

**High Energy Astrophysics**  
**X-RAY SPECTROSCOPY AND**  
**ATOMIC DATA**

*Ehud Behar*

Columbia University

# Collaborators

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## Columbia University:

Steven M. Kahn, Frits Paerels, Andy Rasmussen, Daniel Savin,  
Masao Sako, Ali Kinkhabwala, John Peterson

## The *XMM-Newton* / RGS Consortium:

Teams from SRON, MSSL, PSI

## LLNL, EBIT team:

Peter Beiersdorfer, Greg Brown, Jaan Lepson,  
Hui Chen (and Goddard calorimeter team)

# Outline

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- ❖ Introduction:
  - **The Soft X-Ray Band**
  - *Chandra and XMM-Newton*
- ❖ Collisional Plasmas
  - **Cool Stars - Stellar Coronae**
  - **Hot Stars – Shocks in Stellar Winds**
  - **Supernova Remnants**
  - **Elliptical Galaxies**
  - **Galaxy Clusters – Big blobs of gas; Cooling Flows?**
  - **Atomic Data Needs**
    - ❖ Needs, Fe-L
    - ❖ Laboratory Measurements and Status
- ❖ Photoionized Plasmas
  - **Active Galactic Nuclei**
    - ❖ Absorption
    - ❖ Emission
  - **X-Ray Binaries**
  - **Atomic Data Status and Supporting Lab. Measurements**
- ❖ Conclusions

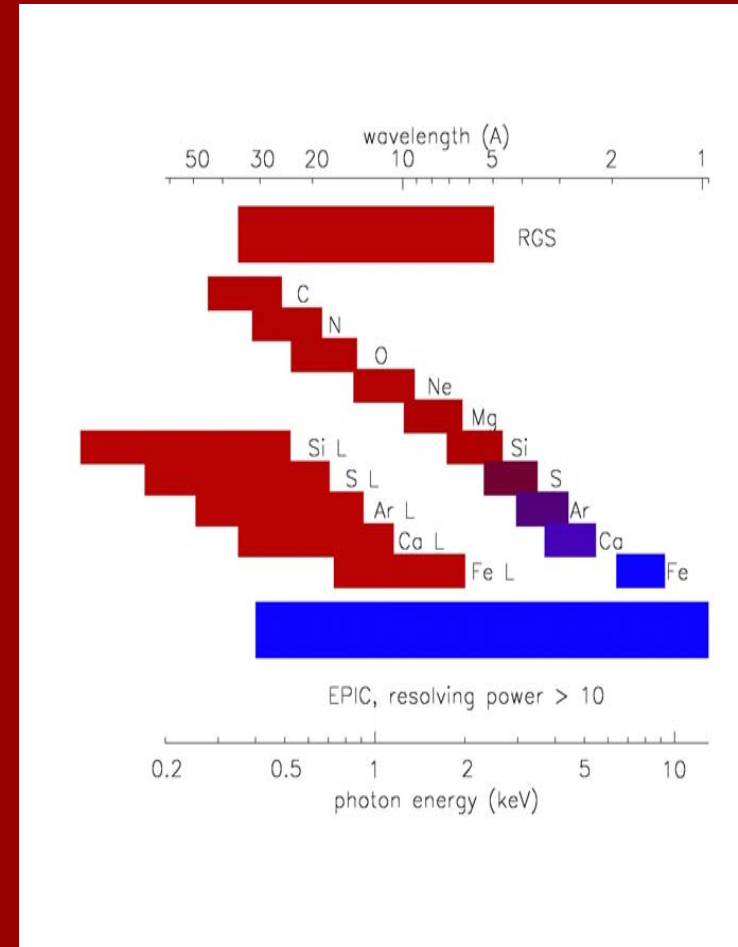
# Introduction

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- ❖ X-Ray Astronomy was born in 1962 with the discovery of Scorpius X-1.
- ❖ Over the years x-ray observatories have revealed a diverse collection of x-ray sources ranging from nearby stars to distant galaxies.
- ❖ However, it wasn't until the recent launches (1999) of *Chandra* and *XMM-Newton* that x-ray line-resolved spectra have become available.
- ❖ With this recent achievement, the x-ray branch of astronomy now joins other wavebands in using spectroscopy to perform quantitative investigations of cosmic objects.

# Features of the X-Ray Band: Highly Ionized Atoms

- ❖ The conventional (soft) x-ray band (1 to 100 Å or  $\sim 0.2 - 10$  keV) comprises emission lines from many K-shell and L-shell ions pertaining to many elements (C – Ni).
- ❖ The x-ray band is uniquely compact, having several ions appear from each element and many lines being present from each ion.
- ❖ The wealth of lines and ions allows for elaborate plasma diagnostics such as temperatures, densities, ionization state, and elemental abundances.



# A New Era in X-Ray Astrophysics: *Chandra and XMM-Newton*

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- ❖ The *Chandra* Observatory (NASA):
  - Launched July 23, 1999
  - 1 telescope
  - 2 CCD cameras
  - 2 transmission grating spectrometers (spectroscopy mode is alternative to imaging)
- ❖ *XMM-Newton* (ESA):
  - Launched December 10, 1999
  - 3 telescopes
  - 2 reflection grating spectrometers
  - 1 Optical/UV monitor

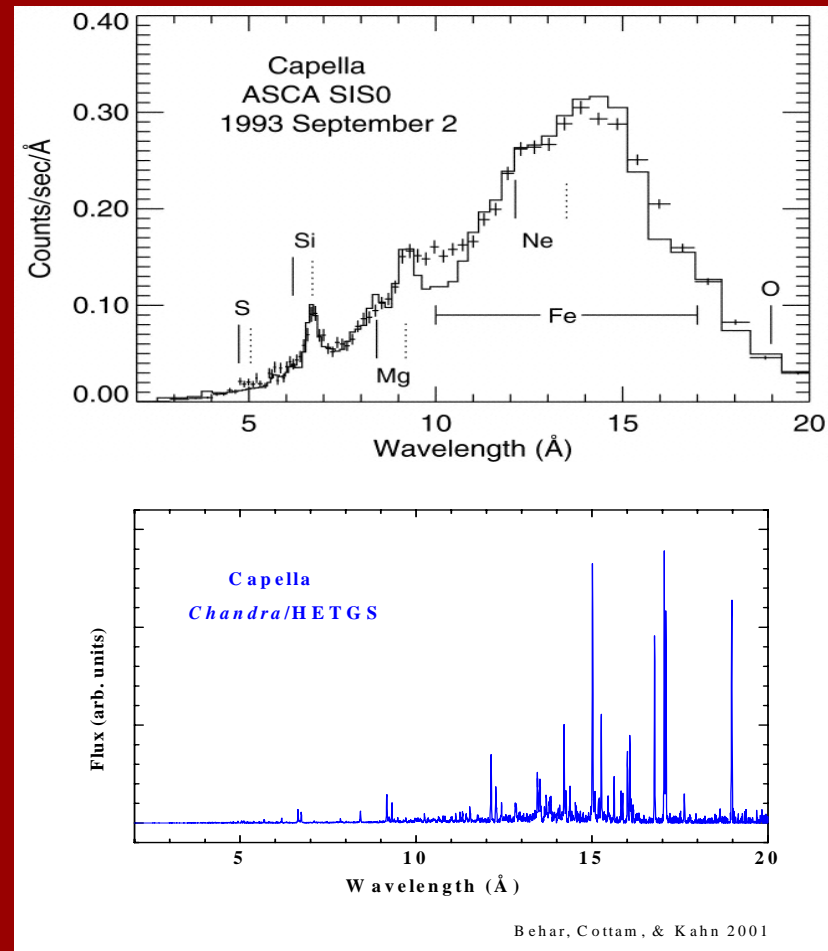


# The Difference High Spectral Resolution Makes

## ❖ CCD spectrum of Capella with ASCA

(Brickhouse, Dupree, Edgar et al. 2000)

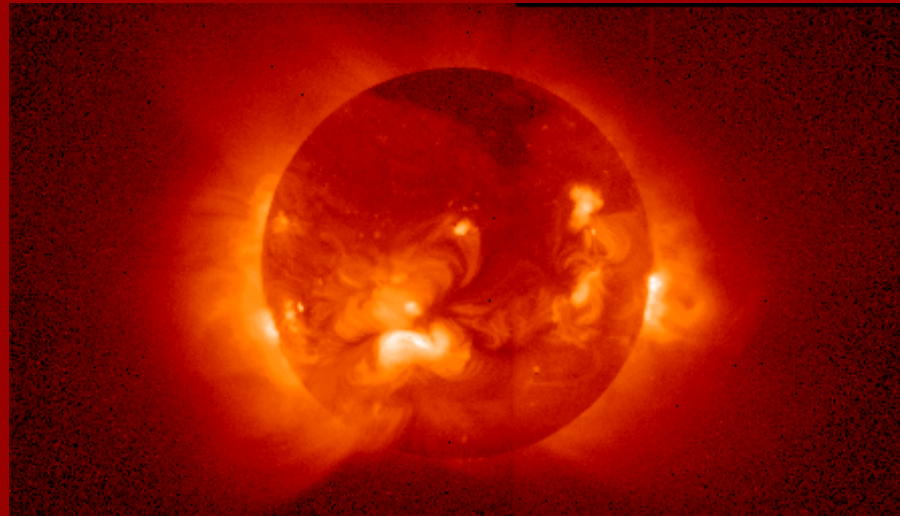
## ❖ Grating spectrum of Capella with Chandra



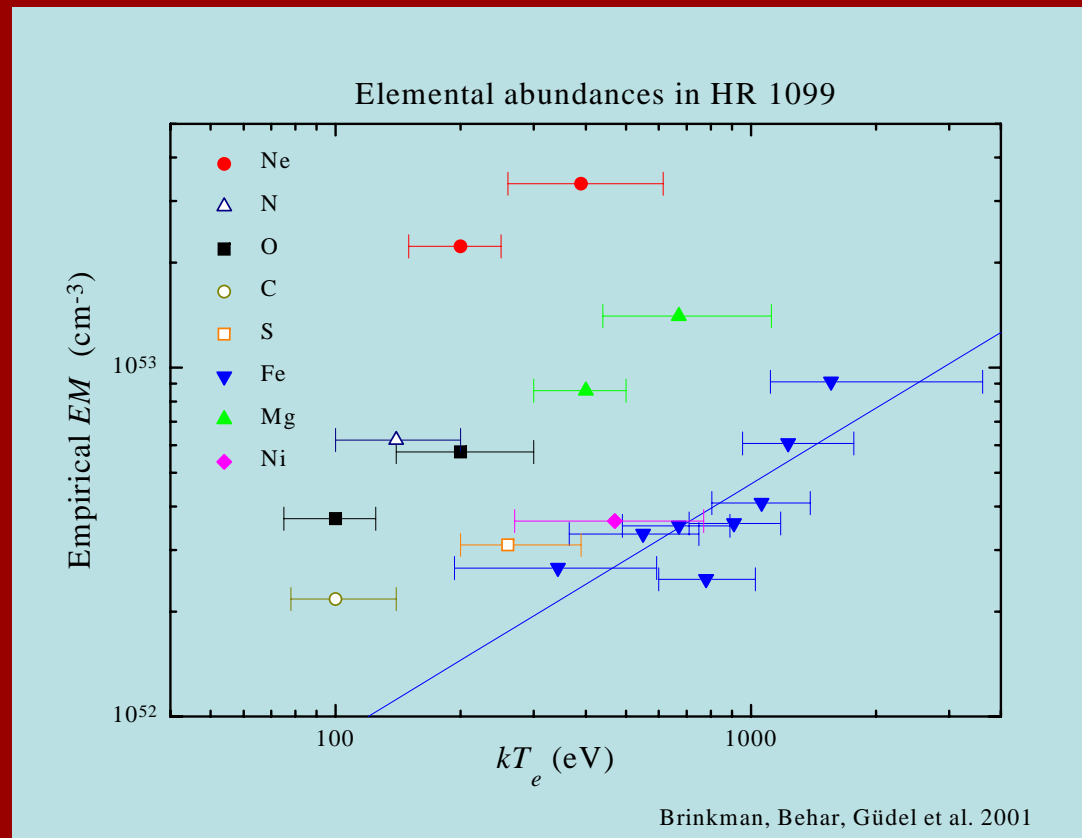
# Stellar Coronae: Hot, Collisional X-Ray Sources

