

# MODELING X-RAY SPECTRA OF ASTROPHYSICAL PLASMAS IMPLICATIONS FOR STATISTICAL ANALYSIS

Randall Smith (CfA)

Collaborators:

N. Brickhouse, A. Foster,

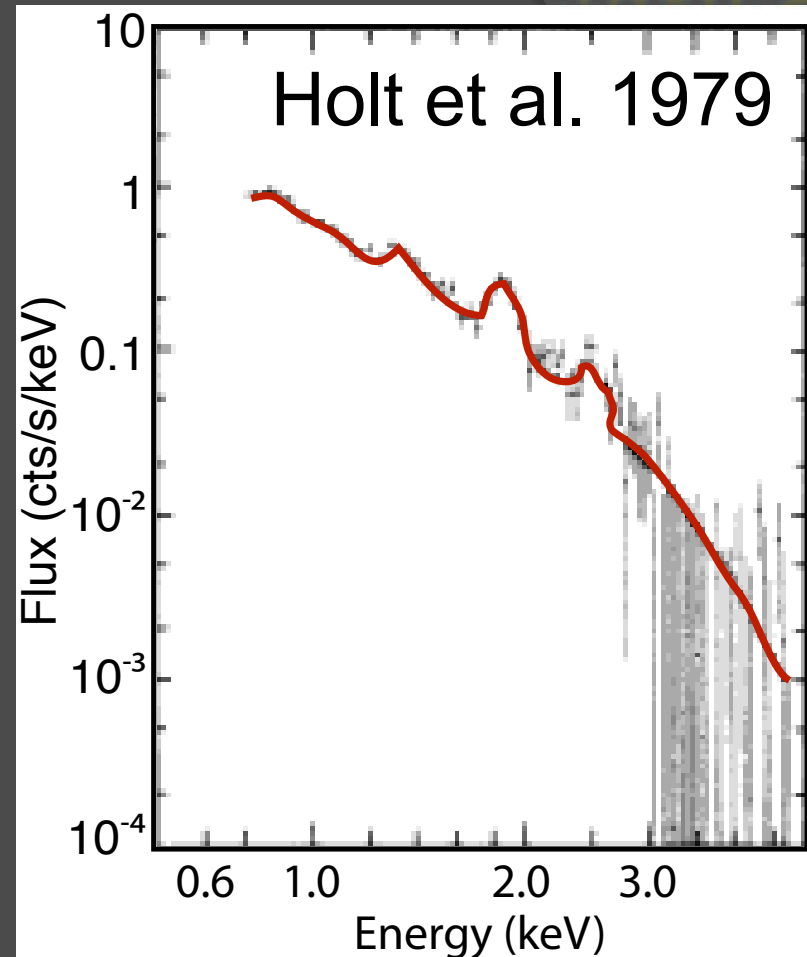
H. Yamaguchi (CfA),

J. Wilms (Erlangen), Li Ji (PMO)

# “X-ray Line Emission from Capella”

1980'S

- Mg, Si, S, and Fe are unambiguously detected
- Inconsistent with an isothermal corona, and requires components between  $6 - 24 \times 10^6$  K for an adequate fit.
- Suggests an X-ray emitting plasma confined to magnetically contained loops explains the data.



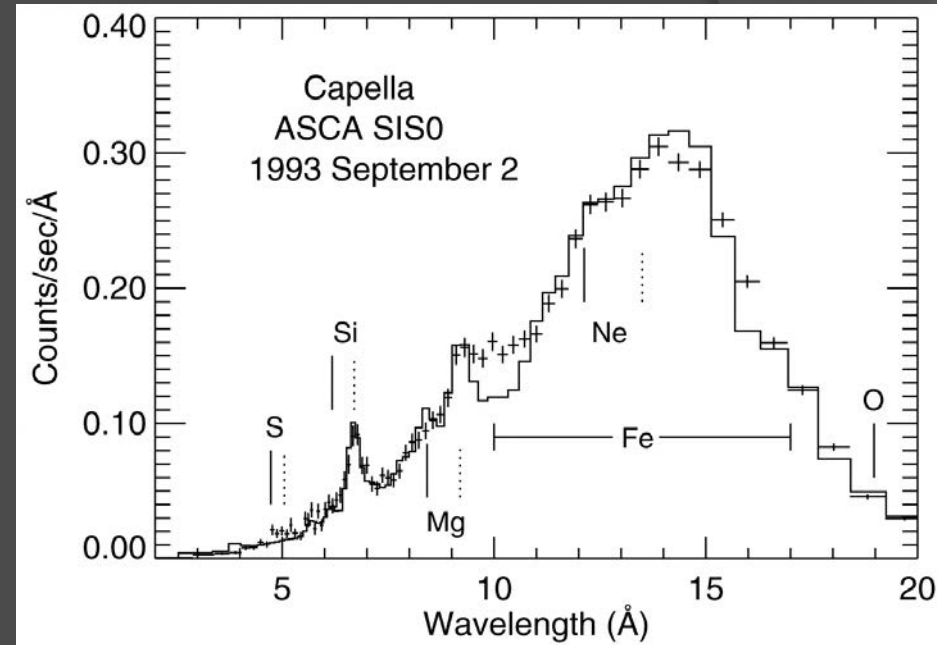
*7 ksec exposure with the Einstein Solid State Spectrometer*

# “X-ray Line Emission from Capella”

1990'S

## Coronal Structure and Abundances of Capella from EUVE and ASCA Spectroscopy

- Collisional plasma models **appear to have flux deficits.**
- **New atomic models** allow reliable determination of elemental abundances.
- **EUVE data are not well fitted with only two temperatures.**
- Mg, Si, S, and Fe consistent with solar photospheric values, while Ne appears to be underabundant by a factor of  $\sim 3$  to 4.

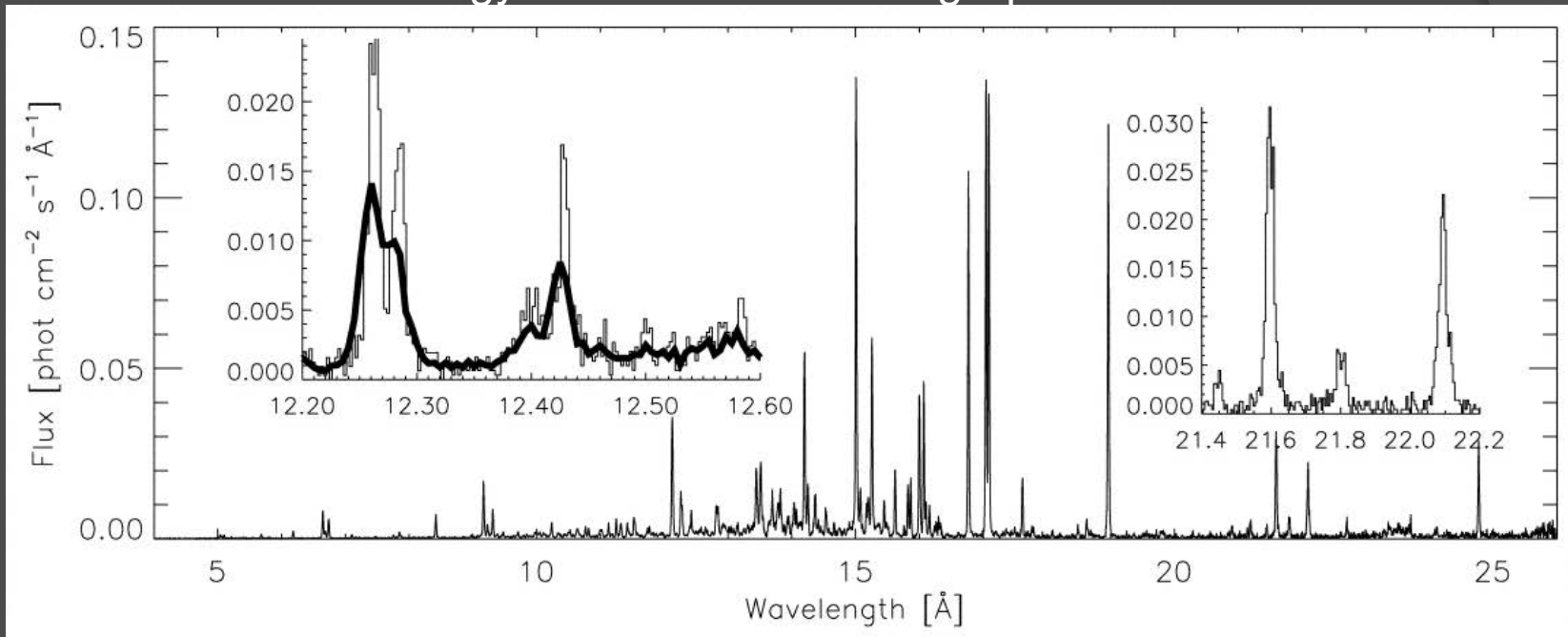


*21 ksec obs. w/ASCA Silicon Imaging Spectrometer (Brickhouse et al. 2000)*

# “X-ray Line Emission from Capella”

2000'S

High-Resolution X-Ray Spectra of Capella: Initial Results from the Chandra High-Energy Transmission Grating Spectrometer



*89 ksec w/Chandra HETG (Canizares et al. 2000)*

- Broad range of temperatures, from  $\log T = 6.3$  to  $7.2$
- The electron density is  $\sim 10^{10} \text{ cm}^{-3}$  at  $T_e \sim 2 \times 10^6 \text{ K}$ .
- The density and emission measure show the coronal loops are significantly smaller than the stellar radius.

# What is an AtomDB?

The AtomDB is database of atomic values – wavelengths & rates – useful for calculating emission & absorption in X-ray spectra, especially from astrophysical plasmas.

It's used by X-ray astrophysicists to identify the elements or ions that create features in an observed spectrum, and also to determine the parameters (temperature, density, etc) of the emitting plasma.

The first version of the AtomDB was released in 2001; it is now the standard source in the field.

## ATOMDB ATOMIC DATA FOR ASTROPHYSICISTS

Features - Comparisons - Physics - FAQ - Download - Contact Us - Login/Register

### Get transition information:

Select an element:

H

### List lines in wavelength region:

Wavelength:   Å  keV

Width:  0.01

Min. Emissivity:  1.e-18 photons cm<sup>3</sup> s<sup>-1</sup>

Elec. Temp. units:  K  keV

### List strong lines in wavelength region at a specific temperature:

Wavelength:   Å  keV

Width:  0.01

Min. Emissivity:  1.e-18 photons cm<sup>3</sup> s<sup>-1</sup>

Elec. Temp.:   K  keV

### Energy level 1

Electron configuration	2p6
Energy above ground (eV)	0
Quantum state	n=2, L=0, S=0.0, degeneracy=1, parity=even
Energy level data source	2006JPhB...39...85L
Photoionization data source	1995A&AS..109..125V

### Energy level 27

Electron configuration	2p5 3d1
Energy above ground (eV)	825.829
Quantum state	n=3, L=1, S=0.0, degeneracy=3, parity=odd
Energy level data source	2006JPhB...39...85L
Photoionization data source	

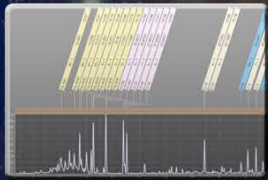
### Level 27 → 1 Interactions

Electron collision rate	Nonzero
Reference	2006JPhB...39...85L
Wavelength (lab/observed)	15.014±0.001Å
Wavelength (theory)	15.0133Å
Transition rate/Einstein A	2.46e+13s <sup>-1</sup>
Transition Type*	E1
Oscillator Strength f <sub>1→27</sub> *	2.4938e+0
Wavelength (lab/observed) reference	
Wavelength (theory) reference	2006JPhB...39...85L
Transition rate reference	2006JPhB...39...85L

Ion	Wavelength Å	Upper Level	Lower Level	Emissivity ph cm <sup>3</sup> s <sup>-1</sup>	Te peak K	Relative Intensity
Fe XIX	14.961	12	1	6.819e-17	1.000e+7	0.03
Fe XIX	14.963	16	4	3.964e-17	1.000e+7	0.02
Fe XX	14.969	49	10	4.275e-18	1.000e+7	0.00
Fe XVIII	14.972	26	1	2.053e-17	7.943e+6	0.01
Fe XX	14.980	29	7	3.143e-18	1.000e+7	0.00
Fe XIX	15.000	26	5	3.323e-18	1.000e+7	0.00
Fe XIX	15.008	15	4	1.697e-17	1.000e+7	0.01
Fe XVII	15.014	27	1	2.228e-15	6.310e+6	1.00
Fe XX	15.047	22	6	1.663e-17	1.000e+7	0.01
Fe XX	15.047	27	7	9.682e-18	1.000e+7	0.00

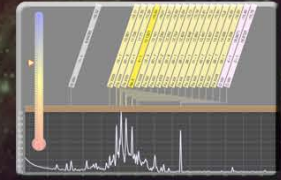


# We even have an iTunes App!



Emission lines  
by wavelengths

Strong lines grouped  
by temperature



H															He				
Li	Be													B	C	N	O	F	Ne
Na	Mg													Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		

AtomDB is an atomic database useful for X-ray plasma spectral modeling. The current version of AtomDB is primarily used for modeling collisional plasmas, those where hot electrons colliding with astrophysically abundant elements and ions create X-ray emission. AtomDB is also useful when modeling absorption by elements and ions or even photoionized plasmas, where X-ray photons interacting with elements and ions create complex spectra.

