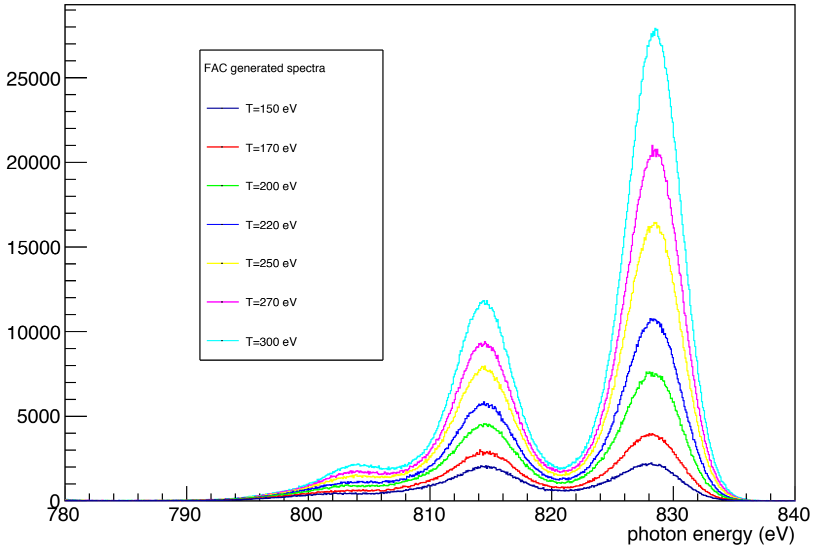
- ❑ Test the MBEB/MRBEB expression for the ionization of ions in several charge states
- ❑ Include results of this expression in a user-friendly website