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- ❖ Physical environment:
  - Magnetic confinement
  - Hot ( $kT \sim 0.1 - 3$  keV)
  - Density ( $n \sim 10^{10}$  cm<sup>-3</sup>)
  - Optically thin
- ❖ Ionization balance:
  - Standard electron-ion collisional processes: CI, RR, as well as EA and DR
- ❖ Line emission:
  - Collisional excitation



# Stellar Coronae (cont.): Emission Measure and Abundances



$$n_e n_H V = \frac{4\pi d^2 F_{ji}}{A_{el} P_{ji} f_q(T_e)}$$

$F_{ji}$  – measured

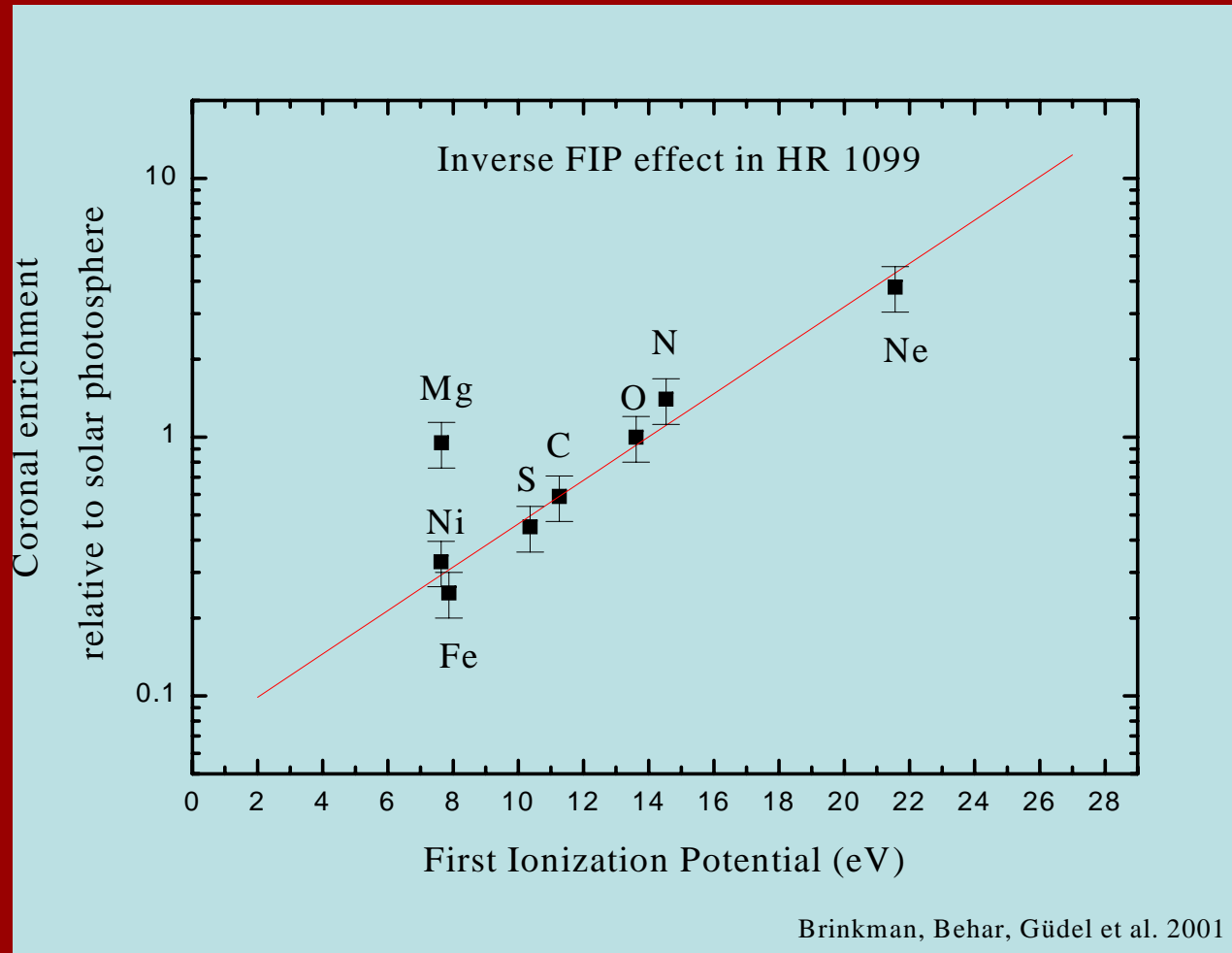
$d$  – known

$A_{el}$  – assumed solar

$P_{ji}, f_q$  – atomic physics

# Stellar Coronae (cont.)

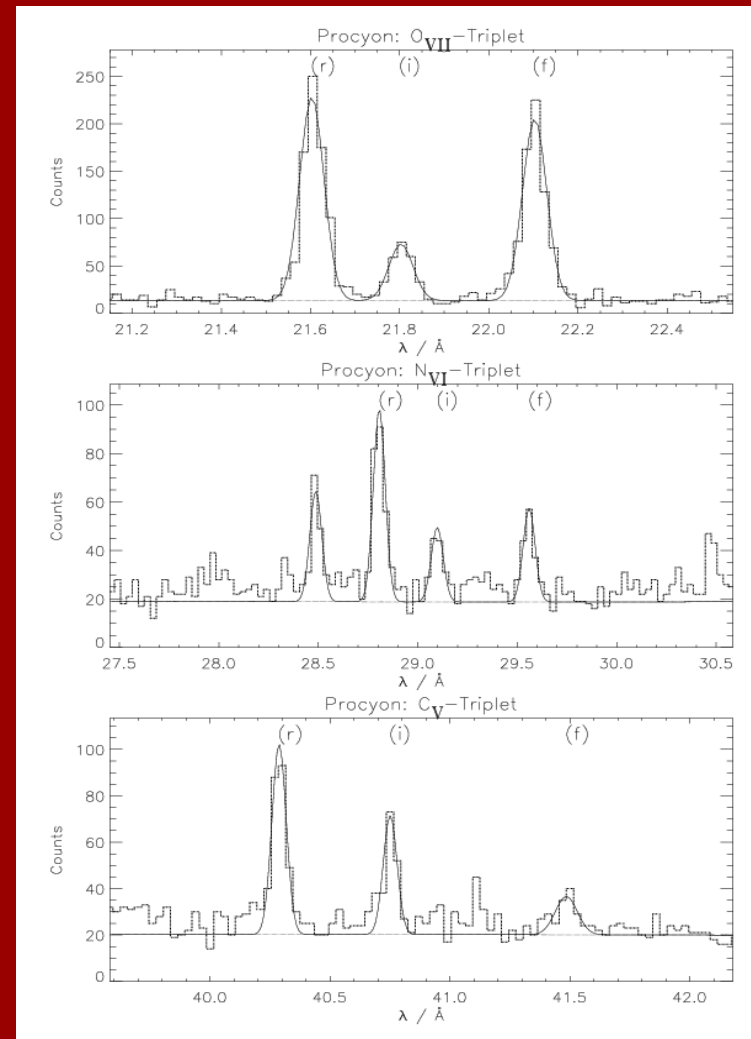
## Inverse FIP Effect



# Density Diagnostics

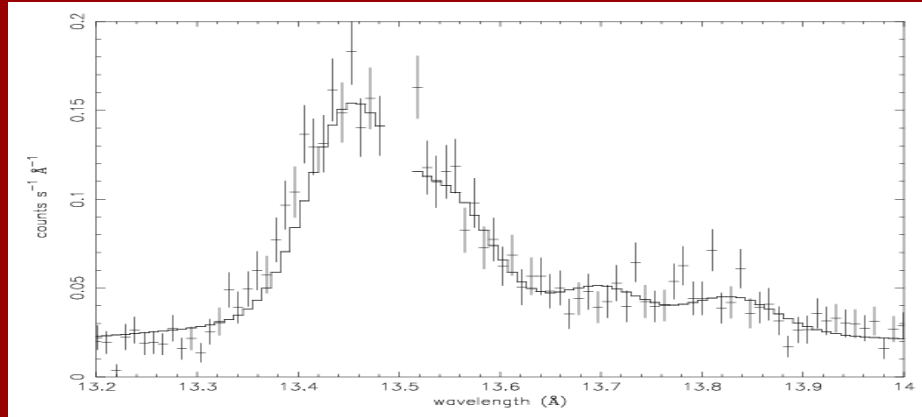
- ❖ Collisional depletion of excited levels of forbidden lines.
- ❖ Most popular are the He-like triplets (Gabriel & Jordan 1969). The 1s-2s forbidden line is suppressed at high densities.
- ❖ Critical density depends on element.

Ness, Mewe, Schmitt et al. 2001



# Hot Stars: UV depletion of excited levels

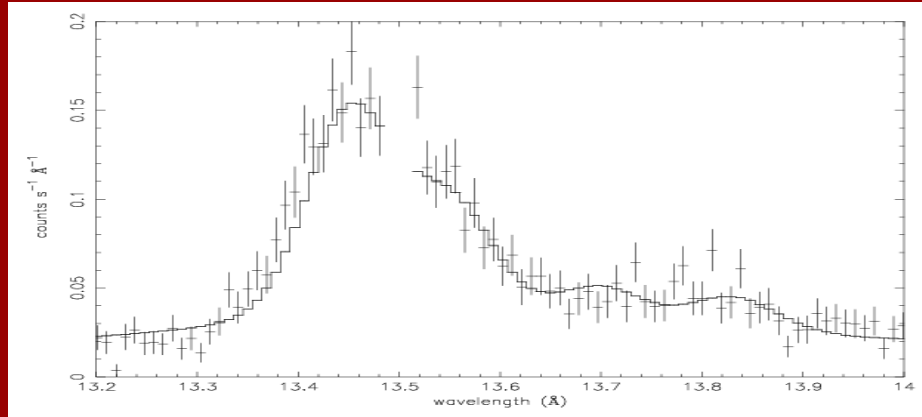
- ❖ UV depletion of excited levels mimics density effects.
- ❖ Example: He-like triplets in  $\zeta$  Pup.
- ❖ Provides measurements of distance from photosphere.