ATOMDB

Web site & download info



References browser



HARVARD-SMITHSONIAN  
CENTER FOR ASTROPHYSICS

**ATOMDB**

ATOMIC DATA FOR  
ASTROPHYSICISTS

v2.0.2 BUILD 4787

February 23, 2012

# AtomDB: Atomic Data for X-ray Astrophysicists

1	1s <sup>2</sup>	0.0000	1	0	0	1	2	0%
2	1s <sup>1</sup> 2s <sup>1</sup>	561.24	2	0	1	3	1	0%
3	1s <sup>1</sup> 2s <sup>1</sup>	569.68	2	0	0	1	1	10%
4	1s <sup>1</sup> 2p <sup>1</sup>	568.81	2	1	1	1	1	15%
5	1s <sup>1</sup> 2p <sup>1</sup>	568.86	2	1	1	3	1	20%
6	1s <sup>1</sup> 2p <sup>1</sup>	568.95	2	1	1	5	1	25%
7	1s <sup>1</sup> 2p <sup>1</sup>	574.79	2	1	0	3	1	30%
8	1s <sup>1</sup> 3s <sup>1</sup>	662.45	3	0	1	3	1	35%
9	1s <sup>1</sup> 3s <sup>1</sup>	664.63	3	0	0	1	1	40%
10	1s <sup>1</sup> 3p <sup>1</sup>	664.48	3	1	1	1	1	45%
11	1s <sup>1</sup> 3p <sup>1</sup>	664.49	3	1	1	3	1	50%
12	1s <sup>1</sup> 3p <sup>1</sup>	664.52	3	1	1	5	1	55%
13	1s <sup>1</sup> 3p <sup>1</sup>	666.11	3	1	0	3	1	60%
14	1s <sup>1</sup> 3d <sup>1</sup>	665.63	3	2	1	3	1	65%
15	1s <sup>1</sup> 3d <sup>1</sup>	665.63	3	2	1	5	1	70%
16	1s <sup>1</sup> 3d <sup>1</sup>	665.64	3	2	1	7	1	75%
								80%
								85%

8      15.9994  
O VII  
 Oxygen  
 1s<sup>2</sup>2s<sup>2</sup>2p<sup>4</sup>

Level	2 → 1										
Electron configuration	1s <sup>1</sup> 2s <sup>1</sup> → 1s <sup>2</sup>										
Energy above ground	561.24 eV → 0.0000 eV										
Quantum state	<table border="1" style="font-size: 0.8em;"> <thead> <tr><th>n</th><th>L</th><th>S</th><th>degeneracy</th><th>parity</th></tr> </thead> <tbody> <tr><td>2 → 1</td><td>0</td><td>1 → 0</td><td>3 → 1</td><td>even → even</td></tr> </tbody> </table>	n	L	S	degeneracy	parity	2 → 1	0	1 → 0	3 → 1	even → even
n	L	S	degeneracy	parity							
2 → 1	0	1 → 0	3 → 1	even → even							
Energy level reference	<a href="#">Whiteford ICFT</a>										
Photoionization reference	<a href="#">1986ADNDT..34..415C</a>										

Electron collision rate	nonzero
Collision rate reference	TBD
Wavelength (theory)	22.0977 Å
Transition rate/Einstein A	912 s <sup>-1</sup>
Transition type	M1
Oscillator strength f <sub>2→1</sub>	2.00296×10 <sup>-10</sup>
Wavelength (theory) reference	<a href="#">Whiteford ICFT</a>
Transition rate reference	<a href="#">Whiteford ICFT</a>

Radiative transition (1 found):

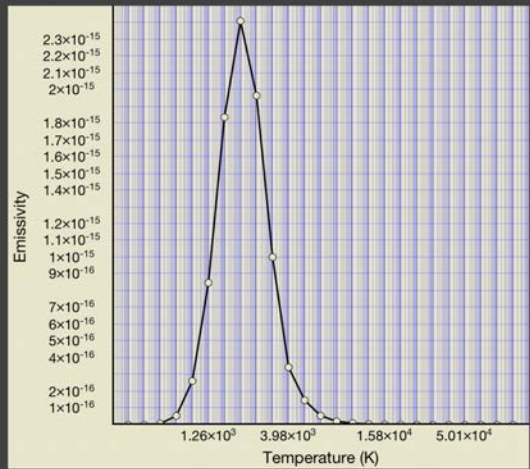
Wavelength (Å)	Wavelength Ref	Einstein A (s <sup>-1</sup> )	Einstein A Ref
----------------	----------------	-------------------------------	----------------

Electron collision rate	nonzero
Collision rate reference	TBD
Wavelength (theory)	22.0977 Å
Transition rate/Einstein A	912 s <sup>-1</sup>
Transition type	M1
Oscillator strength f <sub>2→1</sub>	2.00296×10 <sup>-10</sup>
Wavelength (theory) reference	<a href="#">Whiteford ICFT</a>
Transition rate reference	<a href="#">Whiteford ICFT</a>

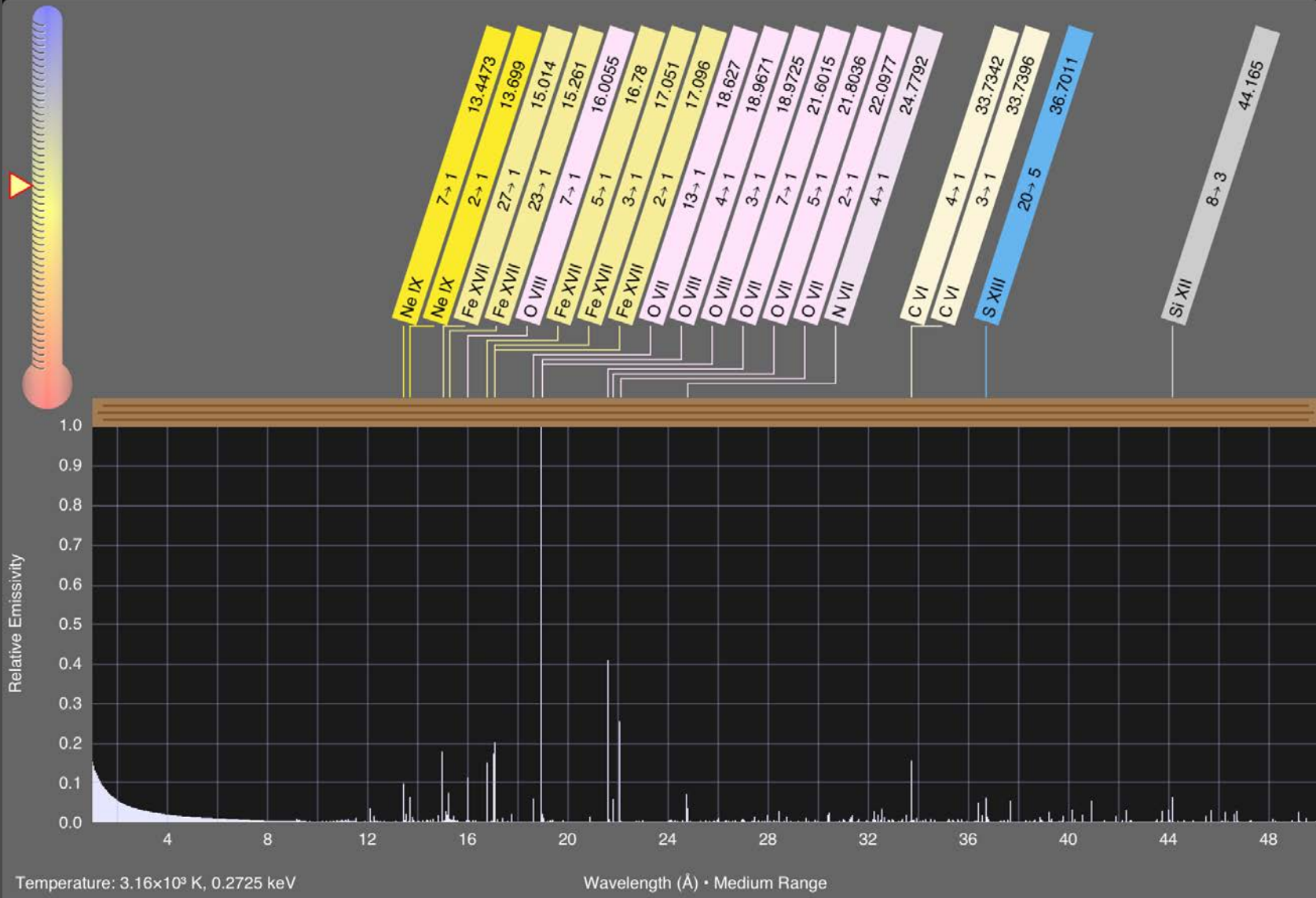
Radiative transition (1 found):

Wavelength (Å)	Wavelength Ref	Einstein A (s <sup>-1</sup> )	Einstein A Ref
22.1 ± 0.007	<a href="#">Whiteford ICFT</a>	912	<a href="#">Whiteford ICFT</a>

Temperature vs. emissivity for O VII 2 → 1:





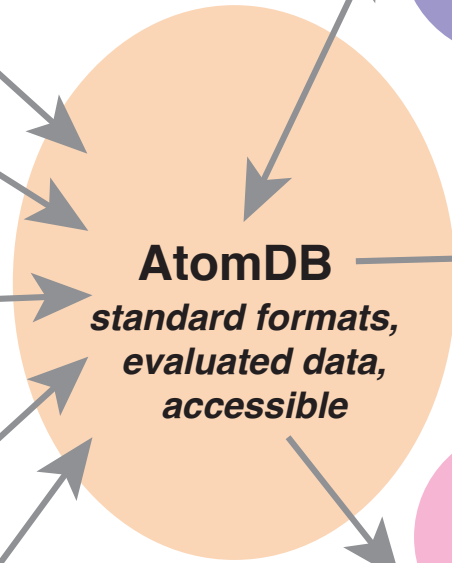


Navigation and control icons: Home, Plot, Legend, Settings, Grid, Zoom, Pan, and other interactive tools.

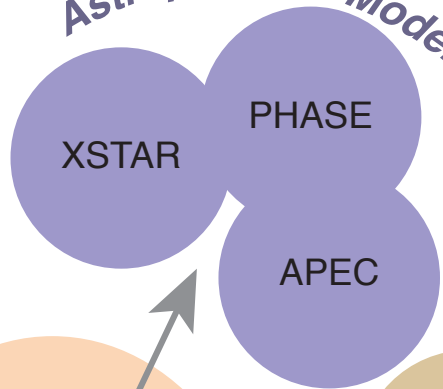
# AtomDB: Rates, Emissivities, and more

*Theoretical and Laboratory Atomic Data (various formats)*

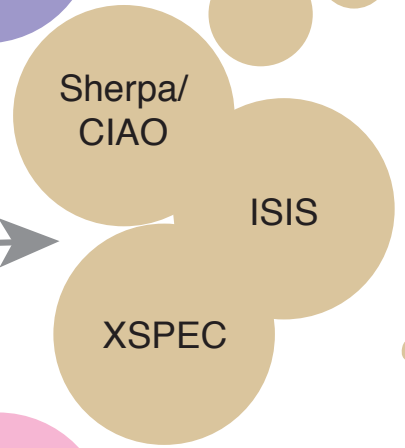
- Wavelengths
- Atomic Structure
- Collisional Rate Coefficients
- Radiative Transition Rates
- Photon Cross Sections