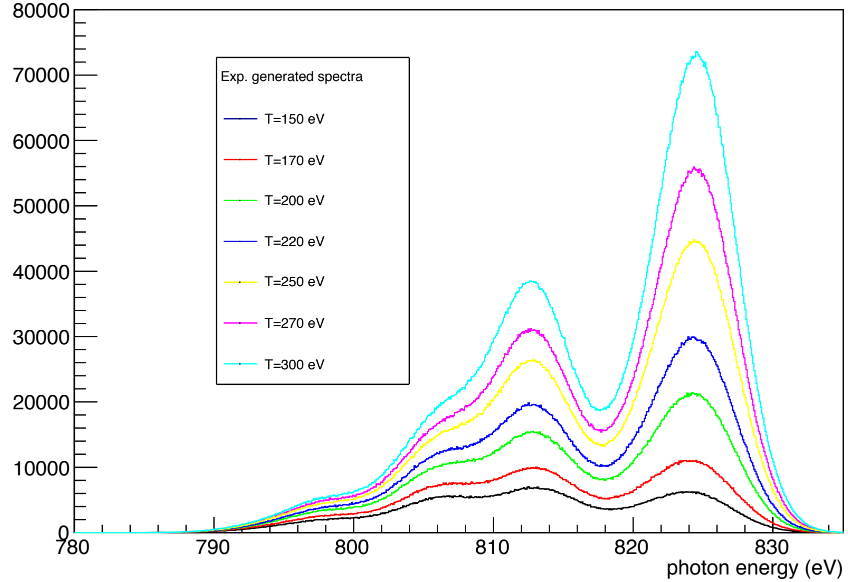
Thanks for your attention

Results 3C+3D+3E CE region Maxwell distribution



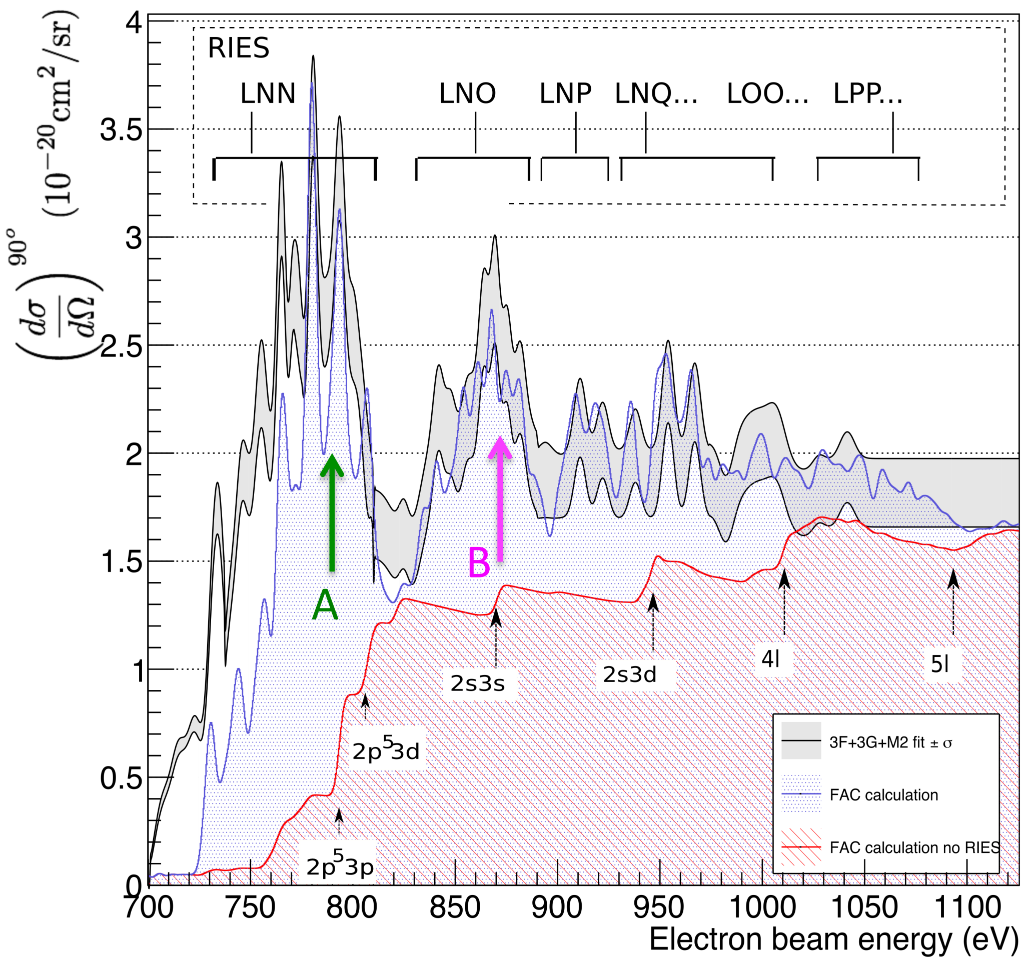


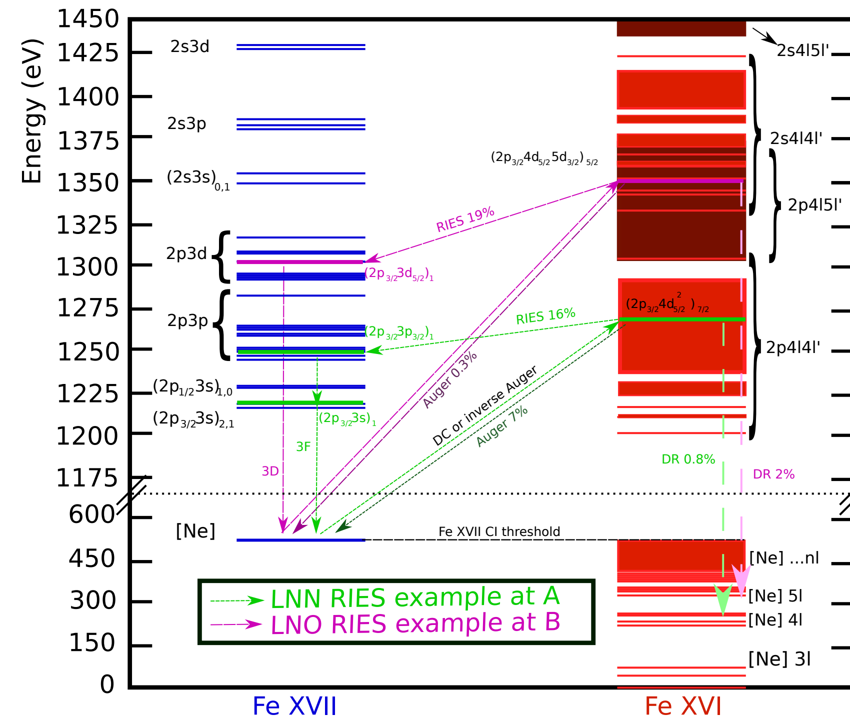




Results 3F+3G+M2

- Region of interest of 3F+3G+M2





Fe XVII purity during scan