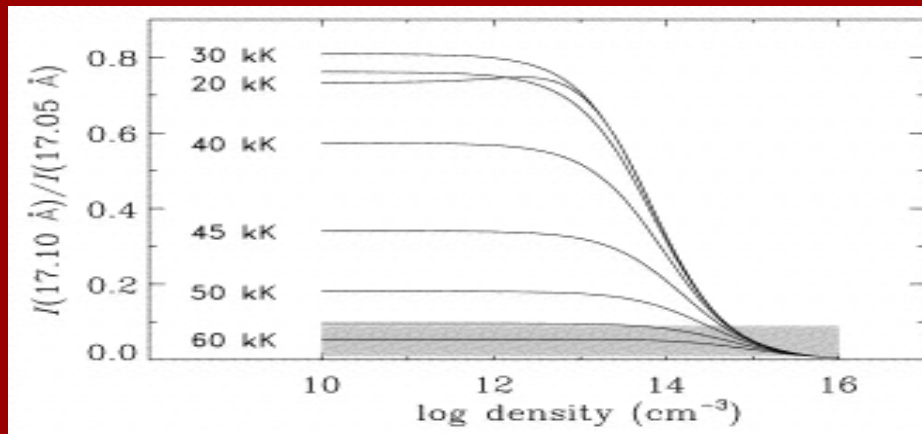
$\zeta$  Pup; Kahn, Leutenegger, Cottam, et al. 2001

# Hot Stars (cont.)

- ❖ UV depletion of excited levels mimics density effects.
- ❖ Example: He-like triplets in  $\zeta$  Pup.
- ❖ Provides measurement of distance from photosphere.
- ❖ Another example: 2p-3s forbidden line of  $\text{Fe}^{16+}$  in the magnetic CV (EX Hya).



$\zeta$  Pup; Kahn, Leutenegger, Cottam, et al. 2001



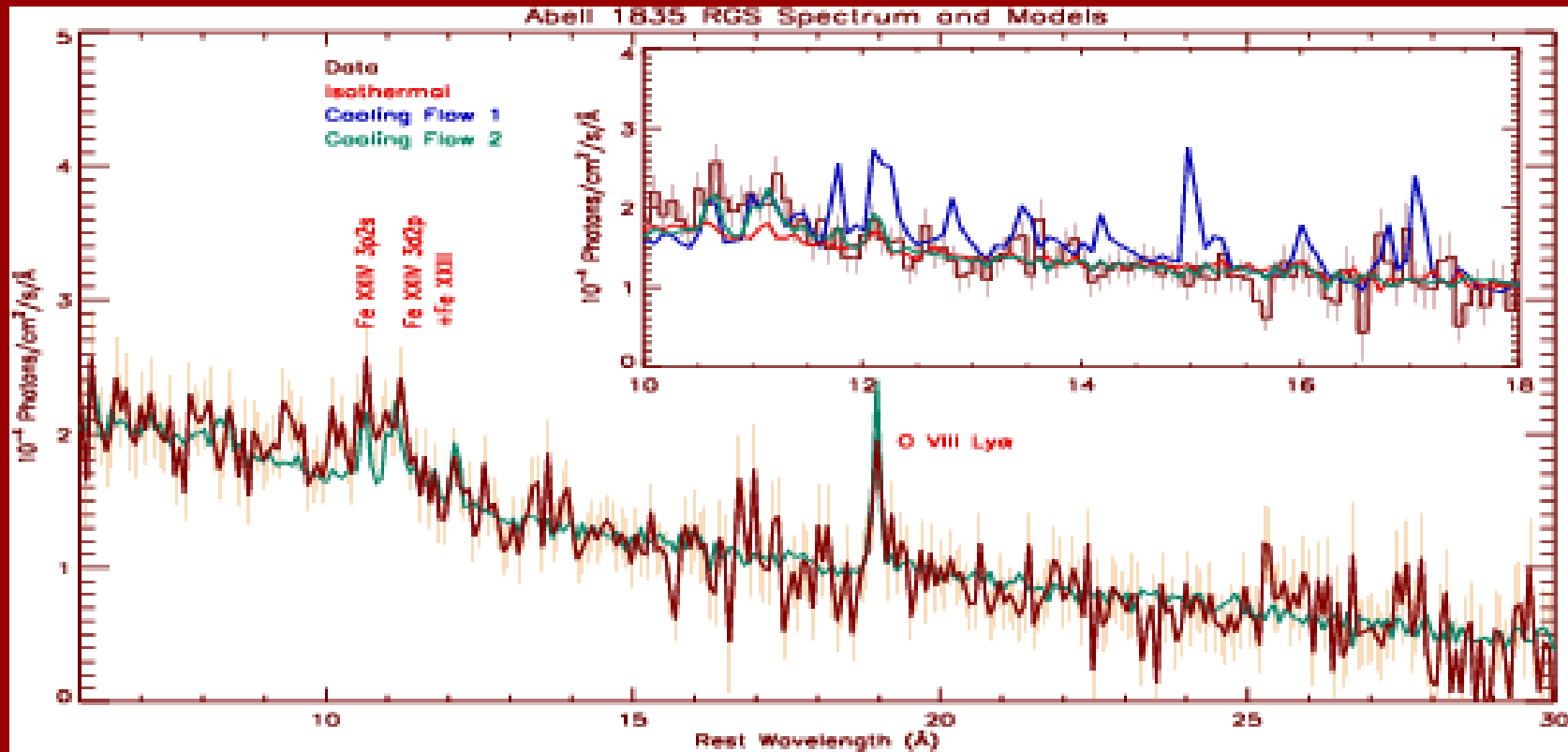
Mauche, Liedahl, & Fournier 2001

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  - **The Soft X-Ray Band**
  - *Chandra and XMM-Newton*
- ❖ Collisional Plasmas
  - **Cool Stars - Stellar Coronae**
  - **Hot Stars – Effect of UV field**
  - **Supernova Remnants**
  - **Elliptical Galaxies**
  - **Galaxy Clusters – Where Are The Cooling Flows?**
  - **Atomic Data Status and Supporting Lab. Measurements**
- ❖ Photoionized Plasmas
  - **Active Galactic Nuclei**
    - ❖ **Emission**
    - ❖ **Absorption**
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  - **Atomic Data Status and Supporting Lab. Measurements**
- ❖ Conclusion and Discussion on Atomic Data Needs

# Galaxy Clusters: What Happened to the Cooling Flows?



Peterson, Paerels, Kaastra et al. 2001

# Collisional Plasmas: Atomic Data Needs

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## ❖ Processes and Data

- Generally important
  - ❖ Wavelengths
  - ❖ Collisional emissivities
  - ❖ Total ionization and recombination rates
- More specific
  - ❖ Transitions among excited states
  - ❖ Ionization and recombination effects on line emission
    - Ionization equilibrium and non-equilibrium
  - ❖ Charge exchange

## ❖ Ions

- K-shell of C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, and Ni
- L-shell, particularly Fe, but also Ne, Mg, Si, S, Ar, Ca, and Ni

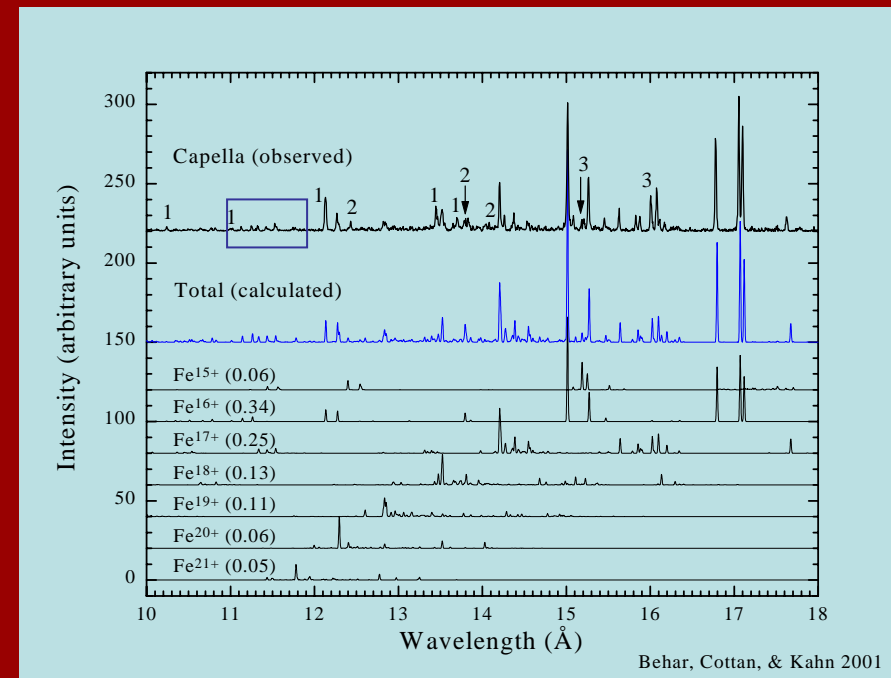
# Fe-L Physics

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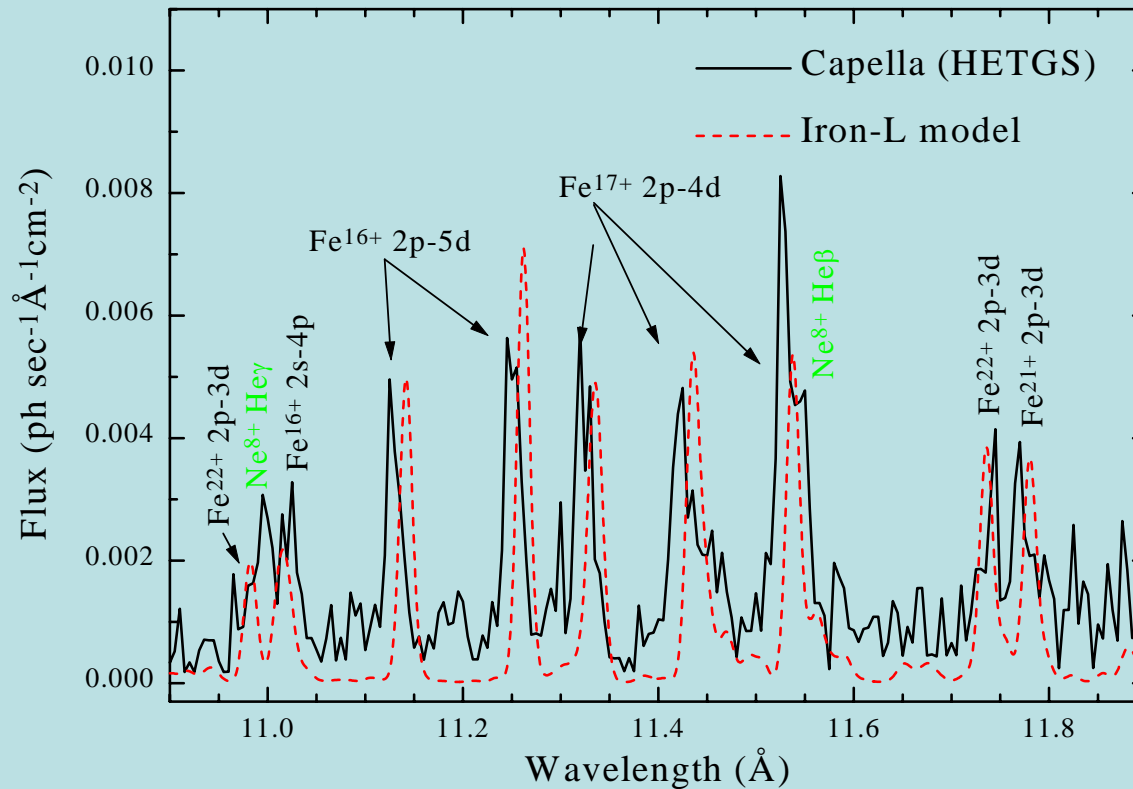
- ❖ 2p-3d and 2p-3s lines of  $\text{Fe}^{16+}$  -  $\text{Fe}^{23+}$  dominate the soft x-ray spectrum of many sources.
- ❖ Lines of different Fe-L ions are easily discernible with contemporary grating spectrometers, which provides a strong, abundance-independent constraint on the charge-state ( $T$ ,  $EM$ ) distribution.
- ❖ For years, Fe-L was the nightmare and scapegoat of many x-ray astronomers. Unjustly so!
- ❖ The Columbia-LLNL Laboratory Astrophysics program has focused on Fe-L, and along with efficient atomic codes has gone a long way to serve us observers and help us exploit the full potential of Fe-L diagnostics.
- ❖ Where possible, it still makes a lot of sense to use single-ion models independent of the ionization balance.