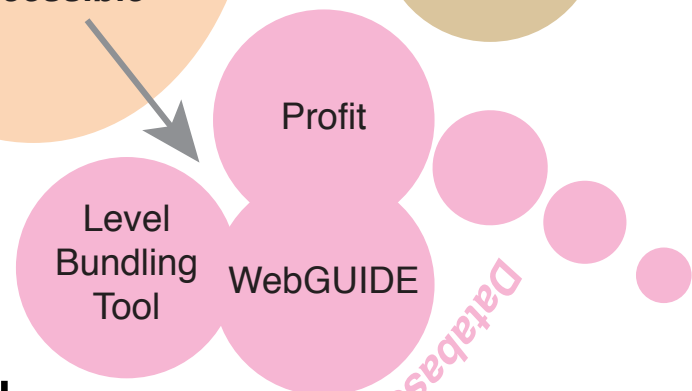
*Astrophysical Models*



*Analysis Tools*

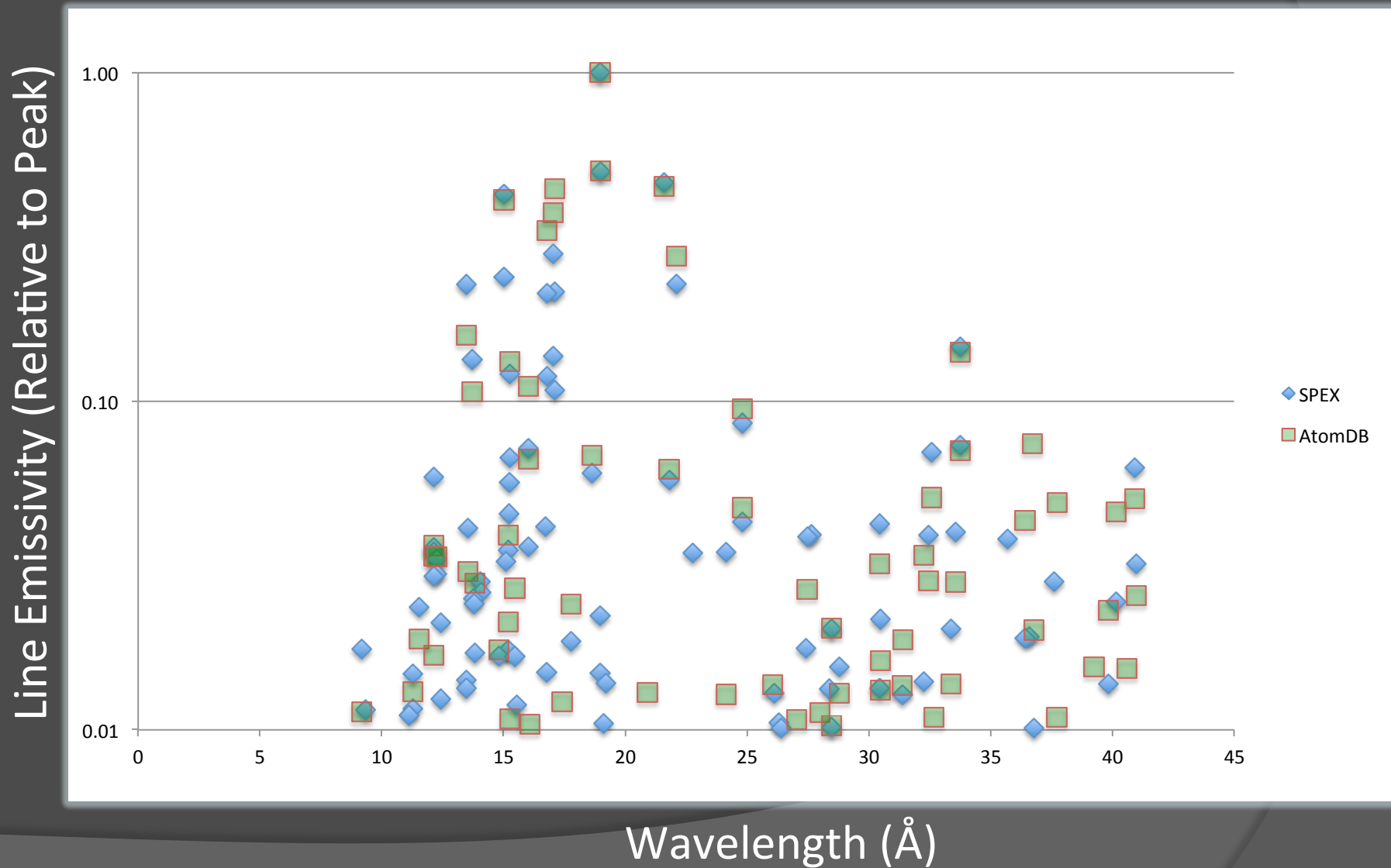


*Database Tools*

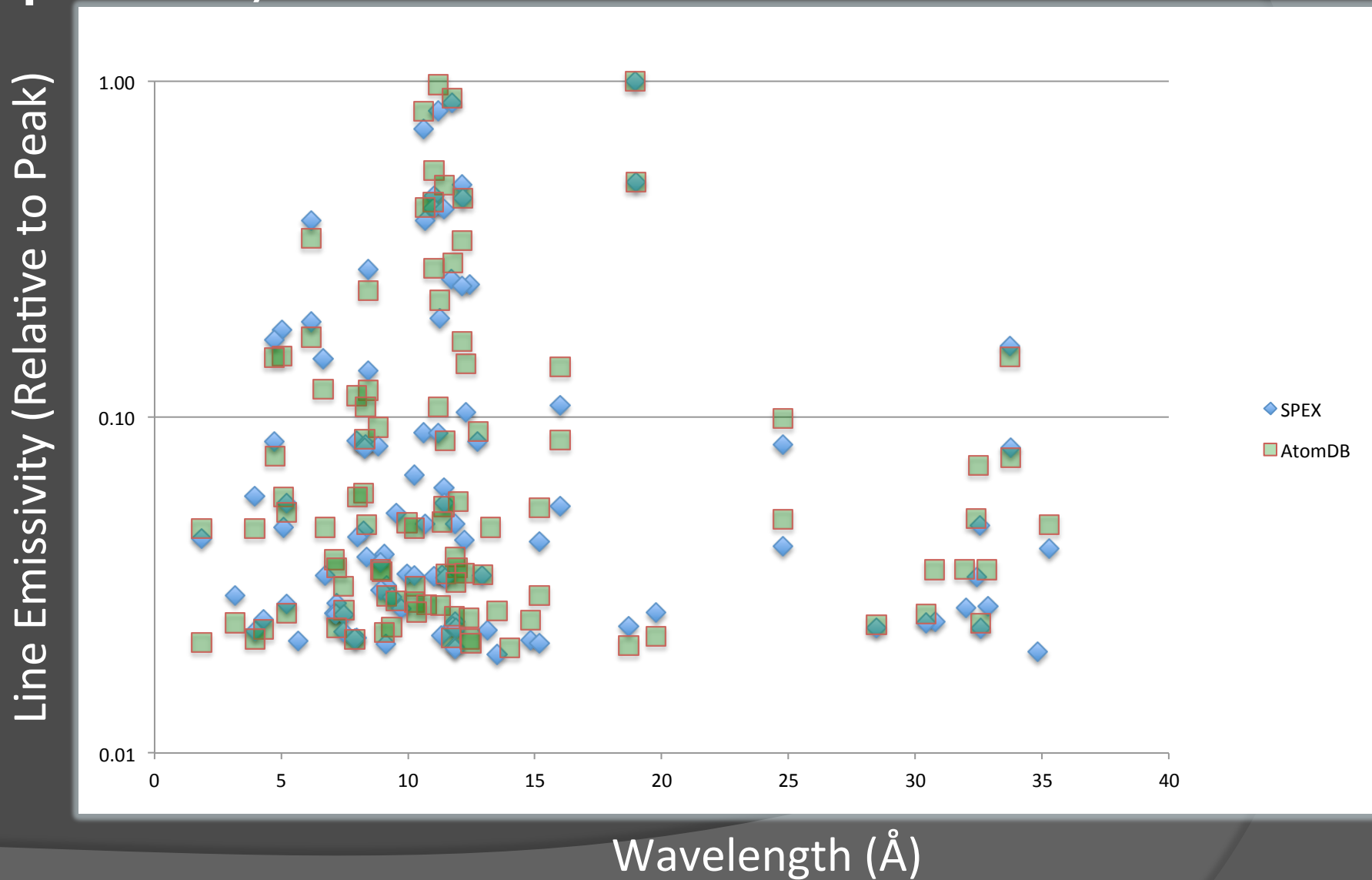


<http://www.atomdb.org>

# 100 strongest lines from a $kT=0.3$ keV plasma, SPEX vs AtomDB

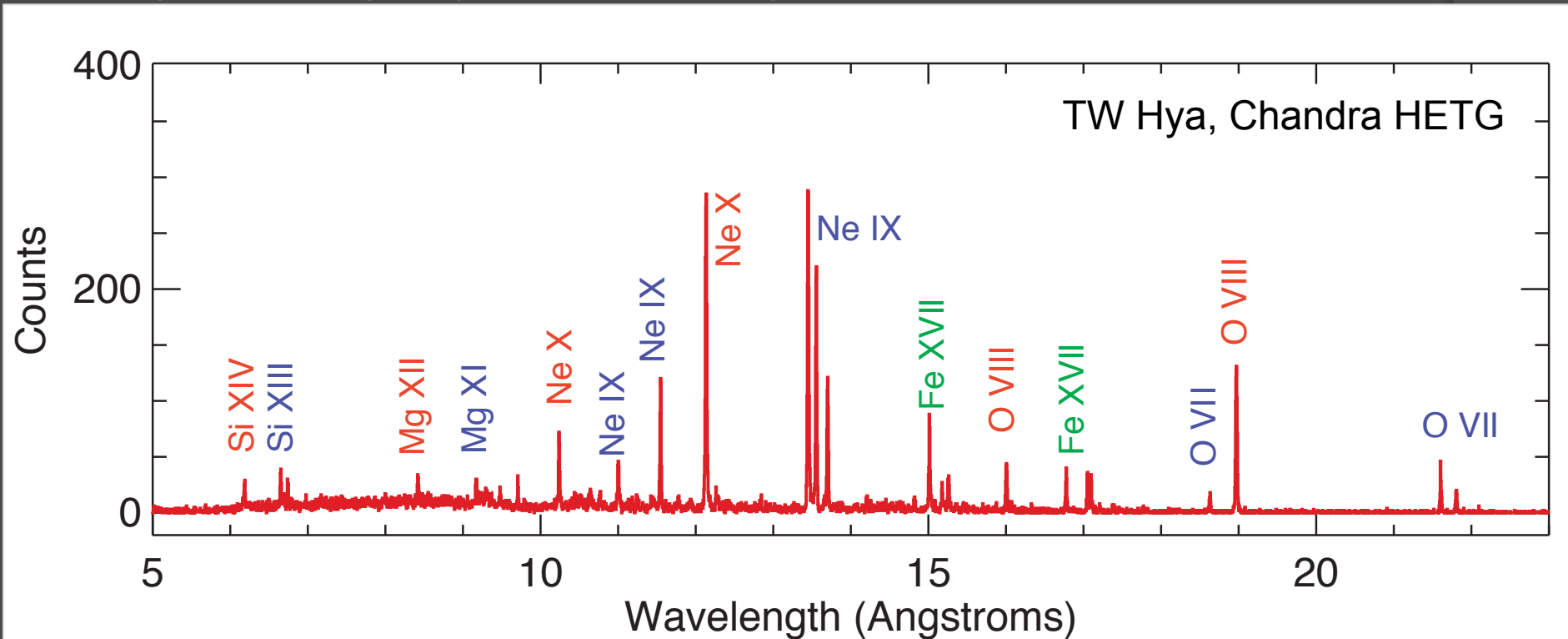


# 100 strongest lines from a $kT=2$ keV plasma, SPEX vs AtomDB



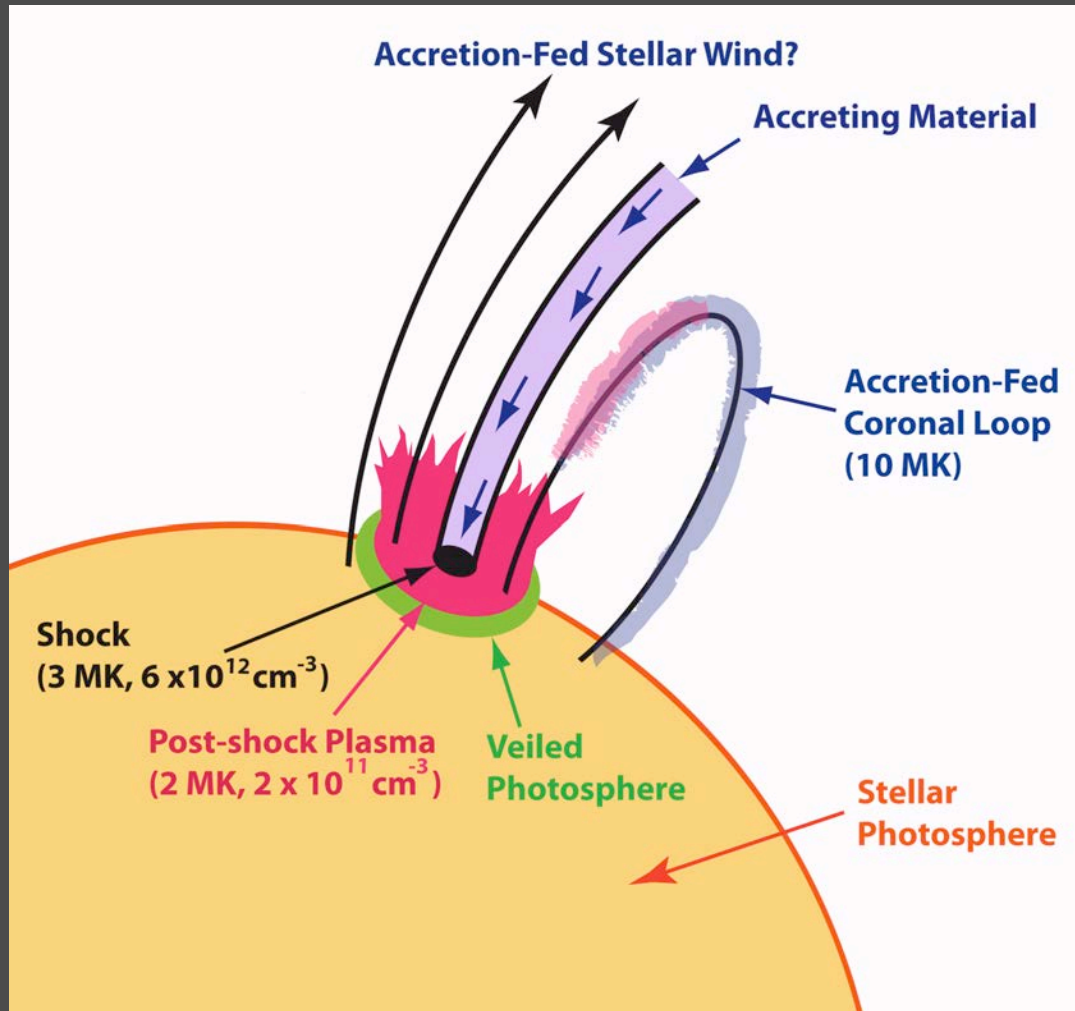
# TW Hya: Accretion & X-rays

TW Hya: A 10 Myr old “Sun” that is still growing by accreting mass from a disk





# TW Hya: Accretion & X-rays

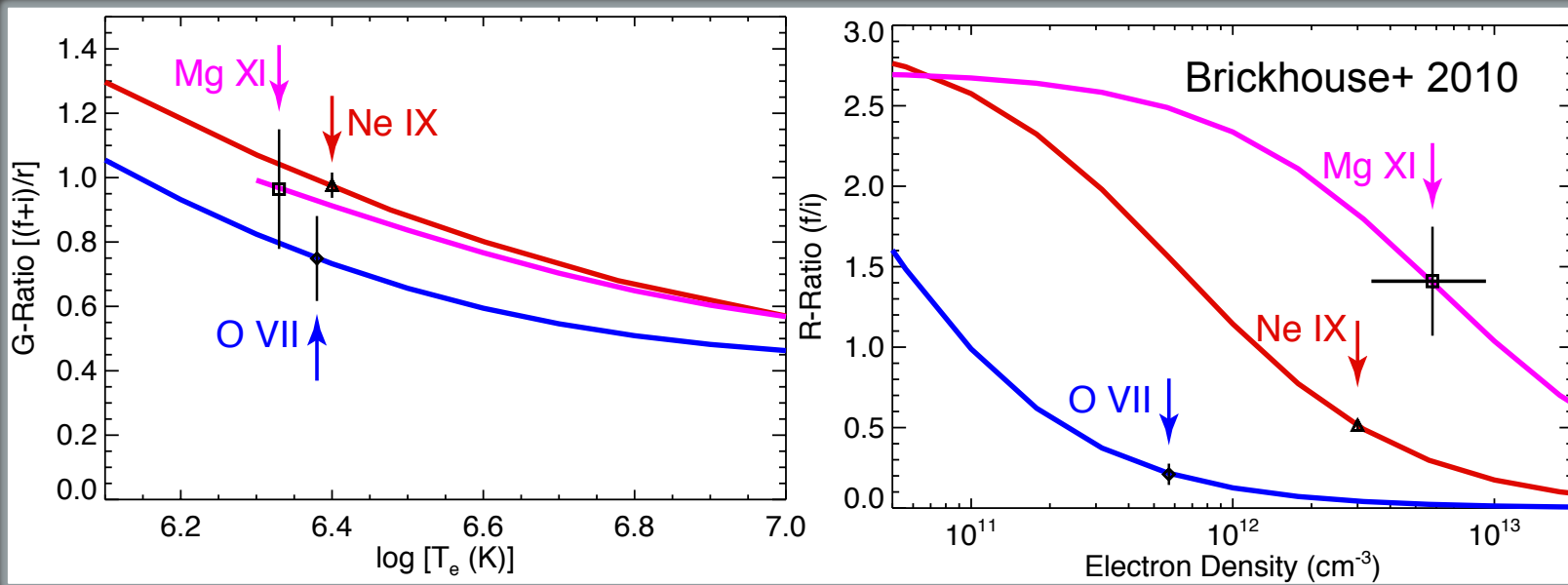


Brickhouse+ 2010

Our current best 'picture' of the situation

Accretion apparently heats a significant amount of coronal gas well beyond the shock itself.

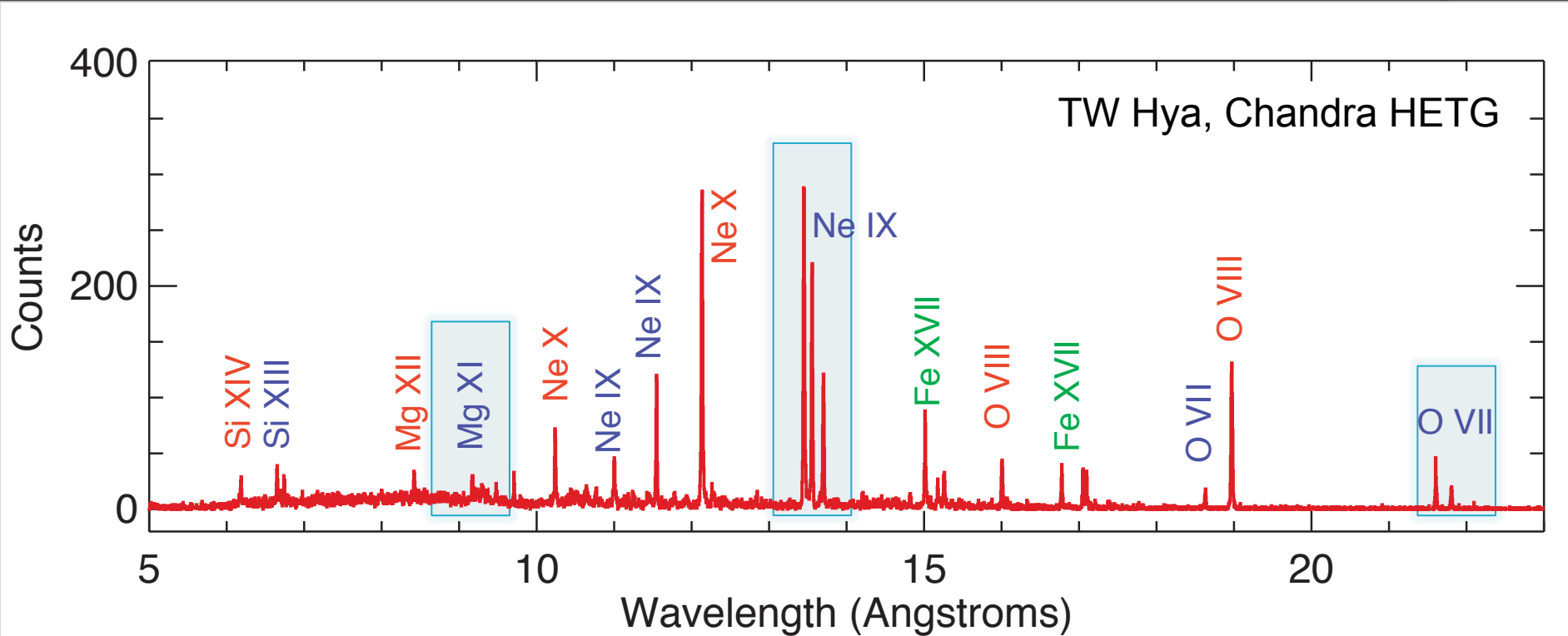
# Helium-like Diagnostics



While the **temperature** diagnostics for Mg XI, Ne IX, and O VII all give roughly the same result, the **density** diagnostics are significantly different.

# TW Hya: Accretion & X-rays

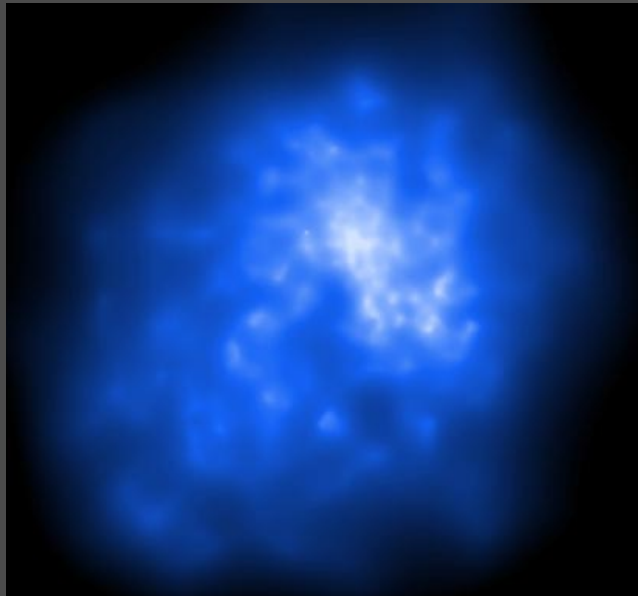
TW Hya: A 10 Myr old “Sun” that is still growing by accreting mass from a disk



How does matter and energy move in and around galaxies?

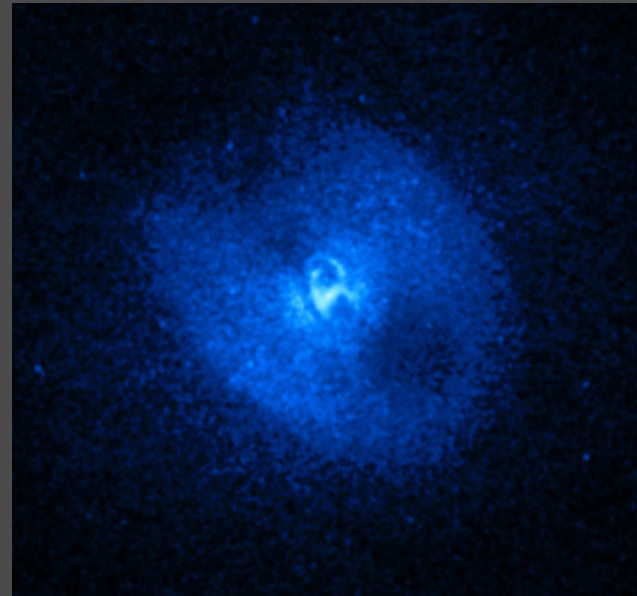
# The Velocity of Intragalactic Gas in Elliptical Galaxies

NGC 5044



NASA/CXC/U. Ohio/T.Statler & S.Diehl

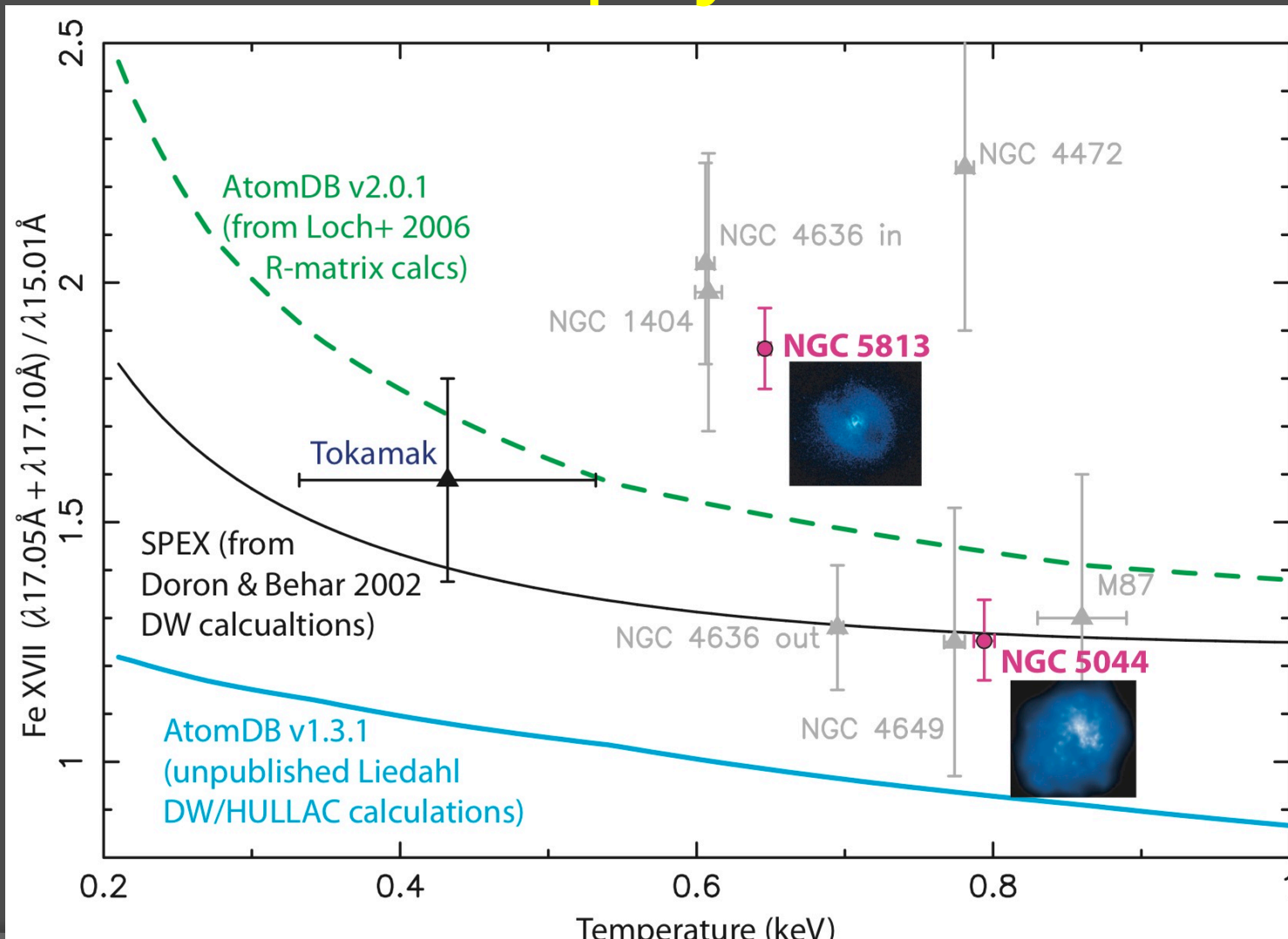
NGC 5813



NASA/CXC/SAO/S.Randall et al.

How does matter and energy move in and around galaxies?

# Fe XVII: Astrophysics & Theory

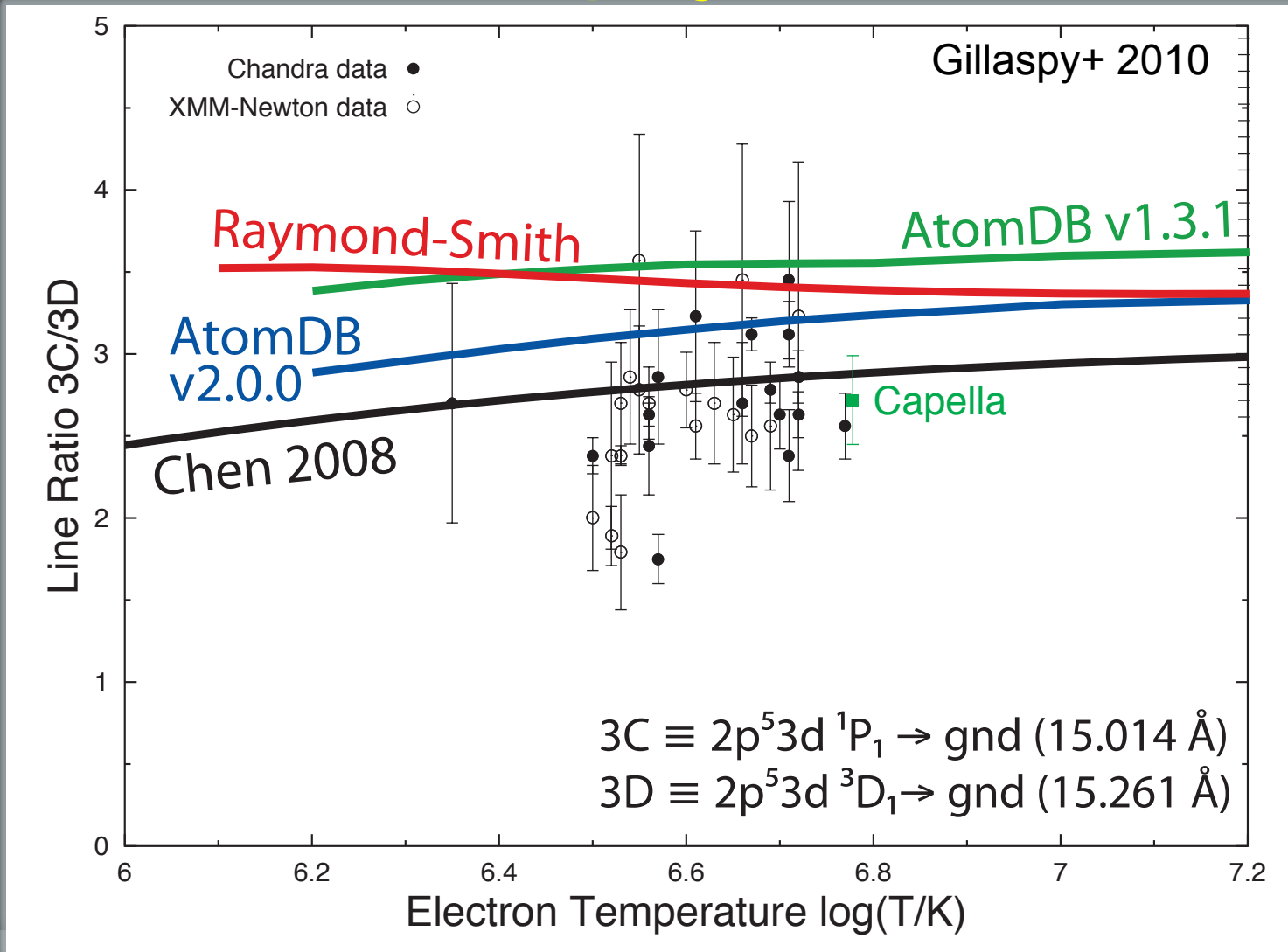


dePlaa+  
2012



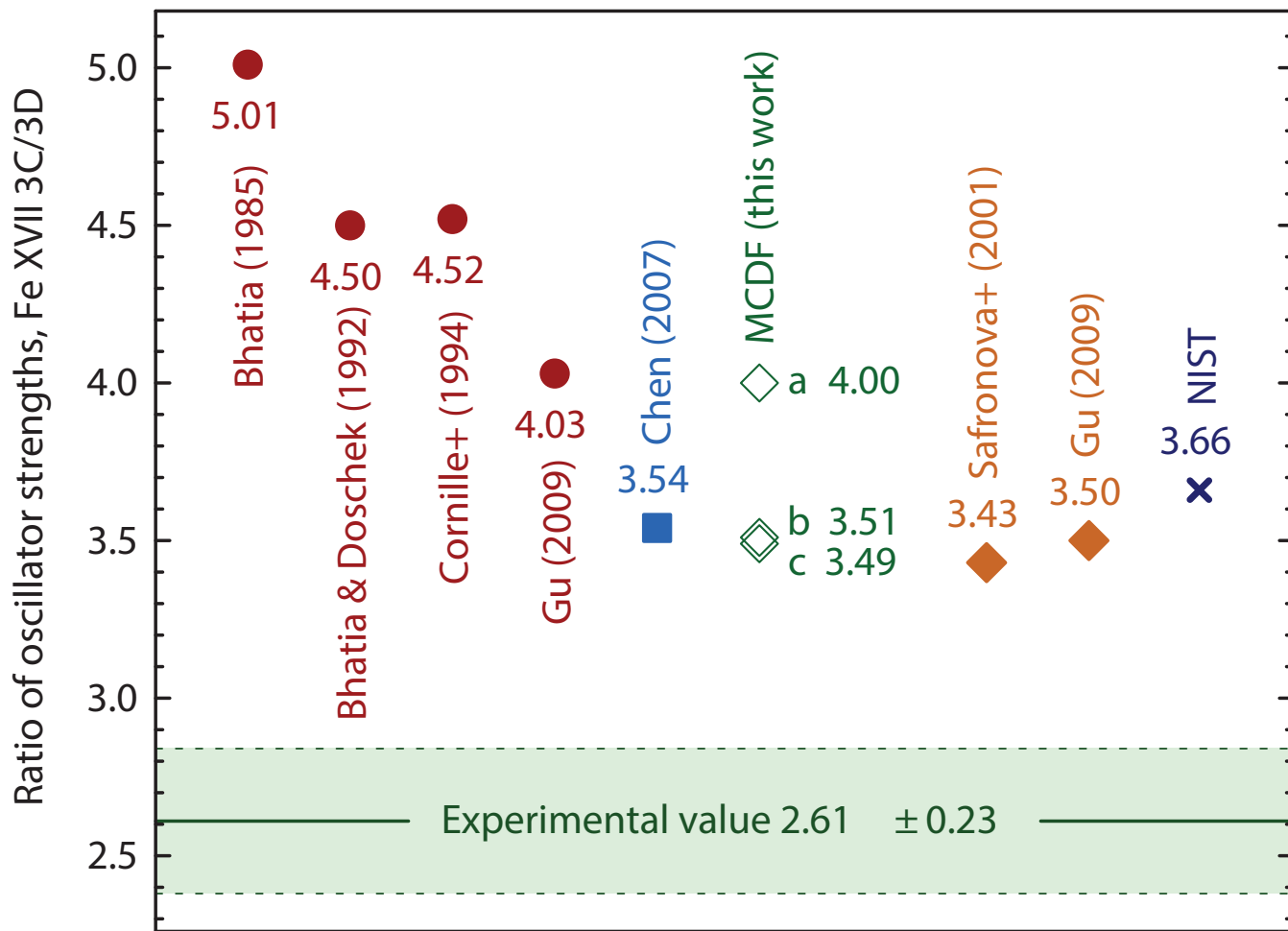
How does matter and energy move in and around galaxies?

# Fe XVII: Astrophysics & Theory



How does matter and energy move in and around galaxies?