# Capella as a Test Case for Fe-L

- ❖ Fe-L dominates.
- ❖ Ab initio DW single-ion calculations (HULLAC) are not so bad.
- ❖ In particular, all lines are identified unambiguously.
- ❖ Most relative line intensities agree to within 20%.
- ❖ Nevertheless, a few outstanding discrepancies remain.

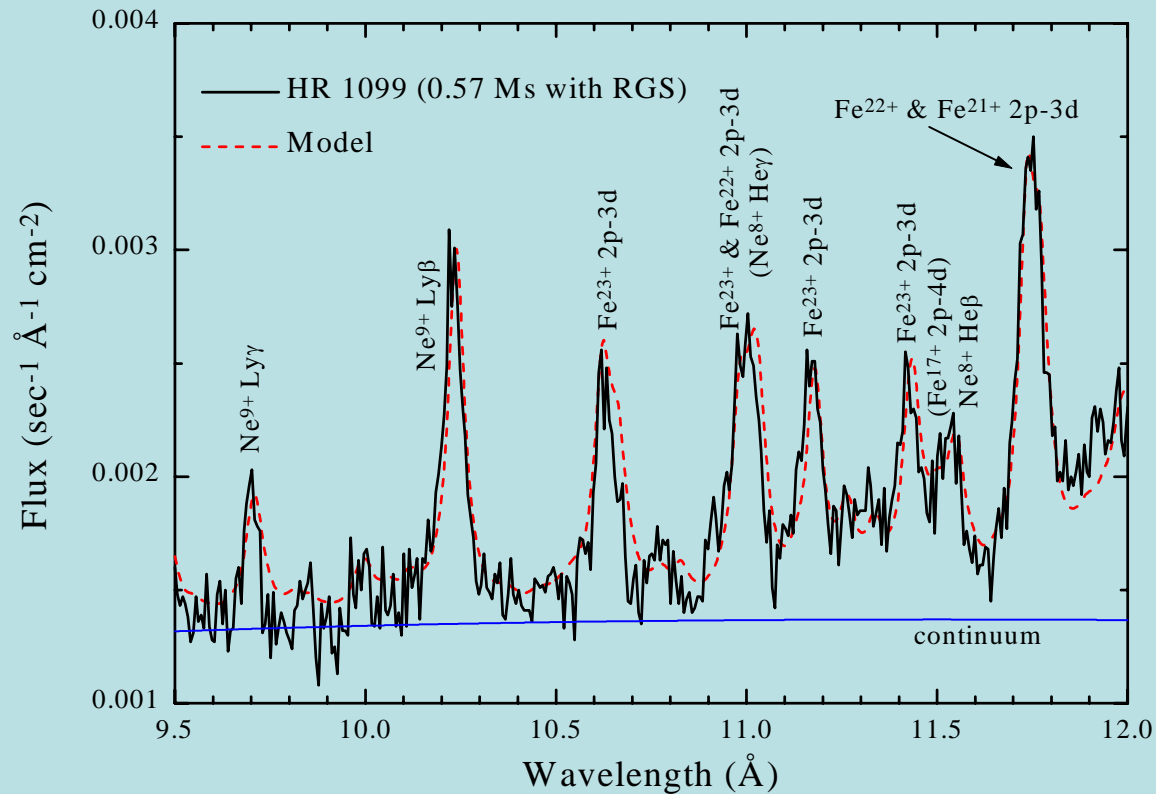


# Are Fe-L Data Really that Bad?



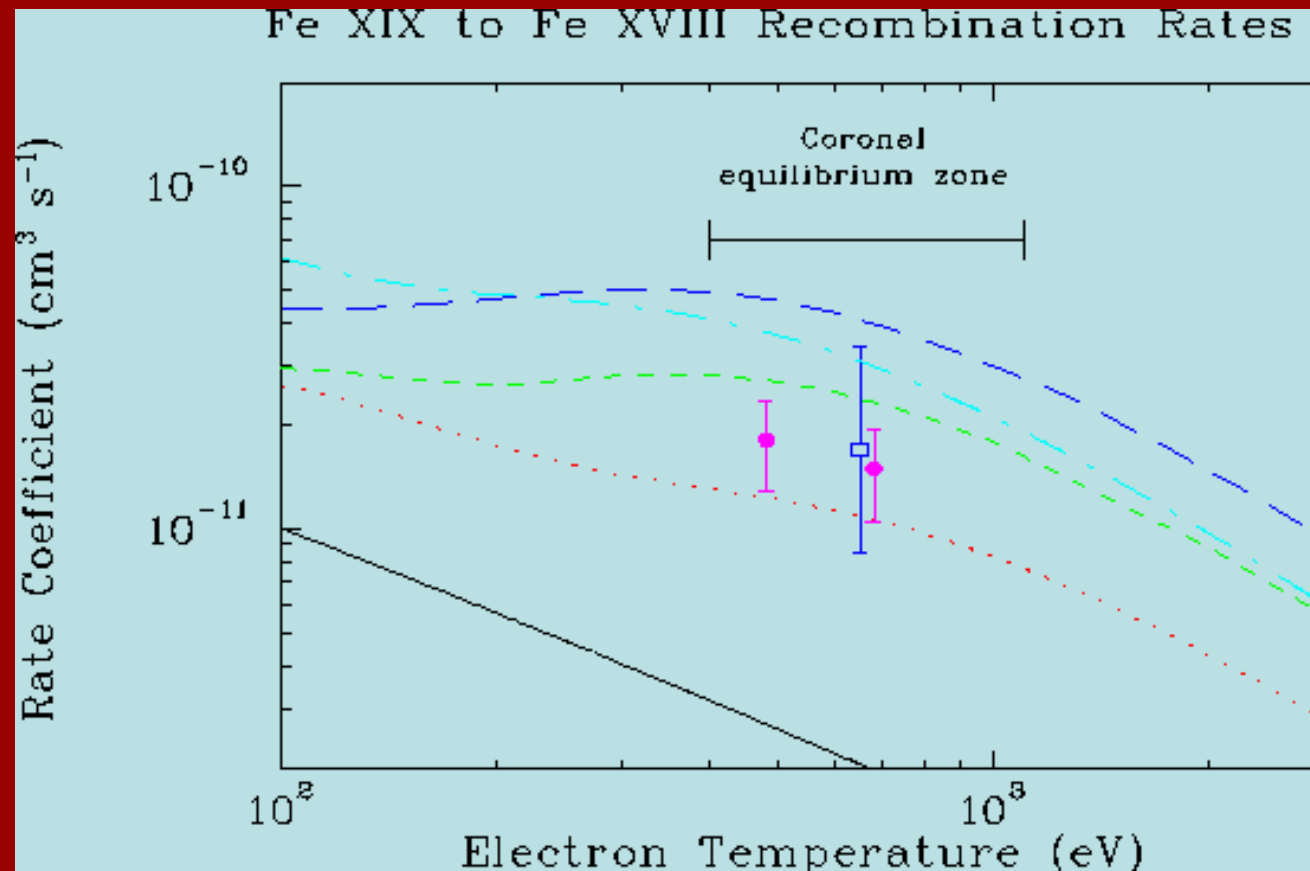
Behar, Cottam, Peterson, et al. 2001

# HR 1099 / RGS: Arguably, The Highest Quality X-Ray Spectrum



Behar, Cottam, Peterson, et al. 2001

# Dielectronic Recombination (DR): Not Doing As Good



Courtesy of Daniel Savin

# Collisional Plasmas: Fe-L Laboratory Measurements

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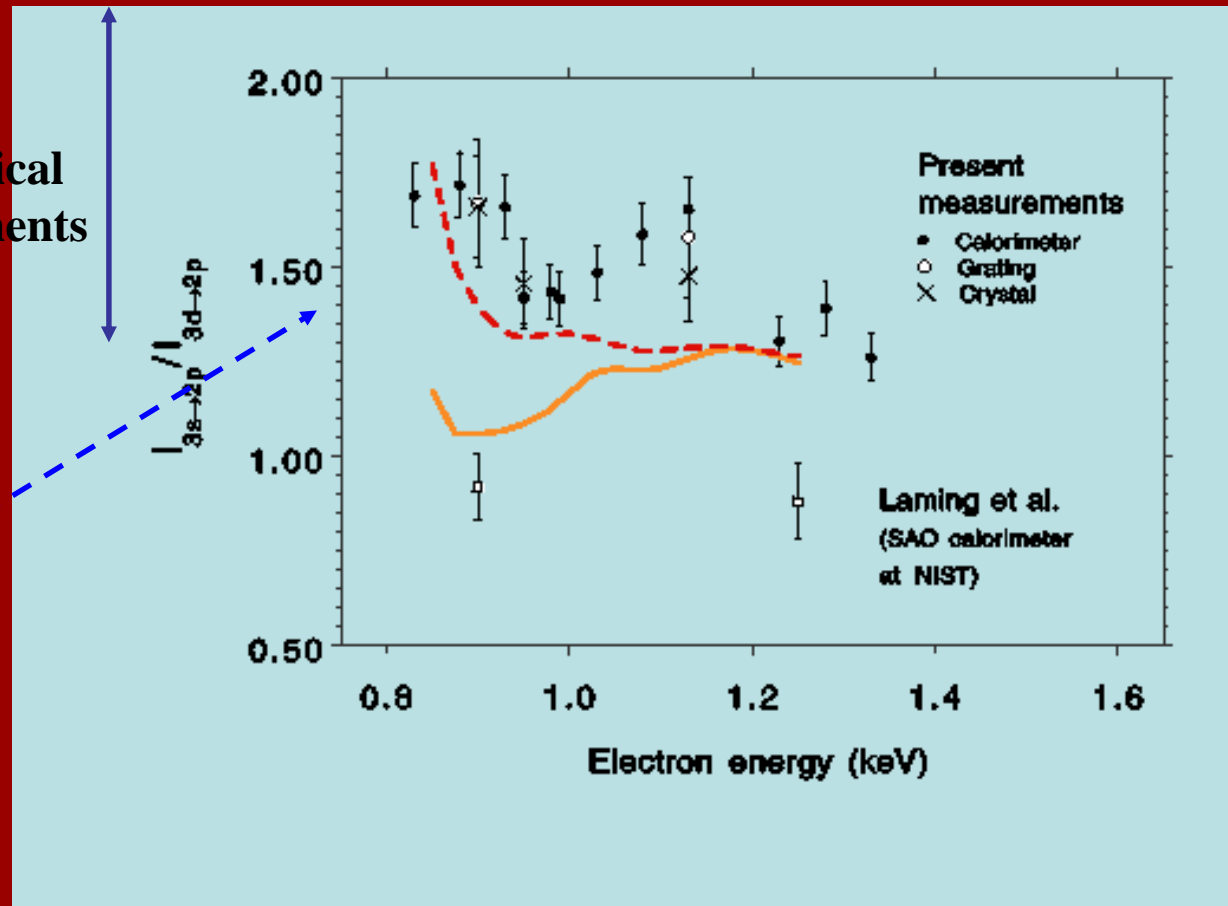
- ❖ Wavelengths
  - LLNL EBIT: Brown et al., 1998, 2000
- ❖ CE rates / line emissivities
  - LLNL EBIT with crystal spectrometer: Savin et al. 1996, Gu et al. 1999, 2001
  - LLNL EBIT with microcalorimeter: Chen et al. 2002
- ❖ Line ratios
  - LLNL EBIT: Brown et al. 1998, 2001
  - NIST EBIT: Laming et al. 2000
  - LLNL EBIT: Beiersdorfer et al. 2002