# Fe XVII: Physics & Theory

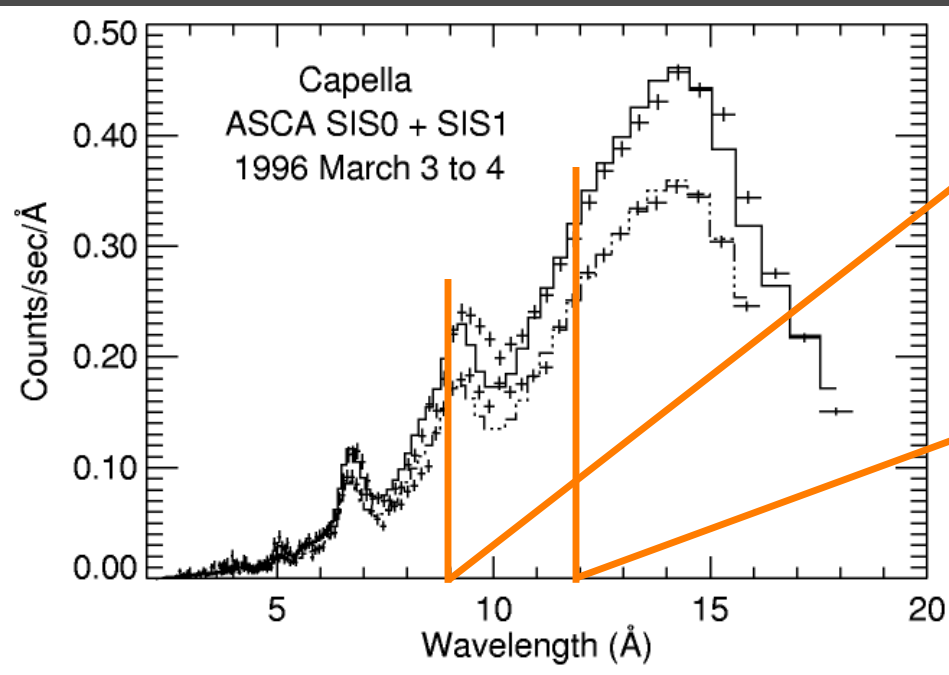
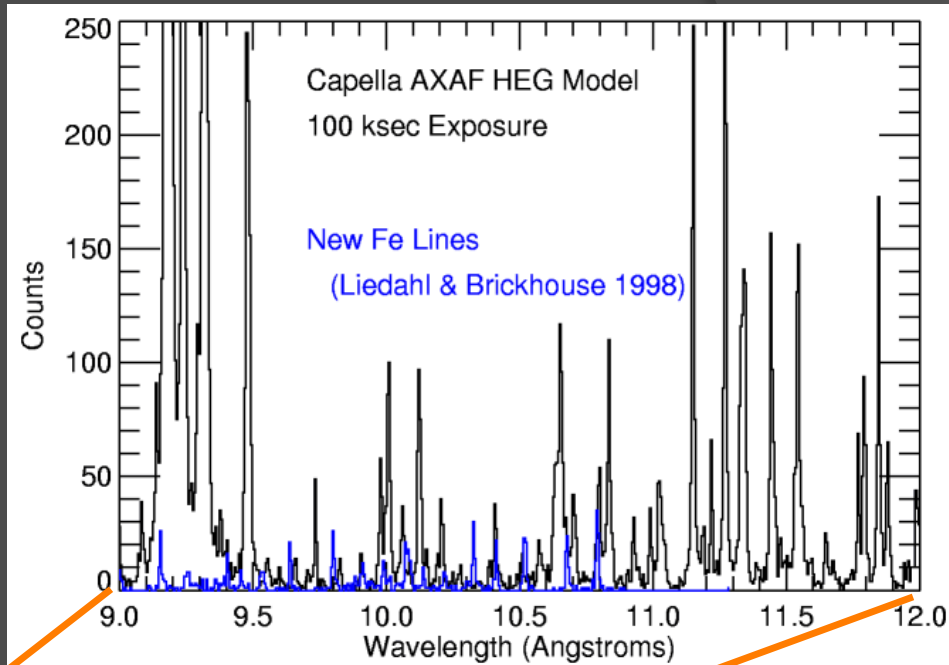


Bernitt+ 2012

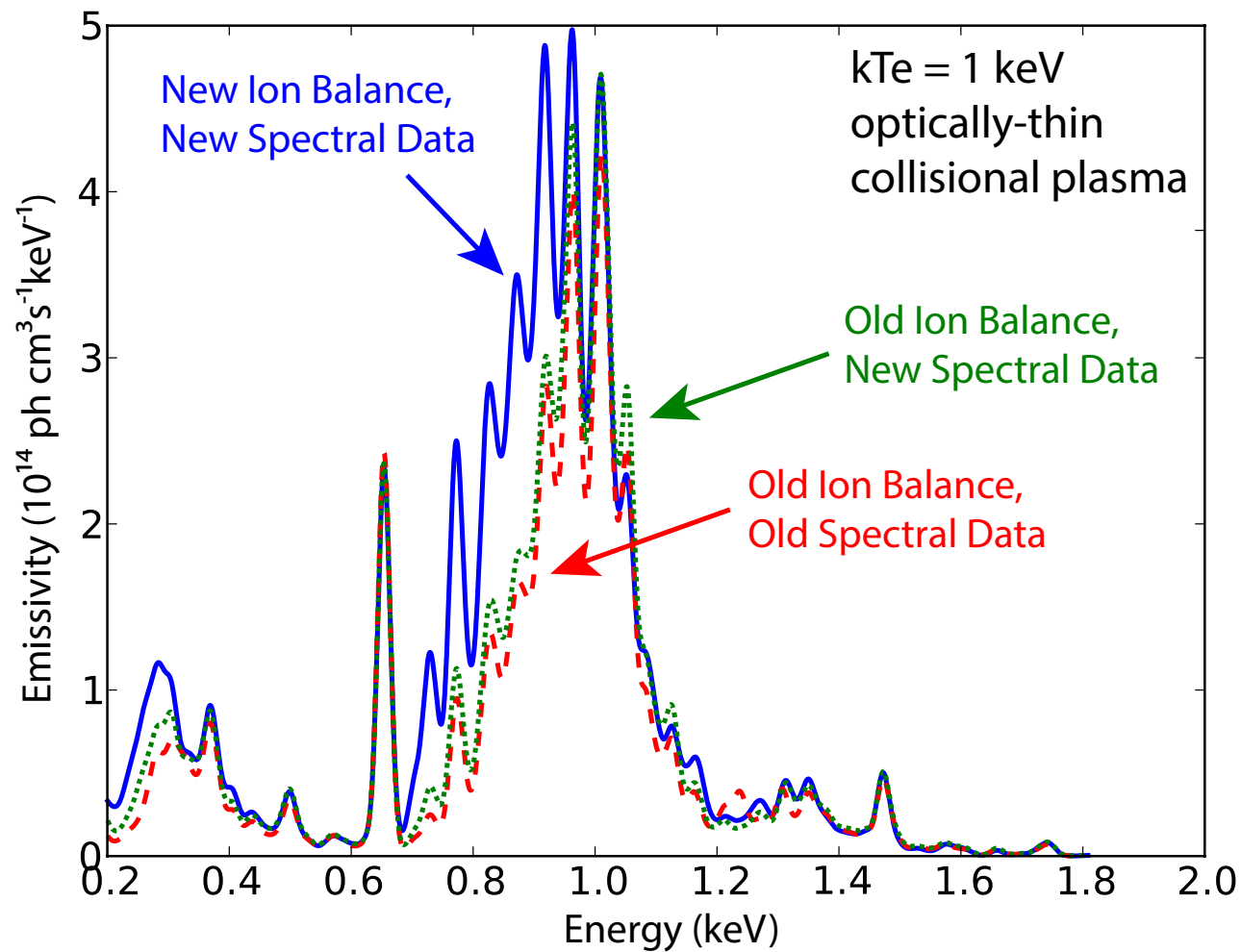
Data from LCLS

# Early Improvements Pre-AtomDB

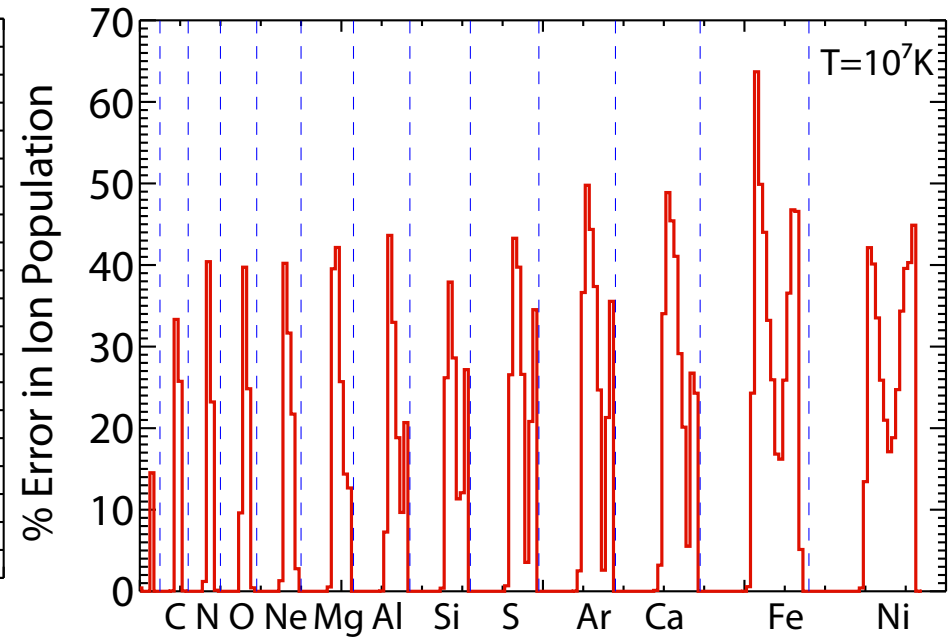
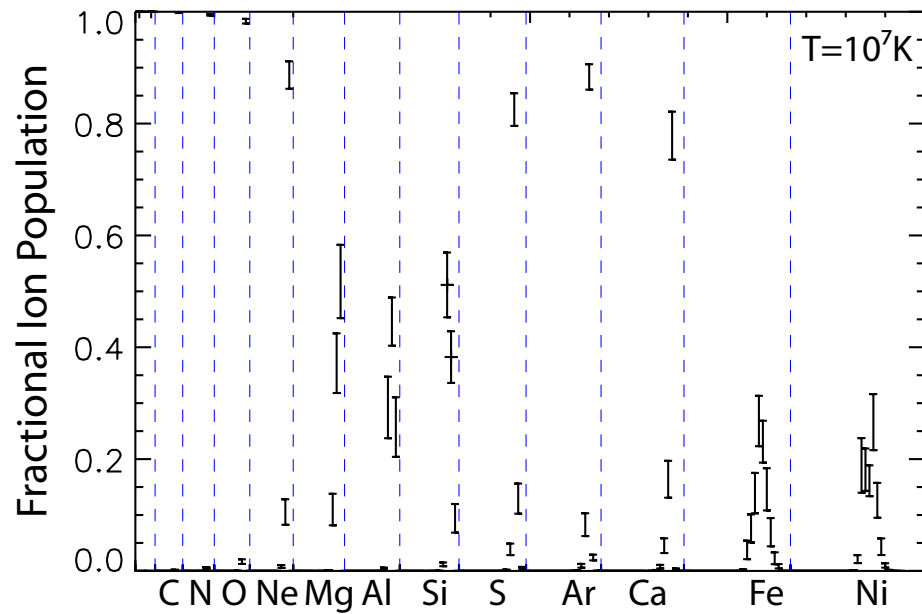
In this case, the poor fit between 9-12 Å is likely due to missing lines, not bad modeling.



# Impact of Data Updates



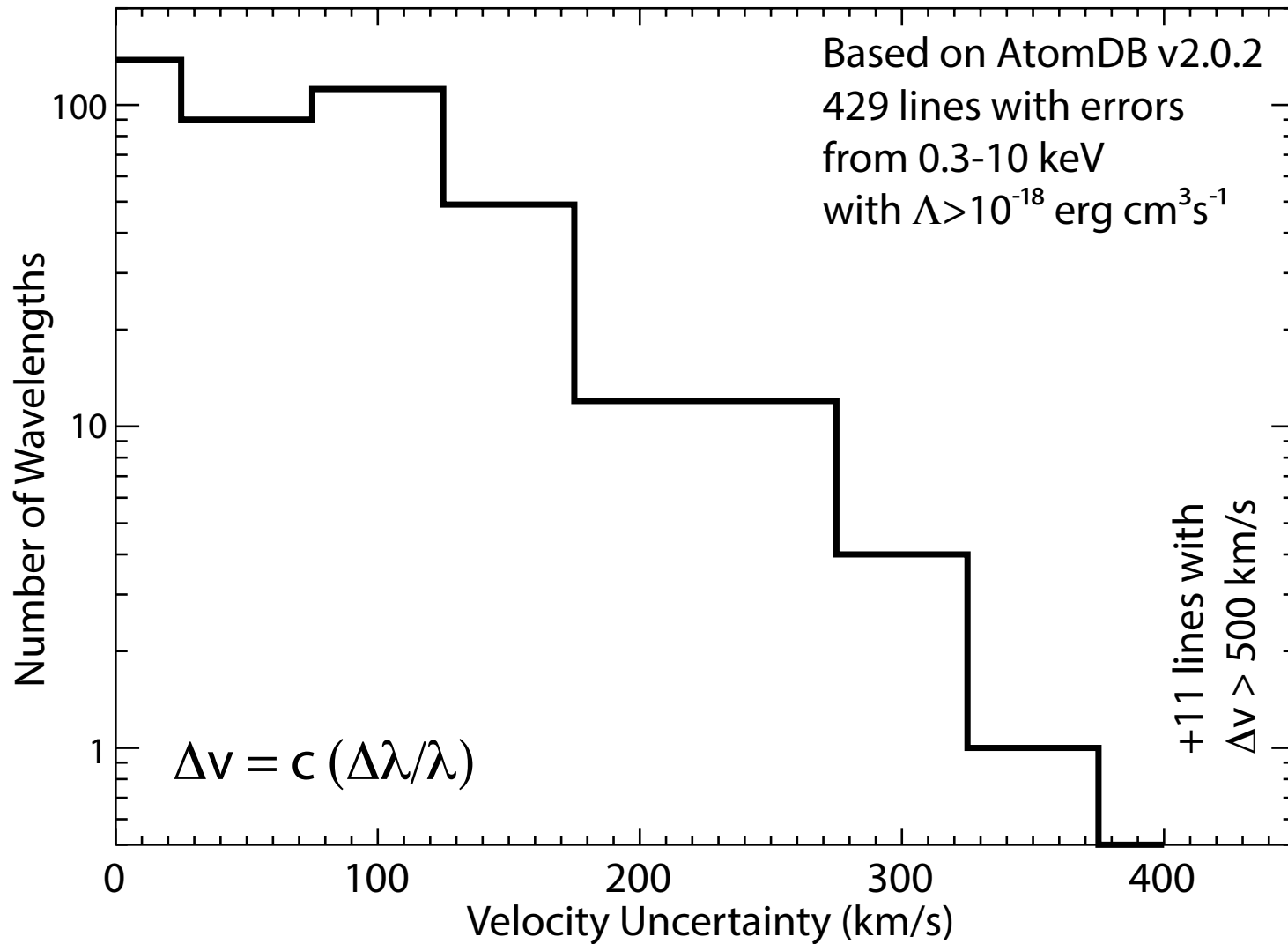
# Current Problems: Ionization Balance



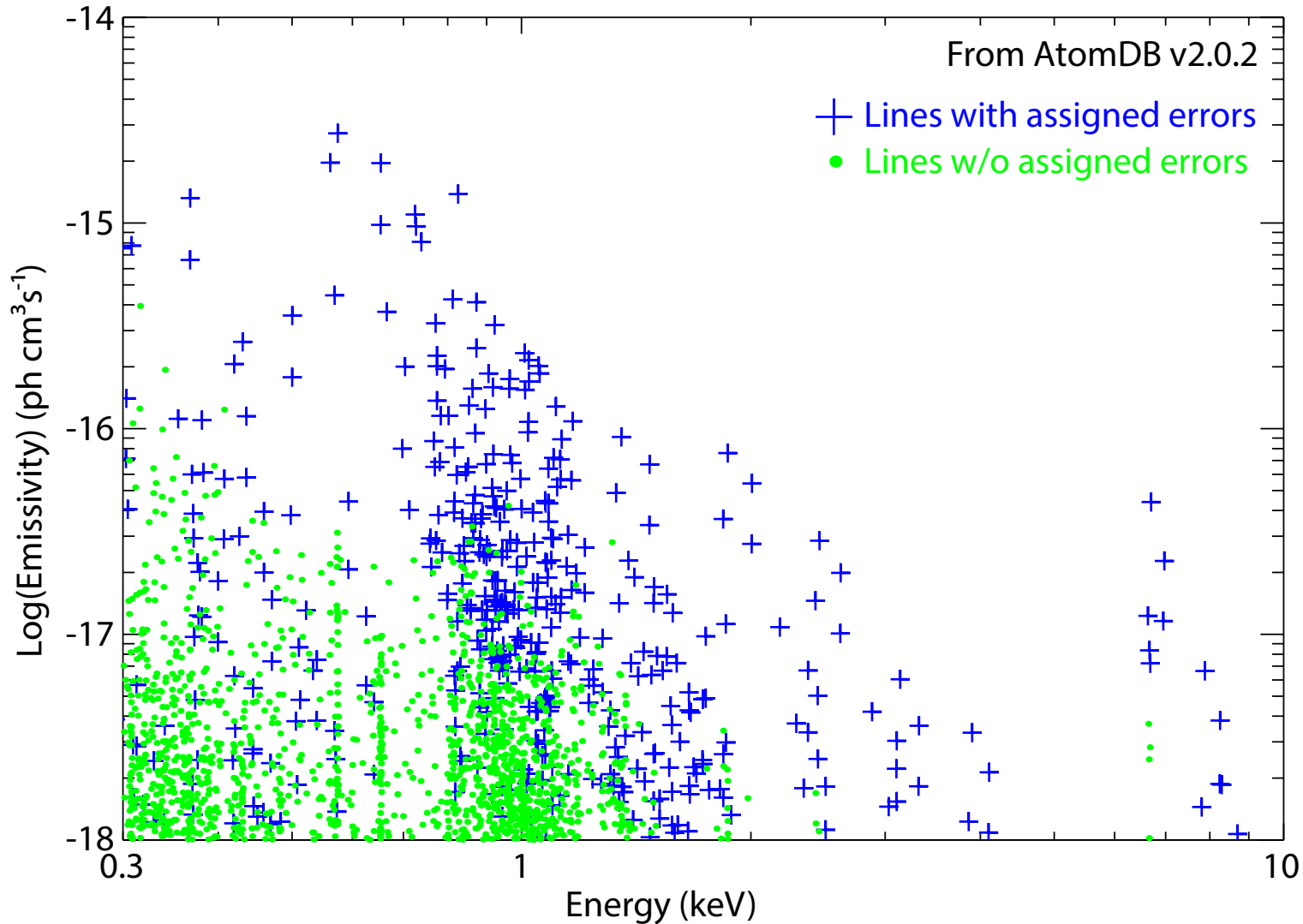
- 30% errors on the ionization & recombination rates leads to  $\sim 30\%$  errors in the ion population.
- However, at the limits of an ion's population, these errors are increased up to 60%.



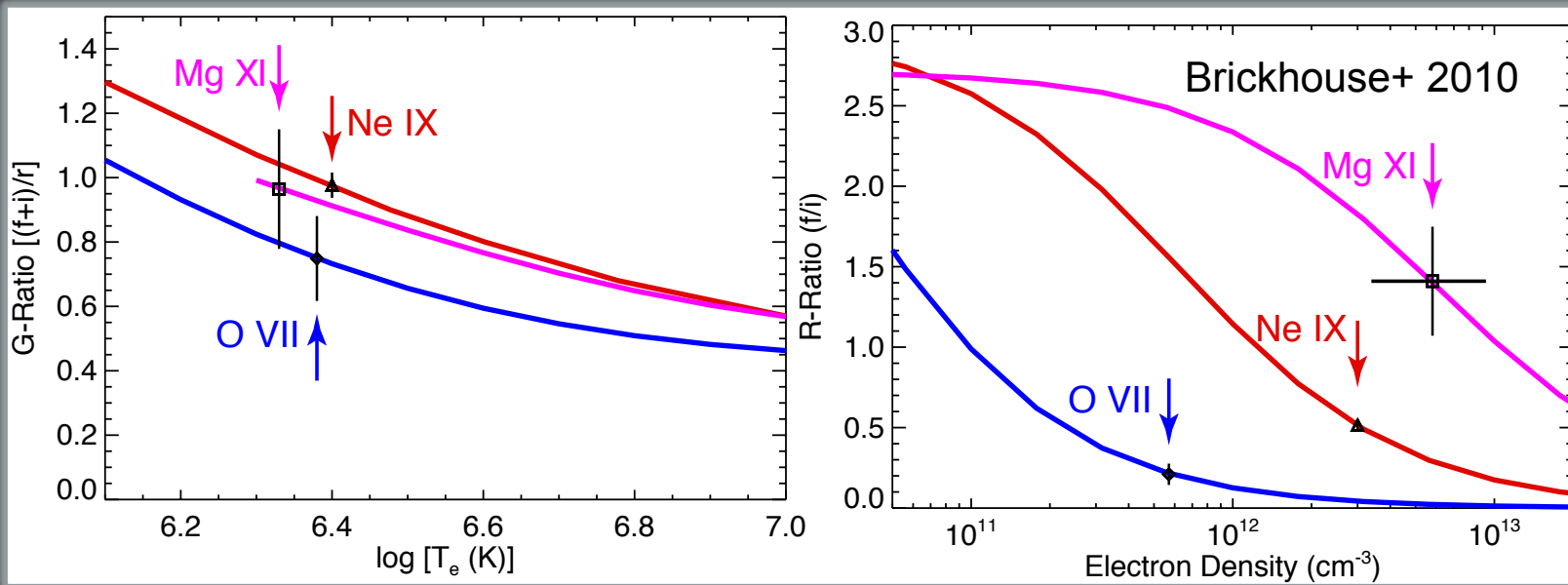
# Wavelength Error Data



# Wavelength errors incomplete

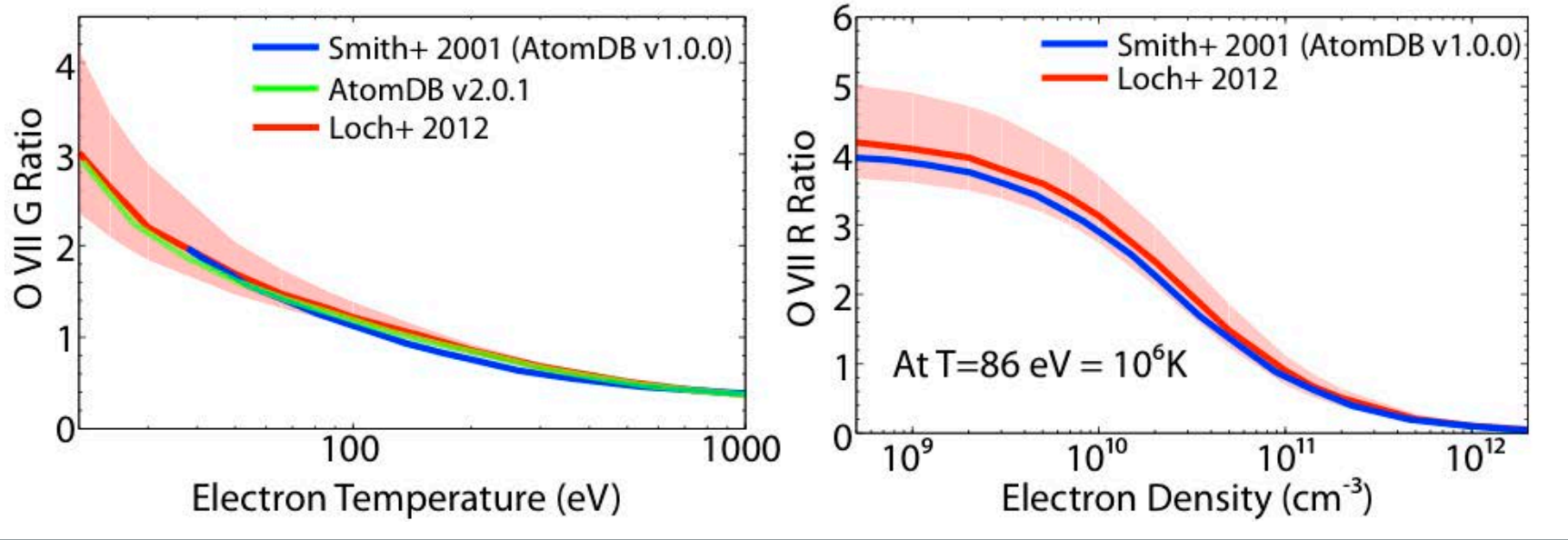


# Helium-like Diagnostics



While the **temperature** diagnostics for Mg XI, Ne IX, and O VII all give roughly the same result, the **density** diagnostics are significantly different.

# Errors / Sensitivity Testing

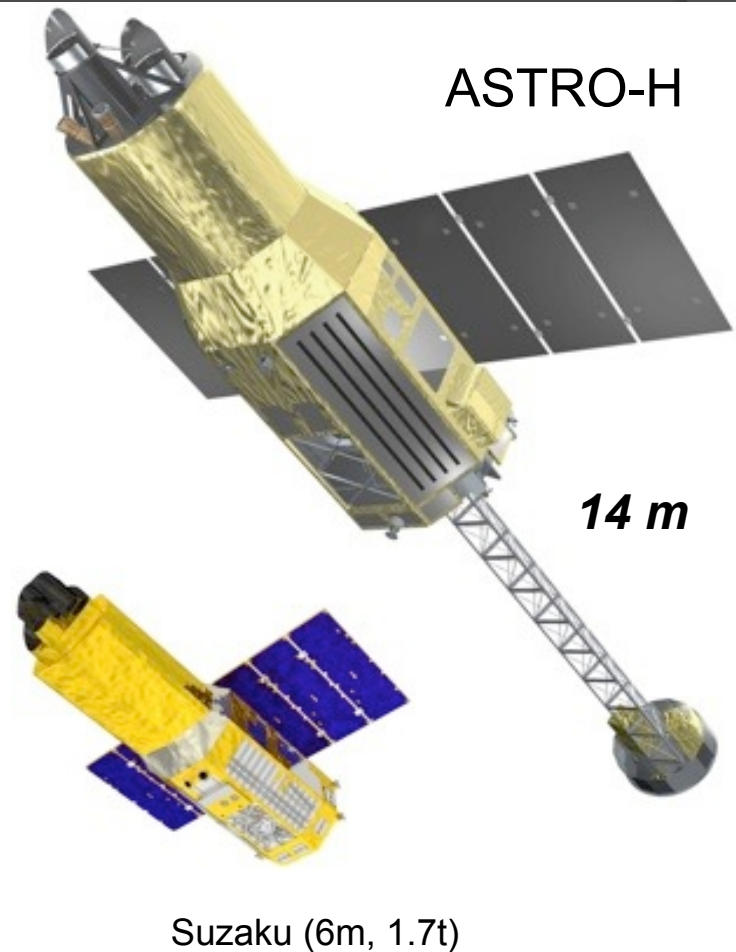


Theoretical calculations can use Monte-Carlo methods, varying the input atomic structure or calculation size to estimate sensitivities. **Care is needed in using these, but they are better than providing no estimate at all.**

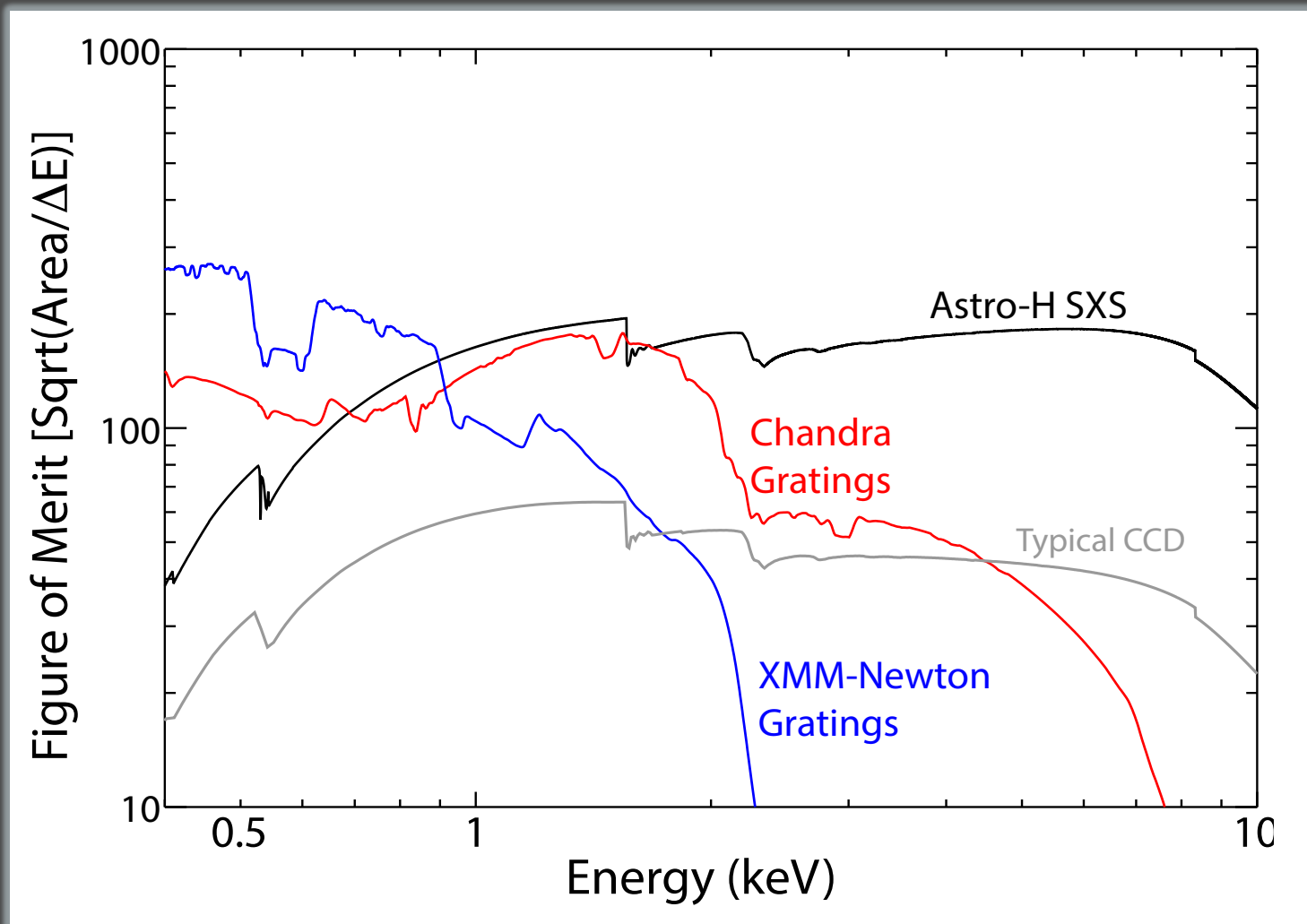
# Astro-H – Launching 2015 (!)