- ❖ Ionization balance
  - TSR: DR rates, Savin et al. 2002
- ❖ Other non-Fe-L works:
  - NIST EBIT: Silver et al. 2000, LLNL EBIT: Lepson et al. 2002

# The Tale of Fe<sup>16+</sup>: What's the matter with the 2p-3s lines?

↑  
Low- $T_e$   
with RE  
(D&B)

High- $T_e$  with DR  
~ 40% effect  
(Doron & Behar)

Various  
astrophysical  
measurements



Beiersdorfer, Brown, Gu et al. 2002

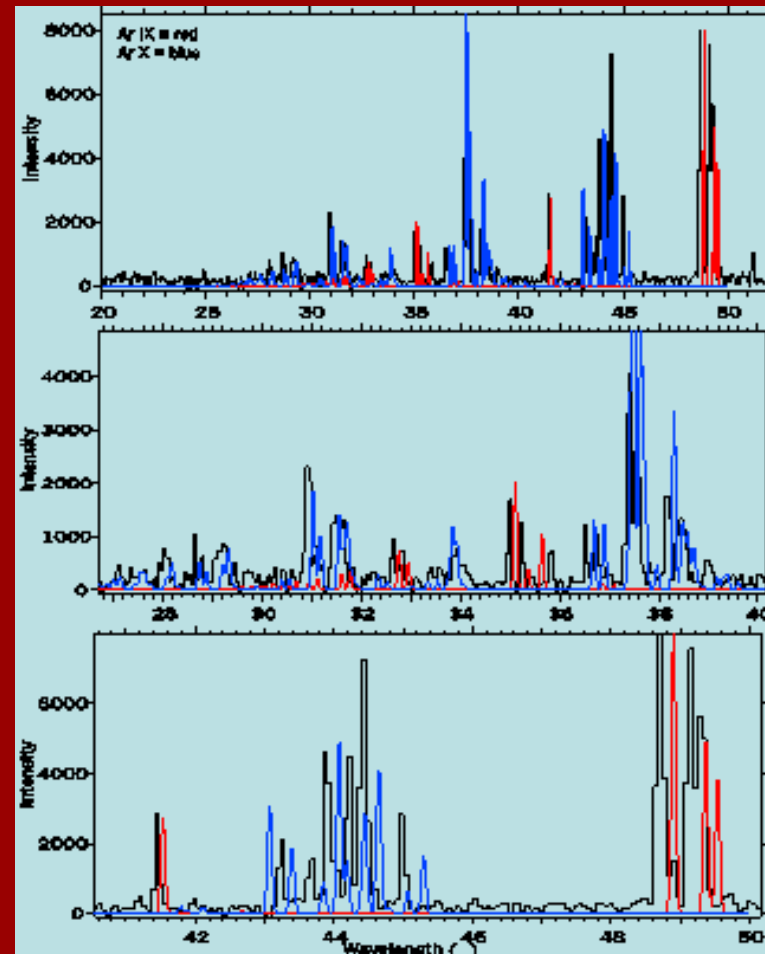
# Collisional Plasmas: Atomic Data Status

Expected Confidence Levels (Ball Park) and Experimental Benchmarking

Data \ Shell	K	K (Fe)	L	L (Fe)
Wavelengths	0.01%	0.01%	0.5%	0.03%
Emissivities	10%	10%	50%	10-20%
Tot. Ionization	20%	20%	30%	30%
Tot. Recomb.	20%	20%	100%	20%
Transitions excited levels	50%	50%	50%	30%

# Ongoing and Future Work: Life After Fe-L

❖ Ar IX & X,  
Lepson et al.:  
EBIT LLNL  
measurements vs.  
HULLAC calculations

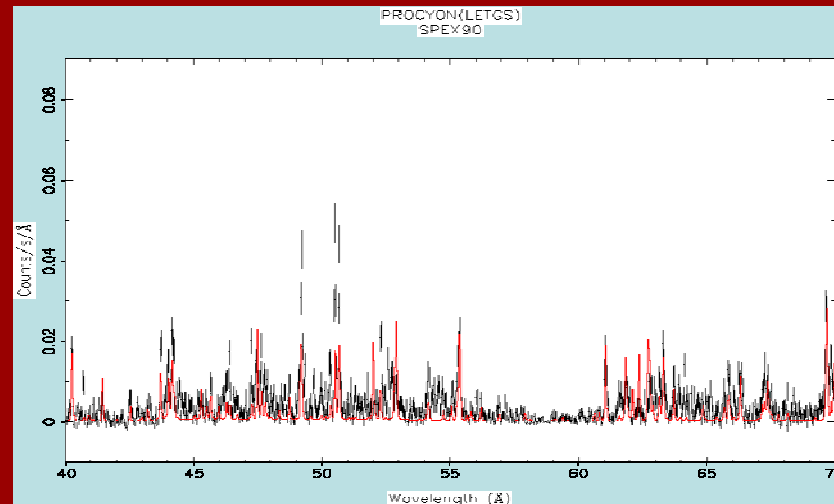


# L-shells of Other Elements (contd.)

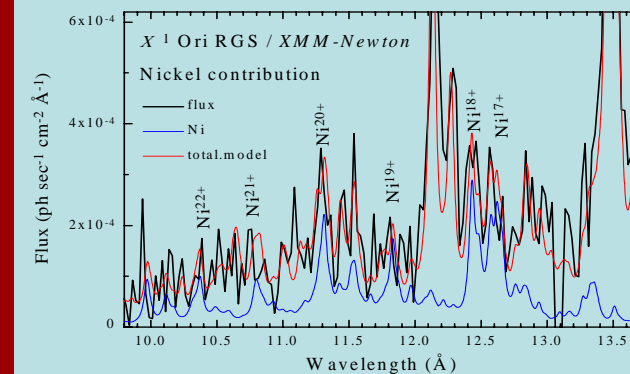
## ❖ Procyon (LETGS)

Raassen, Mewe, Audard,  
et al. 2002

Si, S – L are partially  
missing in the MEKAL  
database.