- **Launch site:**  
Tanegashima Space Center, Japan
- **Launch vehicle:** JAXA H-IIA rocket
- **Orbit Altitude:** 550km
- **Orbit Type:** Approximate circular orbit
- **Orbit Inclination:** ~31 degrees
- **Orbit Period:** 96 minutes

- **Total Length:** 14m
- **Mass:** <2.6 metric ton
- **Power:** <3500 W
- **Telemetry Rate:** > 8 Mbps (X-band)
- **Recording Capacity:** > 12 Gbits
- **Mission life :** > 3 years



# Figure of Merit for Detecting Weak Lines



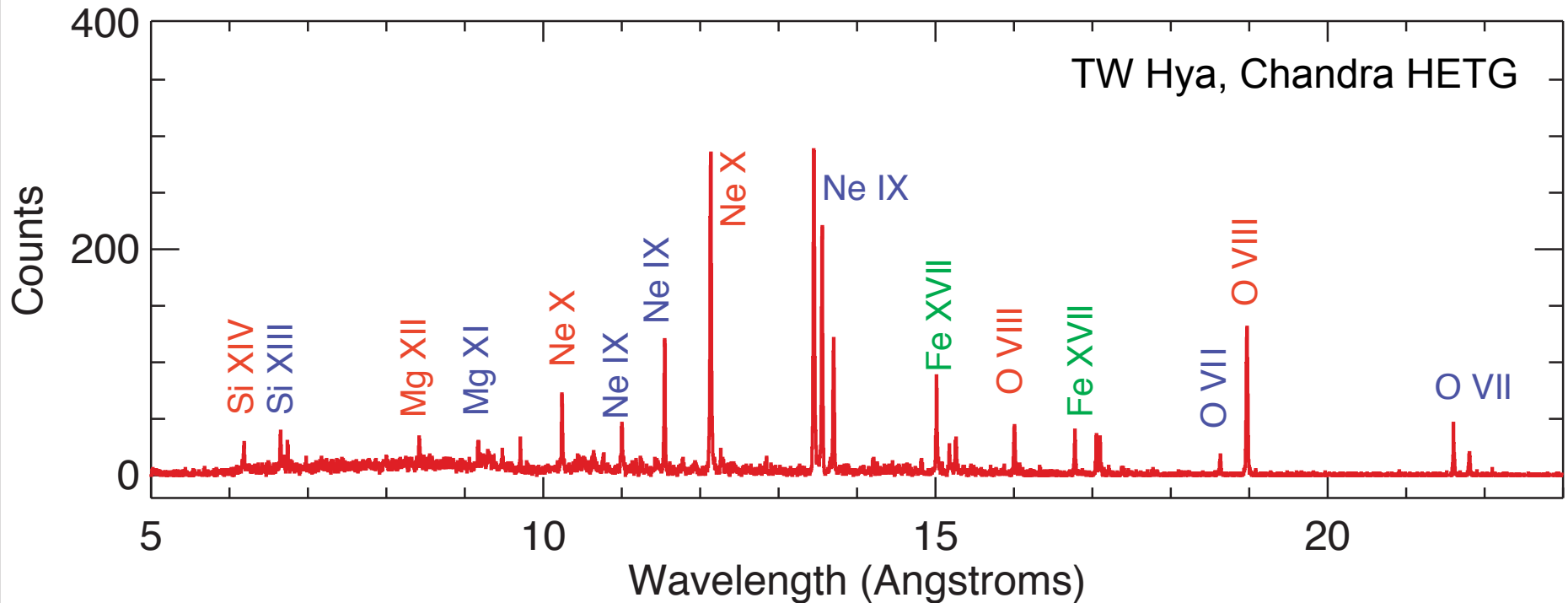
# What Do X-ray Astronomers Need?

*(To be ready for Astro-H)*

- ◎ Precise and accurate data for calibration and interpretation. Ordered by importance:
  - Wavelengths
  - Line widths/shapes/blends
  - Fluxes
- ◎ Reliable and practical estimates of data **accuracy** (especially in X-ray astronomy!)



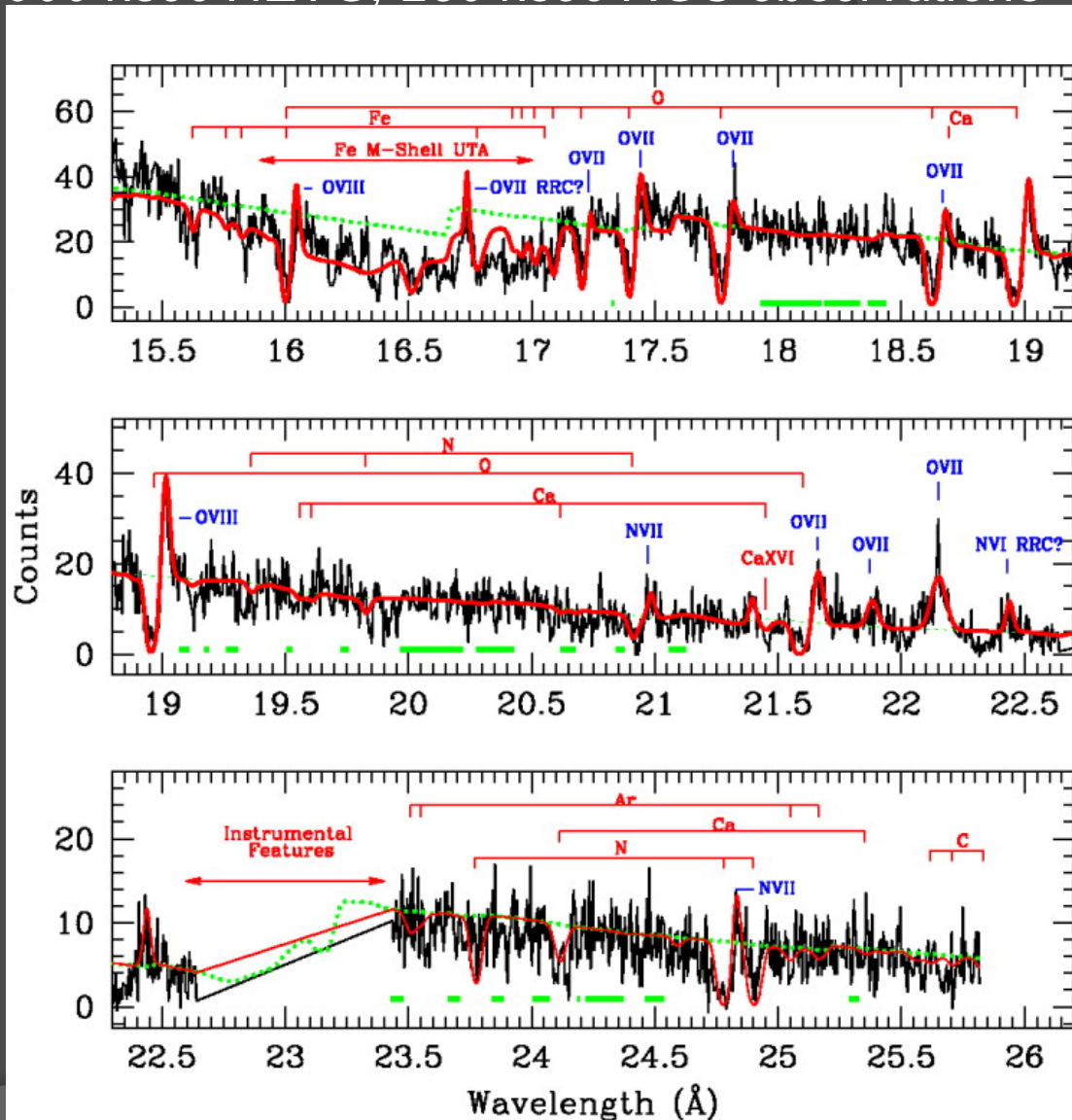
Major needs are the *best possible* **H-like**, **He-like**, and **Fe** (and to a lesser extent Ni) **L-shell** data ( $\lambda$ 's, Einstein A's, collisional  $\sigma(E)$ , etc).



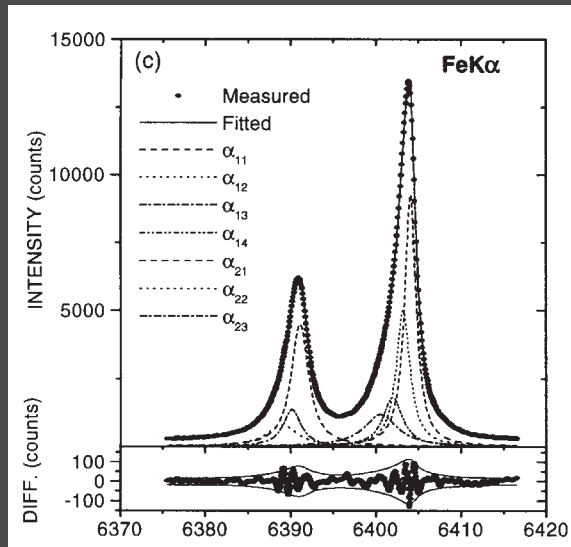
# A Few Words about X-ray Needs

*NGC 3783 – X-ray bright Seyfert galaxy;  
900 ksec HETG, 280 ksec RGS observations*

- Photoionized plasmas are more complex as both collisional and photon cross sections are relevant.
- However, H-like, He-like, and Fe ions are still key (although other ions play a larger role).



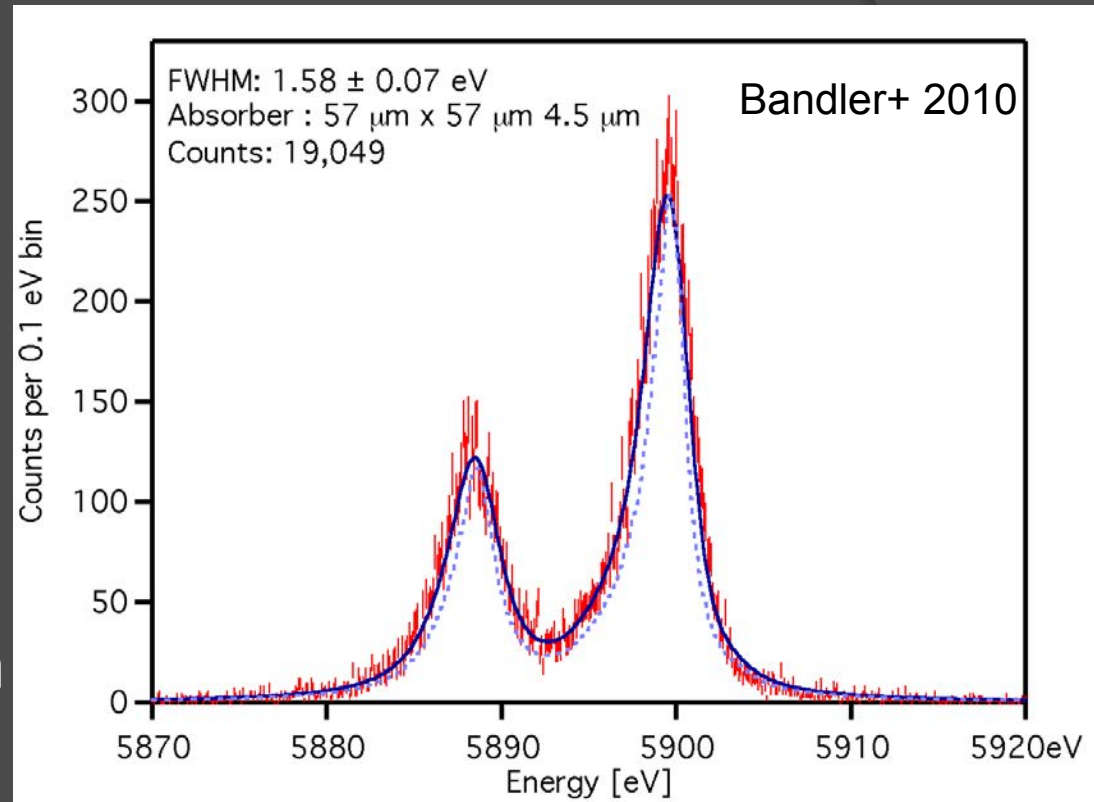
# Calibration: Fluorescent Lines



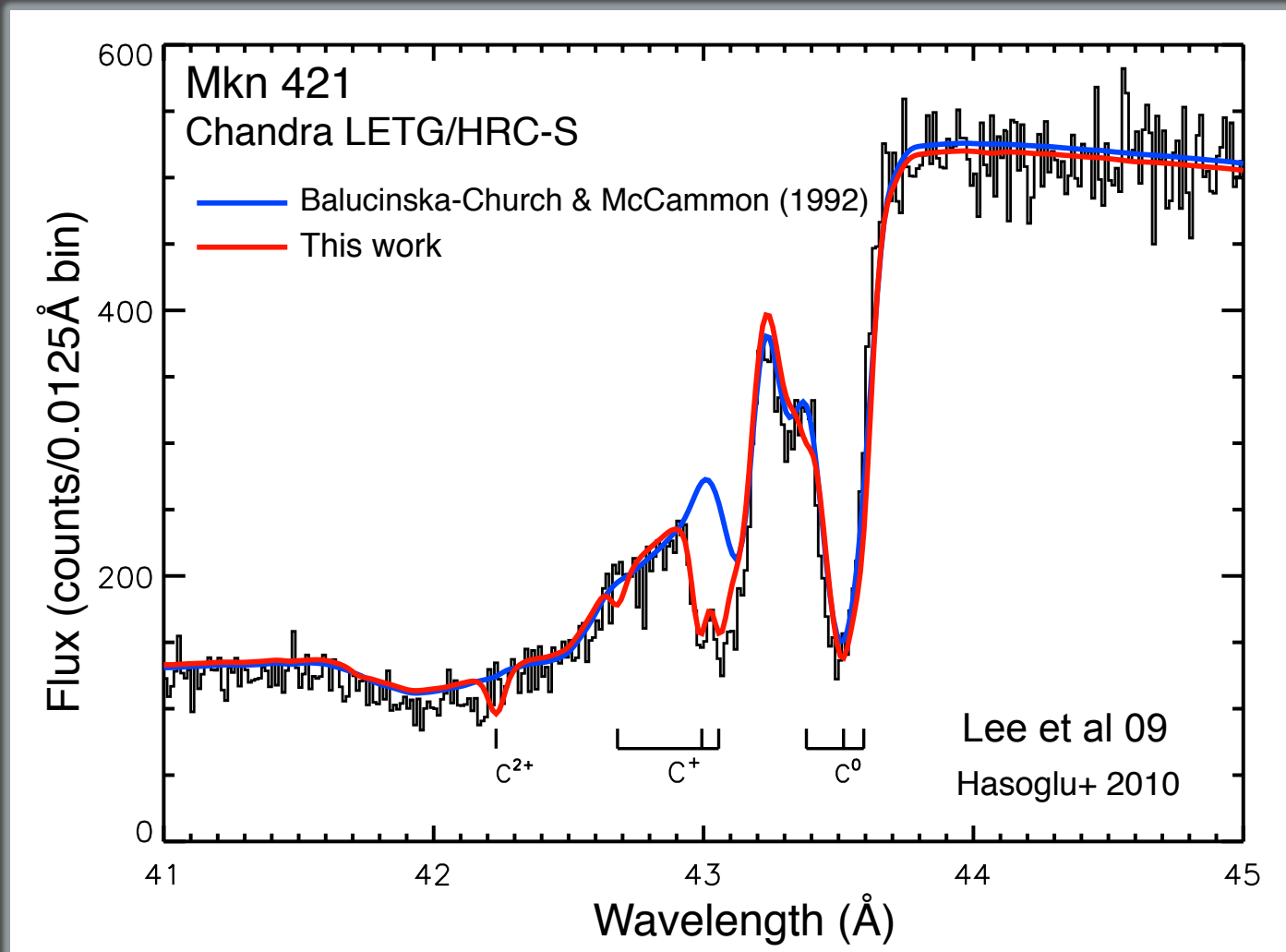
Hoelzer+ 1997

The fluorescent lines from radioactive sources are complex of many lines.

Line widths measured by current calorimeters are dominated by the natural line widths – which are not known for many useful elements!

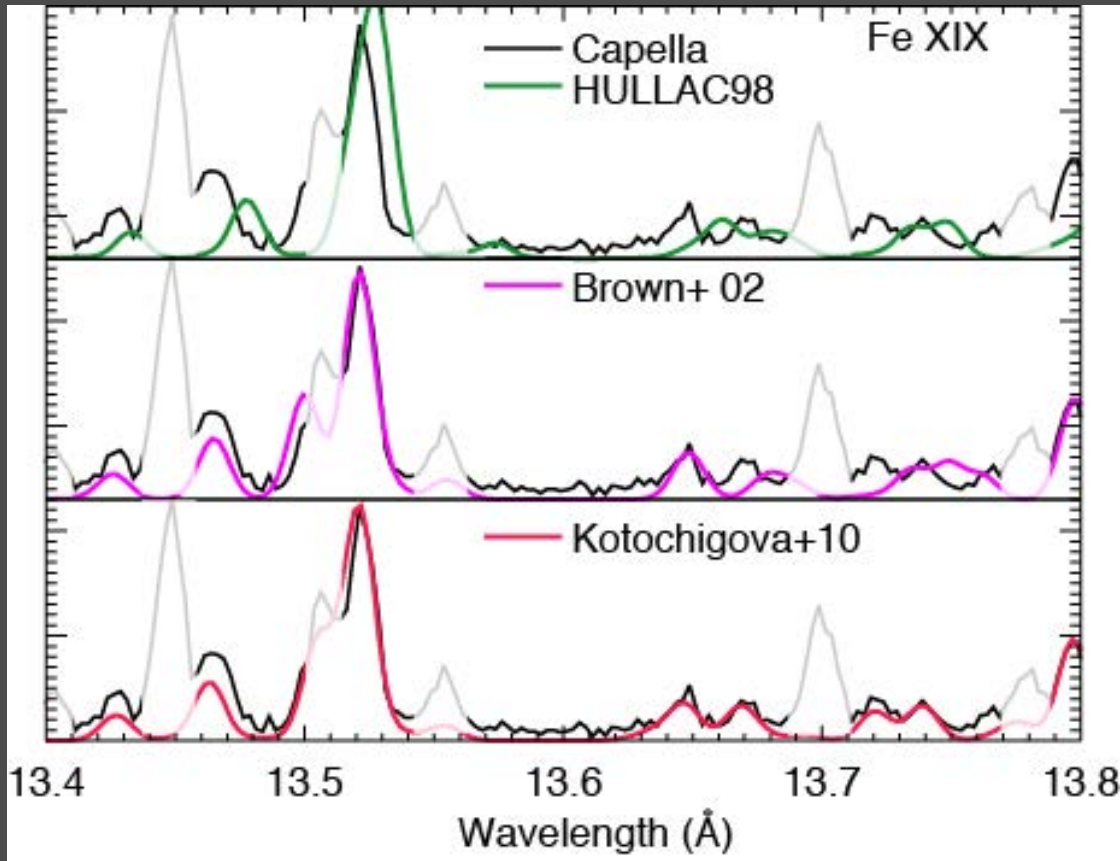


# Calibration: Absorption Cross Sections



Absorption edges and related features still need a lot of work...

# Calibration: Wavelengths



**Fit using 'raw'  
HULLAC  
wavelengths**

**Fit using lab (Brown  
et al. 1998)  
wavelengths**

**Fit using newly  
calculated  
wavelengths**

Kotochigova+ 2010

- By combining laboratory measurements and theoretical structure calculations, can get highly accurate (few mÅ) wavelengths.
- Detectors with  $R > 1000$  require this kind of accuracy!

# Conclusions

## Point #1:

Maintaining a tight connection between identified astrophysical questions and lab astro measurements and calculations is key to motivating progress (and funding).

# Conclusions

Point #2:

15 years ago, we knew existing X-ray spectral models would not survive the imminent arrival of new capabilities from Chandra and XMM-Newton

- Inadequate Fe L shell models with missing lines and inaccurate wavelengths
- Out of date models for H, He-like ions



# Conclusions

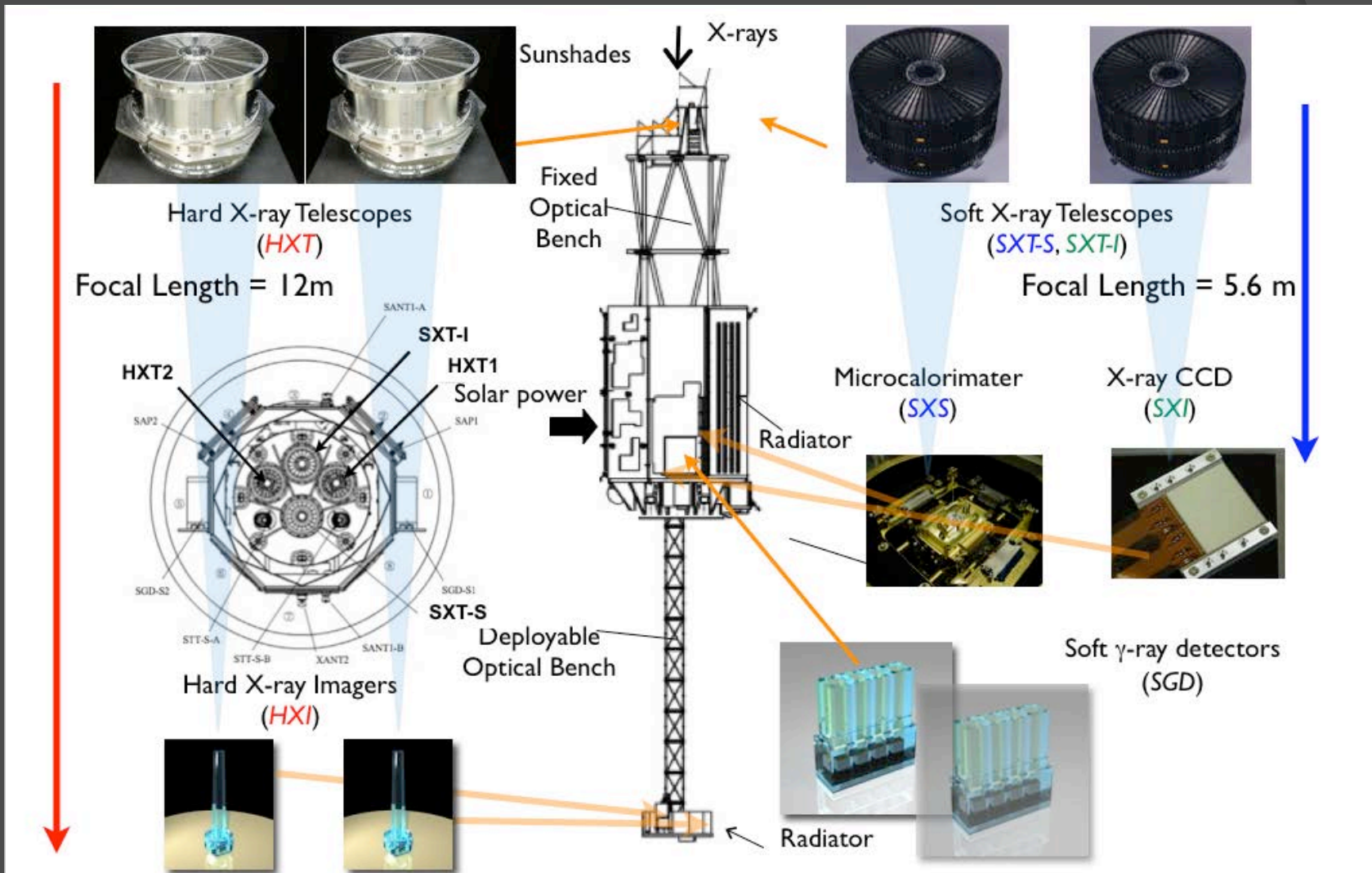
Point #3:

**Astro-H will soon increase the effective area of X-ray spectroscopy 100-fold**

- Some data are still missing: Ni L-shell, Fluorescent lines from select ions, Fe L-shell wavelengths, **AND**
- Current approach of assuming zero spectral model errors will lead to **data that cannot be interpreted.**

# Backup

# Astro-H Instrumentation



# “X-ray Line Emission from the Sun”

Unexpectedly strong solar X-rays were first detected on August 5, 1948 from a repurposed V-2 rocket launch.

The X-rays and optical data on the Solar corona suggested a  $\sim 10^6\text{K}$  plasma was responsible

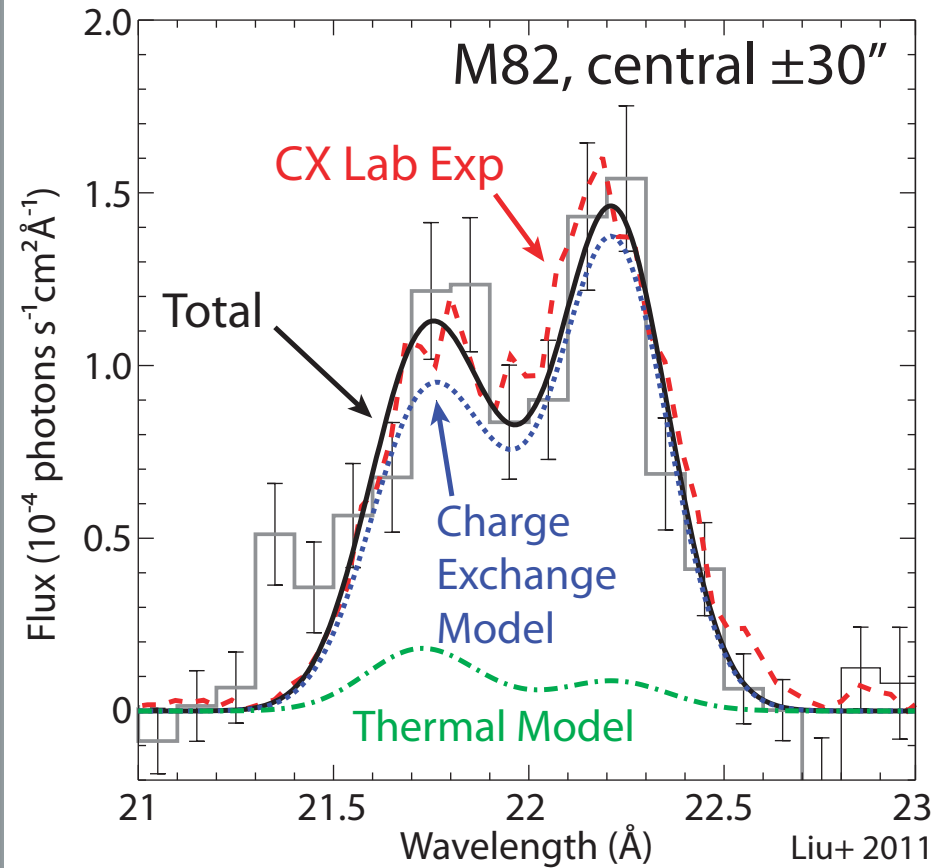
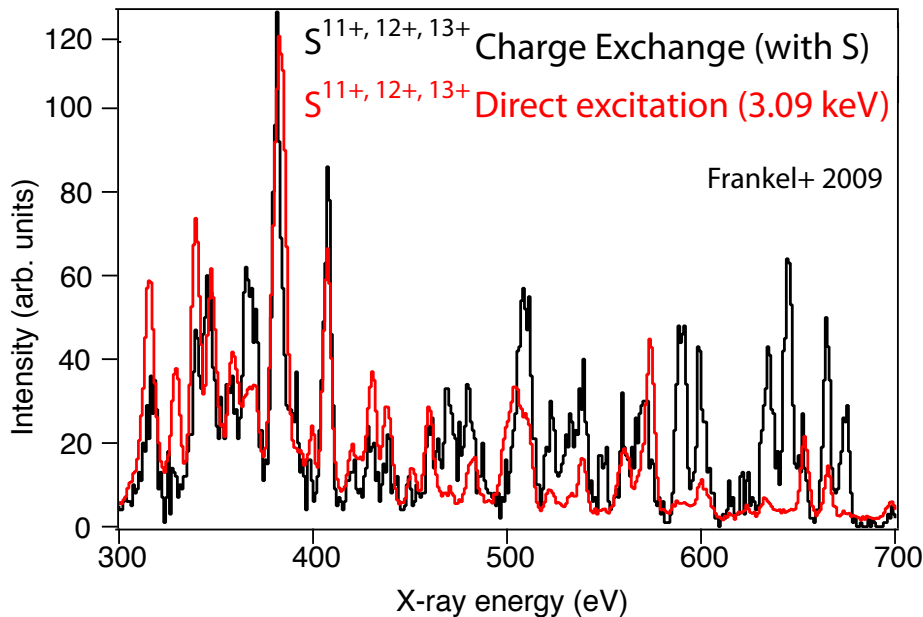
**B12. Soft X-Radiation in the Upper Atmosphere.** T. R. BURNIGHT, *Naval Research Laboratory*.—A simple experiment consisting of small cassettes containing photographic films and plates behind thin aluminum and beryllium windows of various thicknesses have been flown in a number of rockets at White Sands. On August 5, 1948 such an experiment obtained exposures through .076 cm beryllium windows indicating an unexpected intensity of radiation of wave-length shorter than 4 angstroms. On November 18, 1948 an experiment with .00076 and .00153 cm thickness aluminum and .0254 cm beryllium windows was flown with no indication of x-rays being obtained. On December 9, 1948 an identical experiment obtained appreciable blackening through .00076 cm aluminum windows but not through .0254 cm beryllium windows. The sun is assumed to be the source of this radiation although radiation of wave-length shorter than 4 angstroms would not be expected from theoretical estimates of black body radiation from the solar corona. A semiquantitative determination of the intensities indicated has been made, and the possible correlation with solar activity at the time of firing will be presented.

Burnight 1949, Phys Rev 76, 165

# Identifying Recombining Plasmas

## – High-resolution spectra

In the lab...



In the sky...