## ❖ X<sup>1</sup> Ori (RGS): Significant Ni-L contribution.



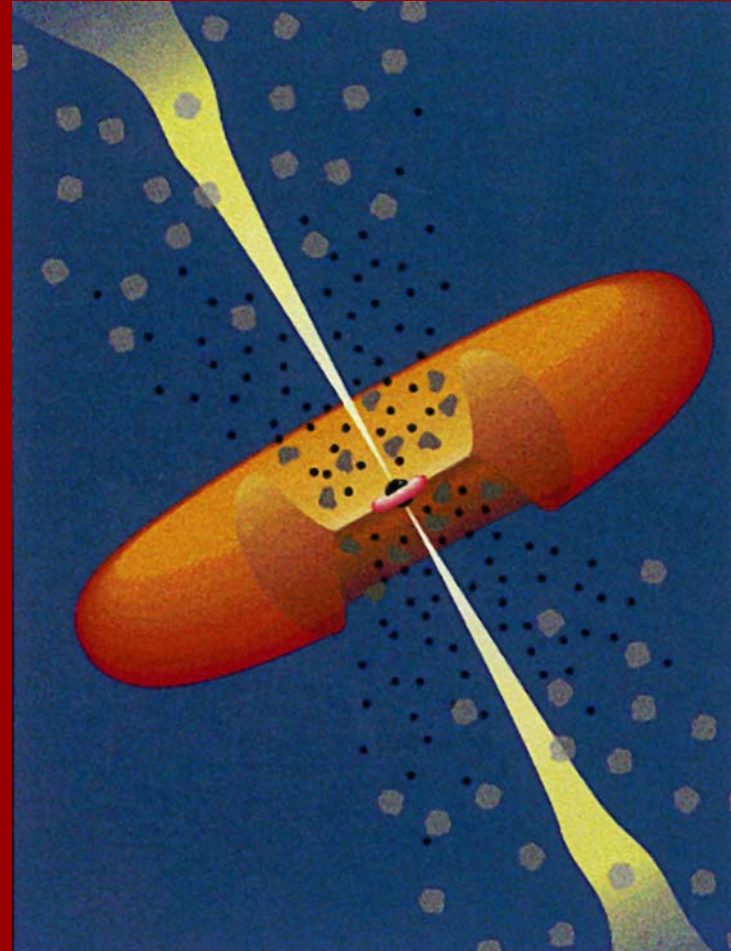
# Outline

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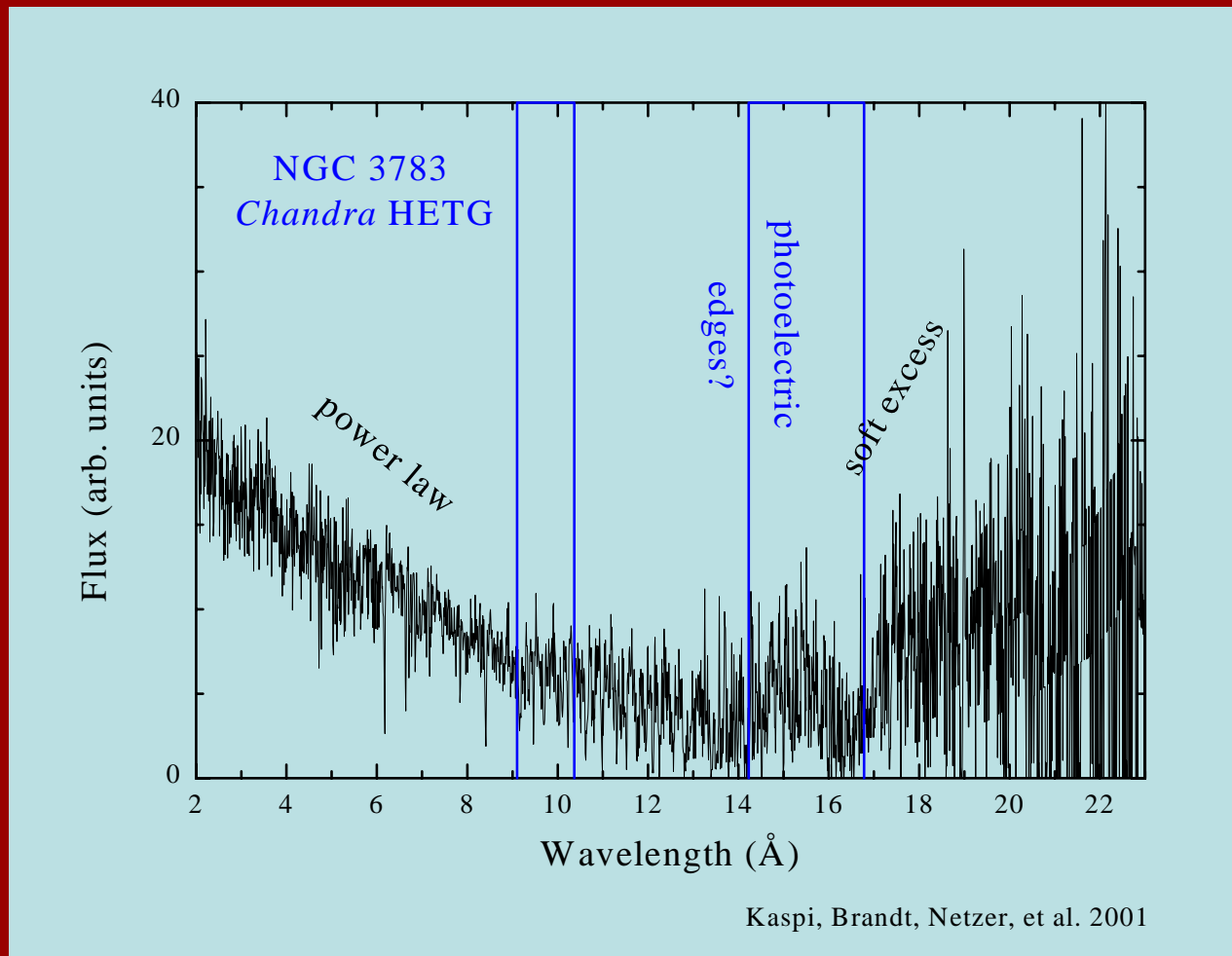
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# Photoionized Plasma

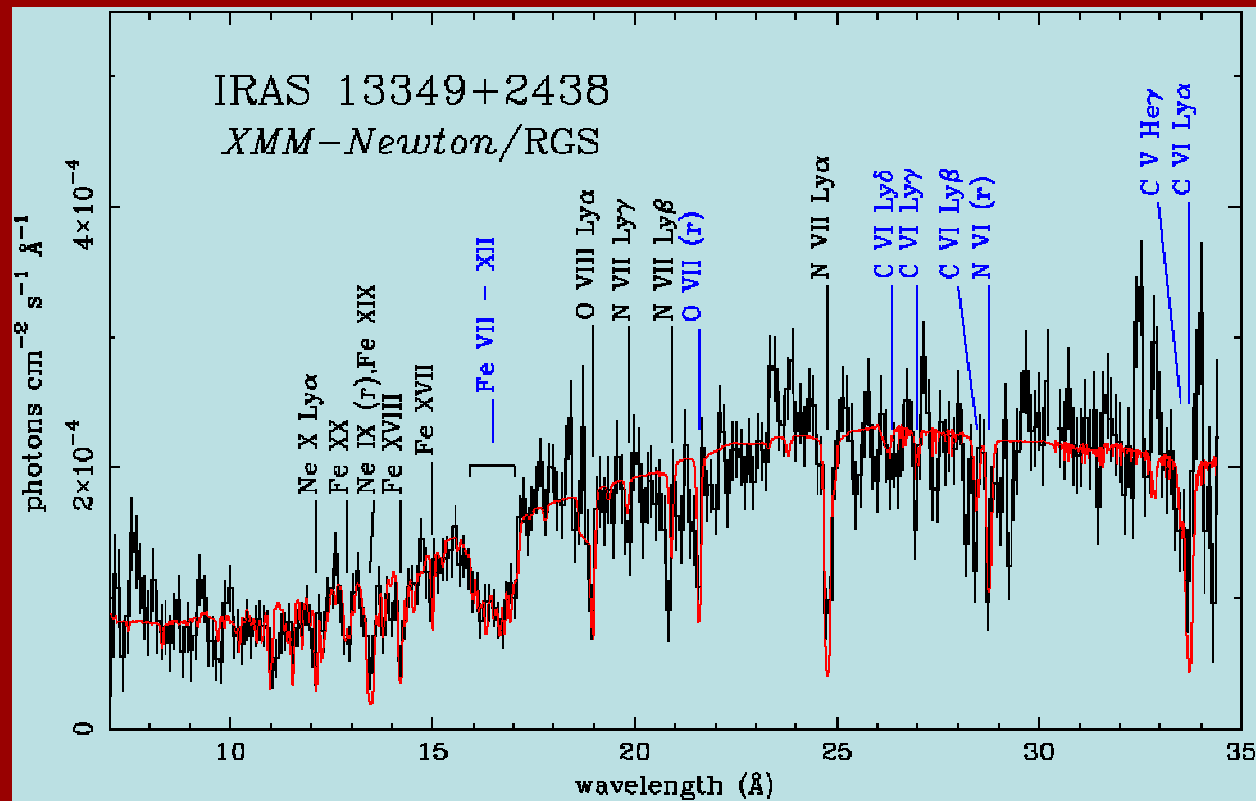
- ❖ Typically, created near accretion sources (X-ray binaries, AGN).
- ❖ Only external source of energy is radiation.
- ❖ Consequently, low temperatures compared to collisional plasma.
- ❖ X-ray emission mechanisms: radiative recombination (ensuing cascades), *photoexcitation*.
- ❖ Ionization balance governed by photoionization and  $\Delta n = 0$  DR.
- ❖ Ionization state determined by ionization parameter ( $\xi$ ).
- ❖ Hard to produce in the laboratory (remarkable exception: Z pinch featuring emission/absorption).



# The Type-I AGN Scenario: Absorption



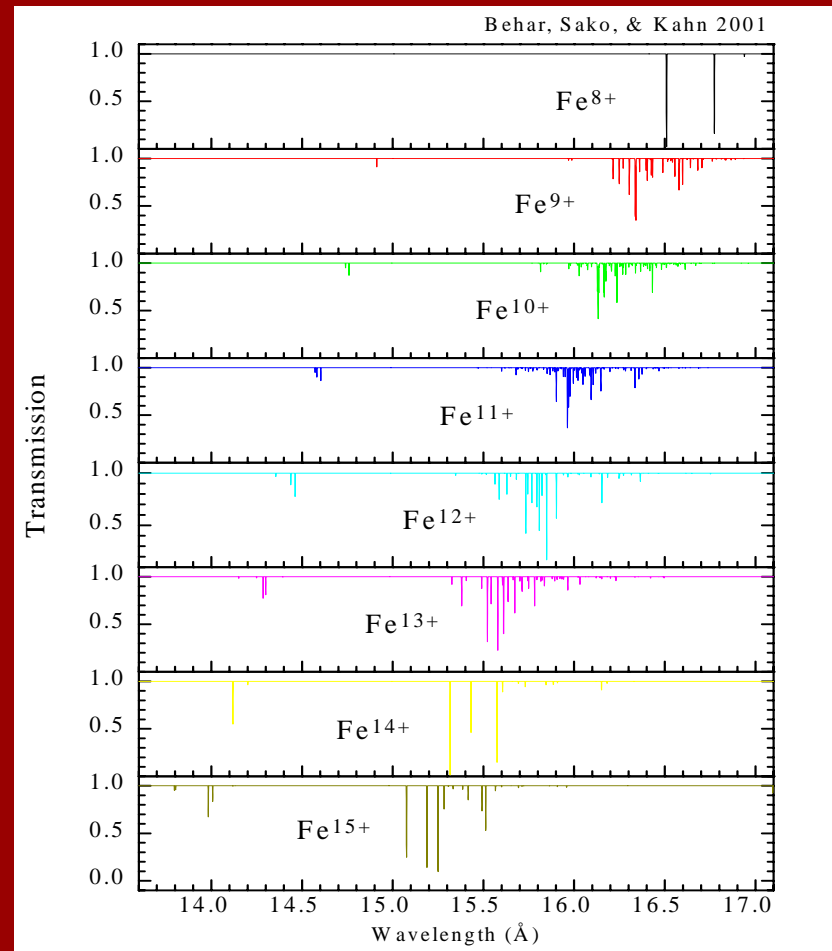
# The Type-I AGN (contd.): Wide Range of Charge States



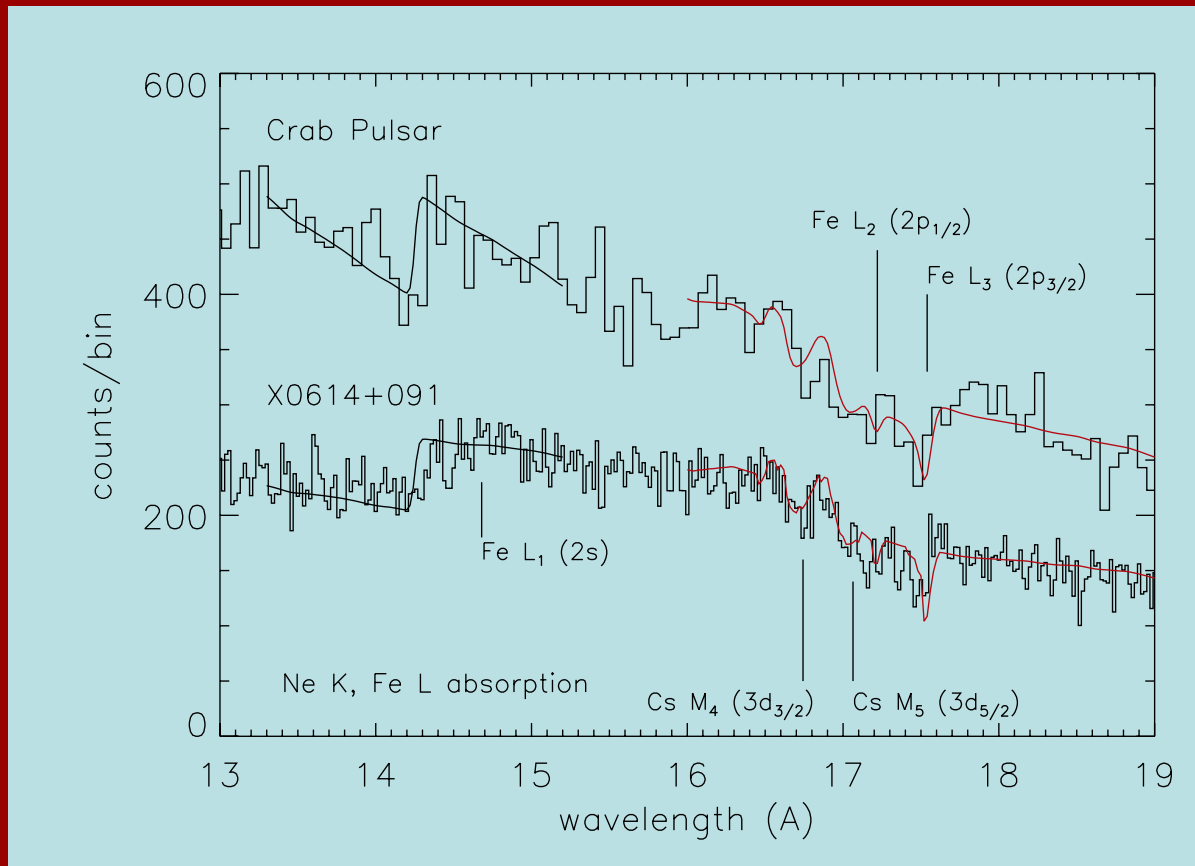
Sako, Kahn, Behar, et al. 2001

# The Fe 2p-3d Unresolved Transition Array (UTA)

- ❖ Absorption by 2p-3d transitions in Fe-M ions creates a UTA between  $\sim 15 - 17 \text{ \AA}$ .
- ❖ Has been observed in several AGN.
- ❖ Incidentally, similar feature has been observed in a very dissimilar laser plasma (Chenais-Popovic, Merdji, Misalla, et al. 2000).
- ❖ Wide range of charge states is very useful for diagnostics, especially for  $\xi$ .
- ❖ Astrophysical origin not totally clear (torus?).
- ❖ Data have been calculated and incorporated in x-ray codes.



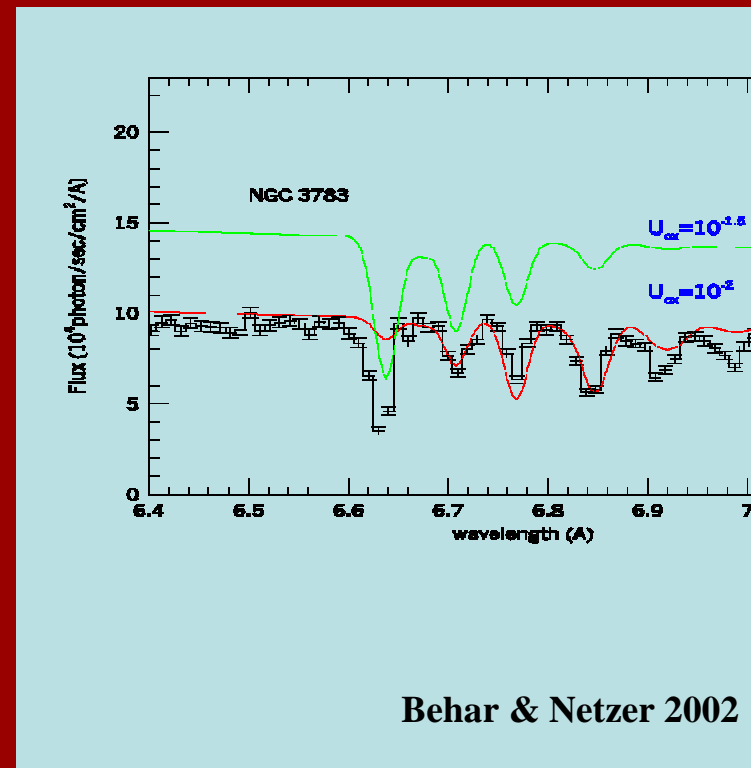
# Chemistry of the ISM Using X-Ray Inner-Shell Absorption



**X0614+091: Paerels, Brinkman, van der Meer et al. 2001**

# 1s-2p ( $K\alpha$ ) Inner-Shell Absorption

- ❖ L-shell ions (Li-like to F-like) have vacancies in their 2p sub-shell.
- ❖ This makes the 1s-2p resonance absorption lines possible.
- ❖ Have been observed in many sources and for many elements.
- ❖ Very useful in probing the ionization state(s) of the absorbing plasma.



# 1s-2p Inner-Shell Line Comparison

Wavelengths (Å) and  $f$ -values

Code Ion	R-Matrix	HULLAC	Cowan	
O <sup>5+</sup>	22.05 ( $f= 0.384,0.192$ )	22.01 (0.351,0.174)	22.05	
O <sup>4+</sup>	22.35	22.33	22.38	
O <sup>3+</sup>	22.73	22.73	22.77	
Fe <sup>23+</sup>	1.860 (0.491) 1.864 (0.146)	1.861 (0.469) 1.864 (0.147)	---	

# Inner-Shell Line Comparison

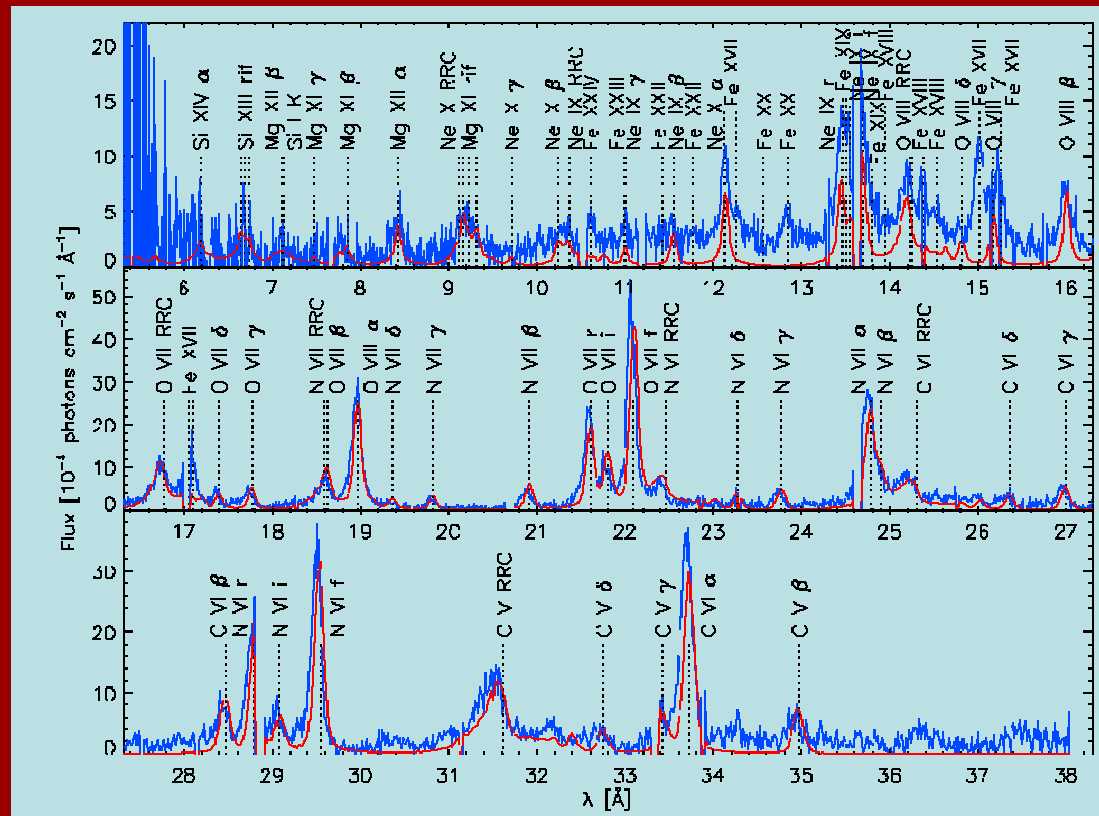
Wavelengths ( $\text{\AA}$ ) and  $f$ -values

Code Ion	R-Matrix	HULLAC	Cowan	NGC 5548*
O <sup>5+</sup>	22.05 ( $f= 0.384,0.192$ )	22.01 (0.351,0.174)	22.05	22.01
O <sup>4+</sup>	22.35	22.33	22.38	22.38
O <sup>3+</sup>	22.73	22.73	22.77	22.74
Fe <sup>23+</sup>	1.860 (0.491) 1.864 (0.146)	1.861 (0.469) 1.864 (0.147)	---	---

\* Based on velocity of O<sup>6+</sup> ( $\pm 0.01 \text{\AA}$ ); Courtesy of Jelle Kaastra

**Uncertainty of the order of the outflow velocity we want to measure!**

# The Type-II AGN Scenario: Emission

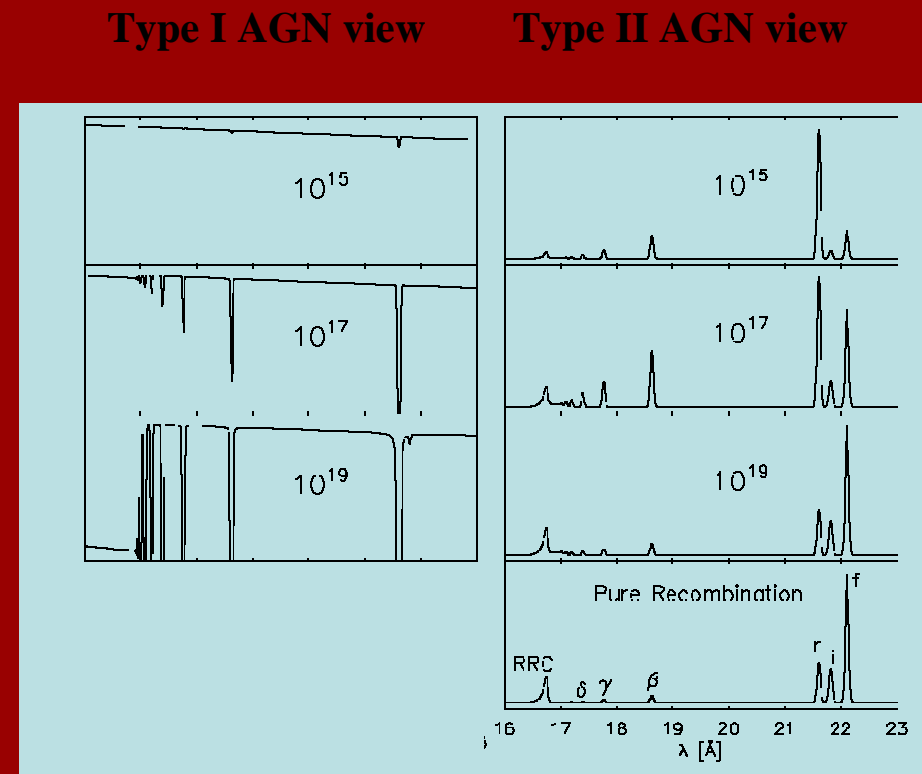


**NGC 1068 / RGS**

Kinkhabwala, Sako, Behar, et al. 2002

# Measuring Column Density Perpendicular to the Line of Sight

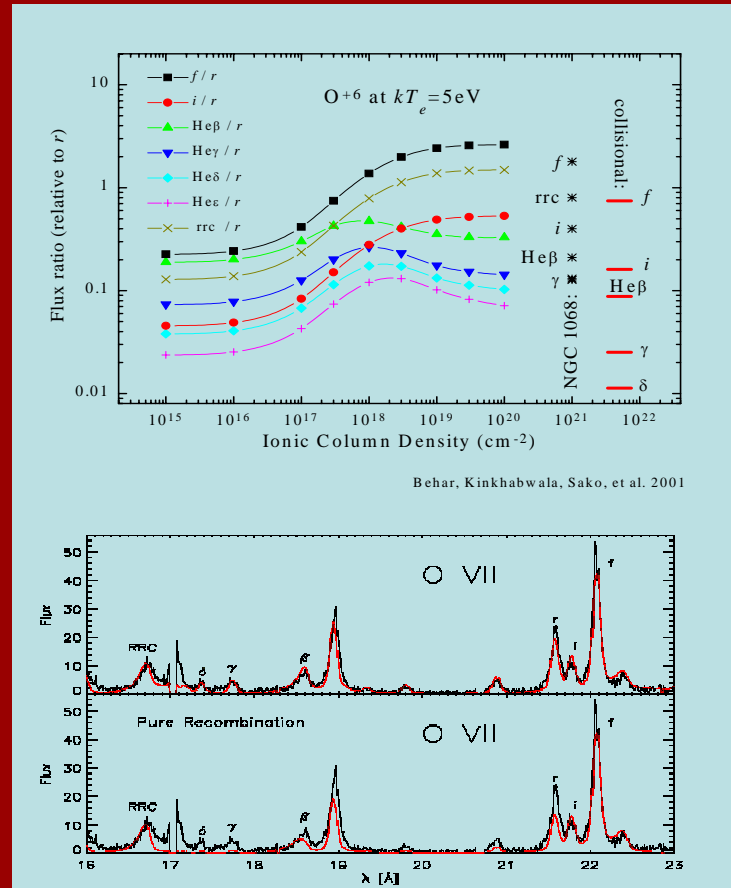
- ❖ Line and RRC (re)emission depends strongly on the balance between recombination and photoexcitation (PE), which, in turn, depends directly on the column density (and velocity).
- ❖ When the resonance lines saturate the PE contribution is turned off, while recombination persists.
- ❖ Superficially, the PE effect can be somewhat mimicked by hot collisional gas.
- ❖ This has caused confusion in the x-ray community in the context of the very popular topic of the AGN-Starburst connection.
- ❖ But, the high- $n$  lines save the day.



Kinkhabwala, Sako, Behar, et al. 2002

# Measuring Column Density (contd.)

- ❖ The high- $n$  lines provide a clear distinction between AGN and SB.
- ❖ The spectra of all type II AGN (e.g. NGC 1068) we've looked at so far can be explained by pure photoionization models (i.e., no SB).
- ❖ Atomic data seem to be adequate. Still working on Fe-L.



Behar, Kinkhabwala, Sako, et al. 2001

Kinkhabwala, Sako, Behar, et al. 2002

# X-Ray Photoionized Plasmas: Atomic Data Needs

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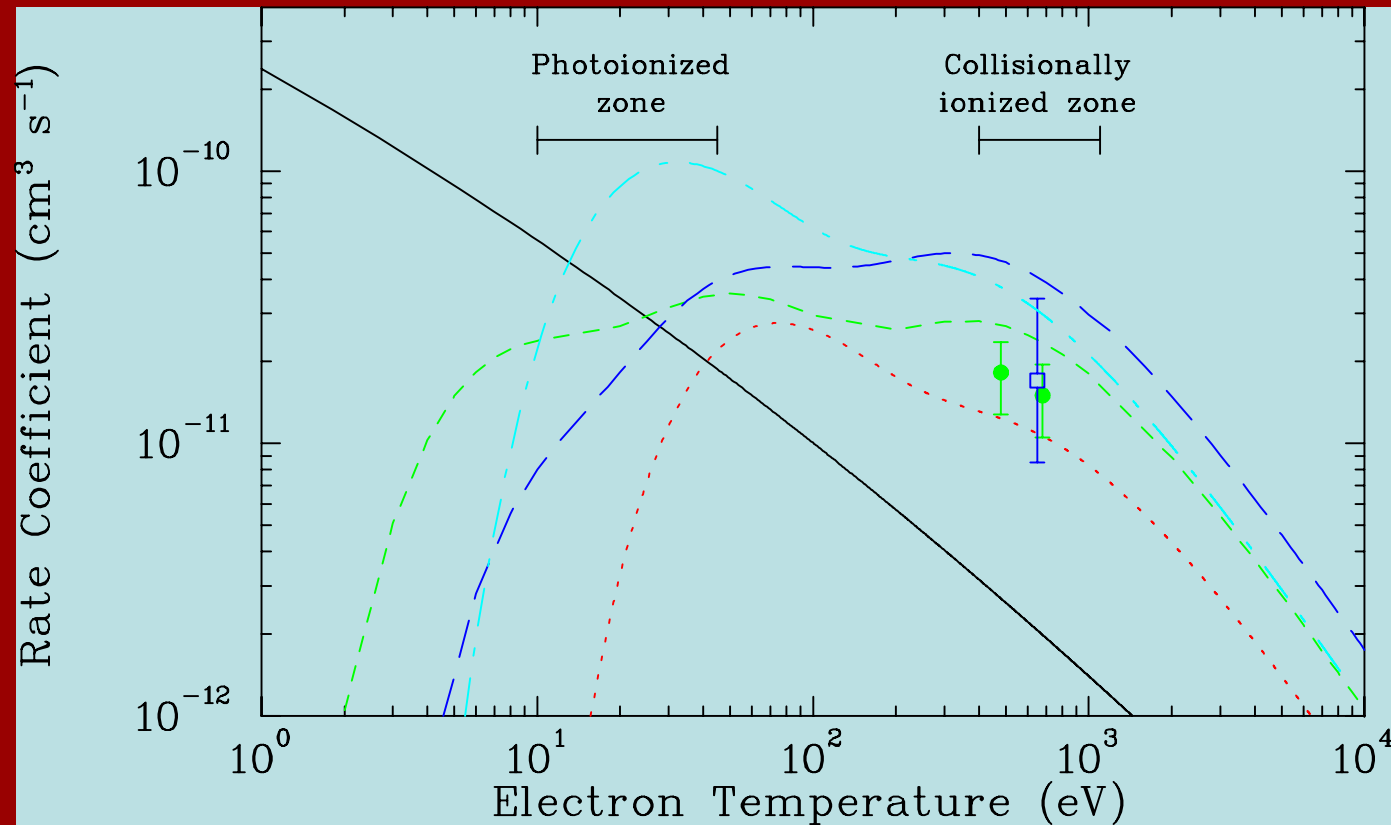
## ❖ Processes and Data

- Generally important
  - ❖ Wavelengths in highly ionized species
  - ❖ Photoionization, recombination, and radiative cascades rates (emissivities)
  - ❖ Photoexcitation (oscillator strengths), **particularly inner-shell**
  - ❖ **Fluorescence yields** (the above + autoionization rates)
  - ❖ Total ionization and recombination rates
- More specific
  - ❖ **X-ray impact on dust and molecules**: absorption wavelengths
  - ❖ Transitions among excited states
  - ❖ Charge exchange

## ❖ Ions

- K-shell of C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe
- L-shell, particularly Fe, but also Ne, Mg, Si, S, Ar, Ca, and Ni
- **But also... all the lower charge states through inner-shell transitions**

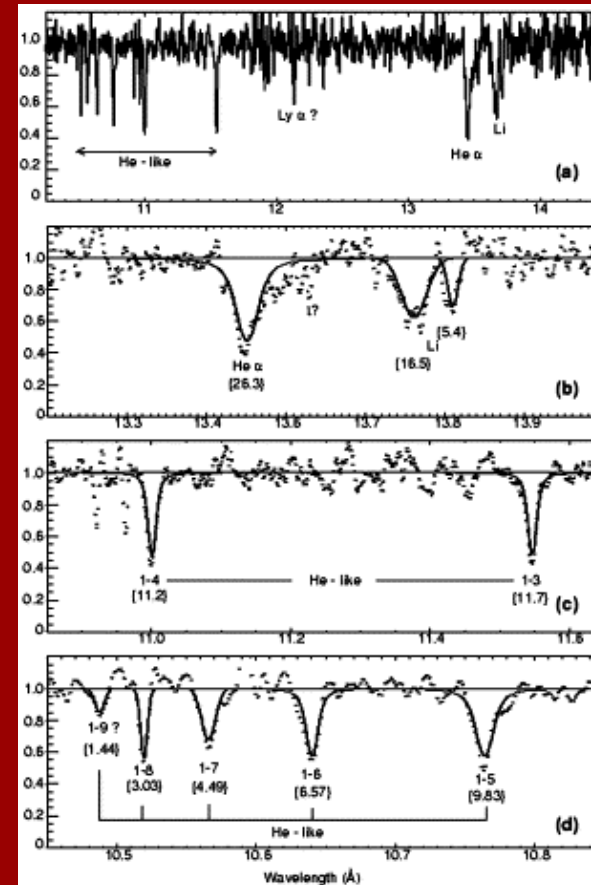
# Fe-L DR, Again, Not Doing So Good



Courtesy of Daniel Savin

# Laboratory Experiments: Z Pinch (& Laser Plasma)

- ❖ Absorption measurements; wavelengths and oscillator strengths.
- ❖ Particularly needed: Inner-shell lines (see my poster).
- ❖ Ionization balance and emission measurements are also possible (Heeter).
- ❖ High laboratory densities might still hinder direct application.



Bailey, Cohen, Chandler, et al. 2001

# Conclusions

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- ❖ High-resolution spectra are constantly being obtained with the gratings on board *Chandra* and *XMM-Newton*. These require high-quality atomic data.
- ❖ For x-ray *collisional plasmas*, much of the available data are of satisfactory quality, allowing for high precision analysis of astrophysical observations.
- ❖ For x-ray *photoionized plasmas*, much, but certainly not all of the available data is of satisfactory quality, both for absorption and for emission.
- ❖ The remaining outstanding problems need to be identified. Some are being addressed by beam experiments such as EBIT and TSR.
- ❖ Fe-L photoionization models remain to be tested.
- ❖ A vast amount of data for inner-shell absorption have been calculated, but these are in urgent need of laboratory verification.