The Impact of Atomic Data Uncertainty on Models

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AtomDB 2020

Spectral model uncertainties

Origin:

- Incompleteness/error on fundamental atomic data affecting line wavelengths, edge energies, line shape, ionization concentration, and emissivity
- Numerical errors (e.g., interpolation between temperature grids)

Why do we care:

- For most of the lines, we do not know their exact uncertainties
- Many line fluxes are uncertain >20%, equal to or higher than the instrumental calibration error
- Seriously affect science (abundance, column density, etc)
- Lab measurements for a few cross sections (more for wavelength)

Current approach (assuming no model error) will lead to wrong interpretation

Atomic data error

Line emissivity for CIE plasma:

$$F_{ij} \propto C_{ion} \times occupation_j \times A_{ji}$$

Ionization-recombination balance (Arnaud-Rothenflug, Bryans, Urdampilleta)

Collisional and resonant excitation, proton excitation, dielectronic recombination, auto-ionization, radiative recombination, charge exchange, radiative transition, etc

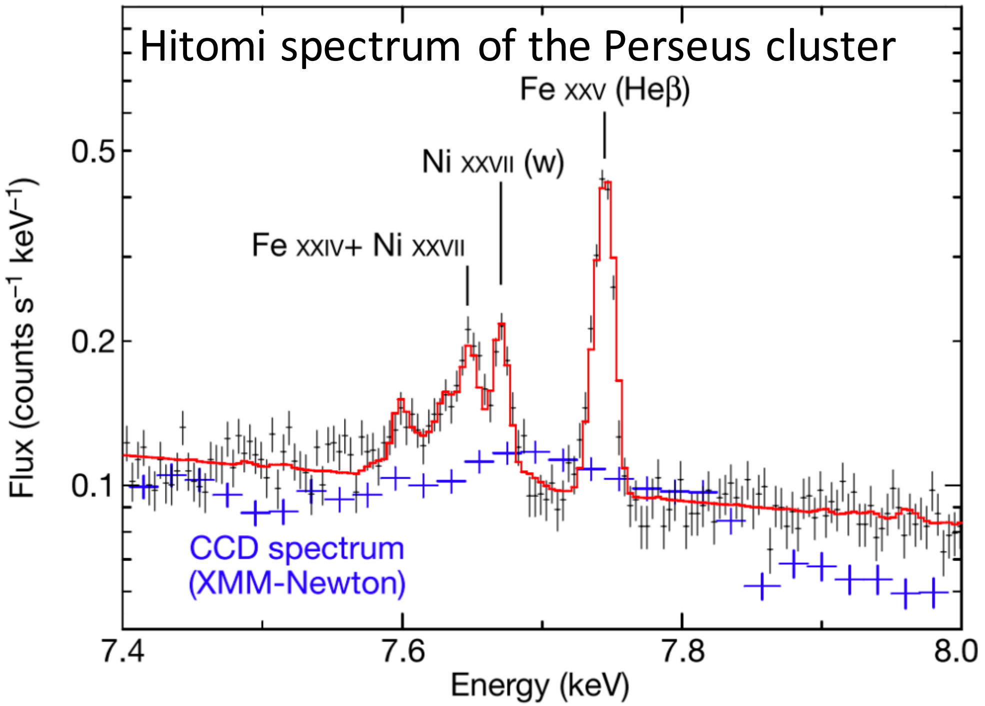
Radiative transition probability, branching ratio

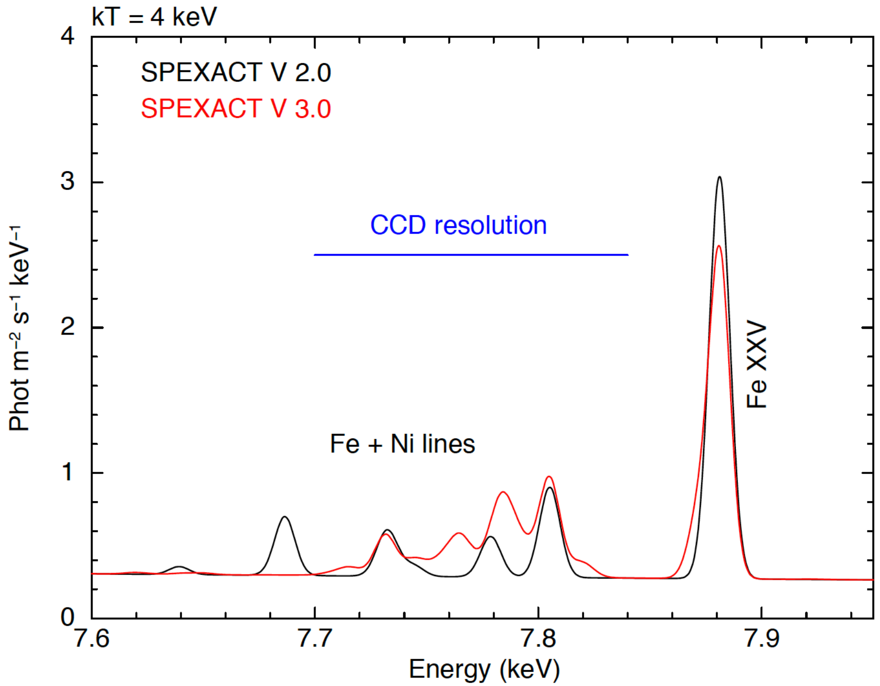
- Present transition data are often a mixture of distorted wave and R-matrix calculations

Wavelength error

Accuracy of transition energies measured in laboratory:

- K-shell: H-like $\sim 10^{-6}$; He-like $\sim 10^{-5}$
- L-shell: Fe, Ni, Si, S $\sim 10^{-4}$
- Innershell: Li-like DR $\sim 10^{-4}$, few data for L-shell

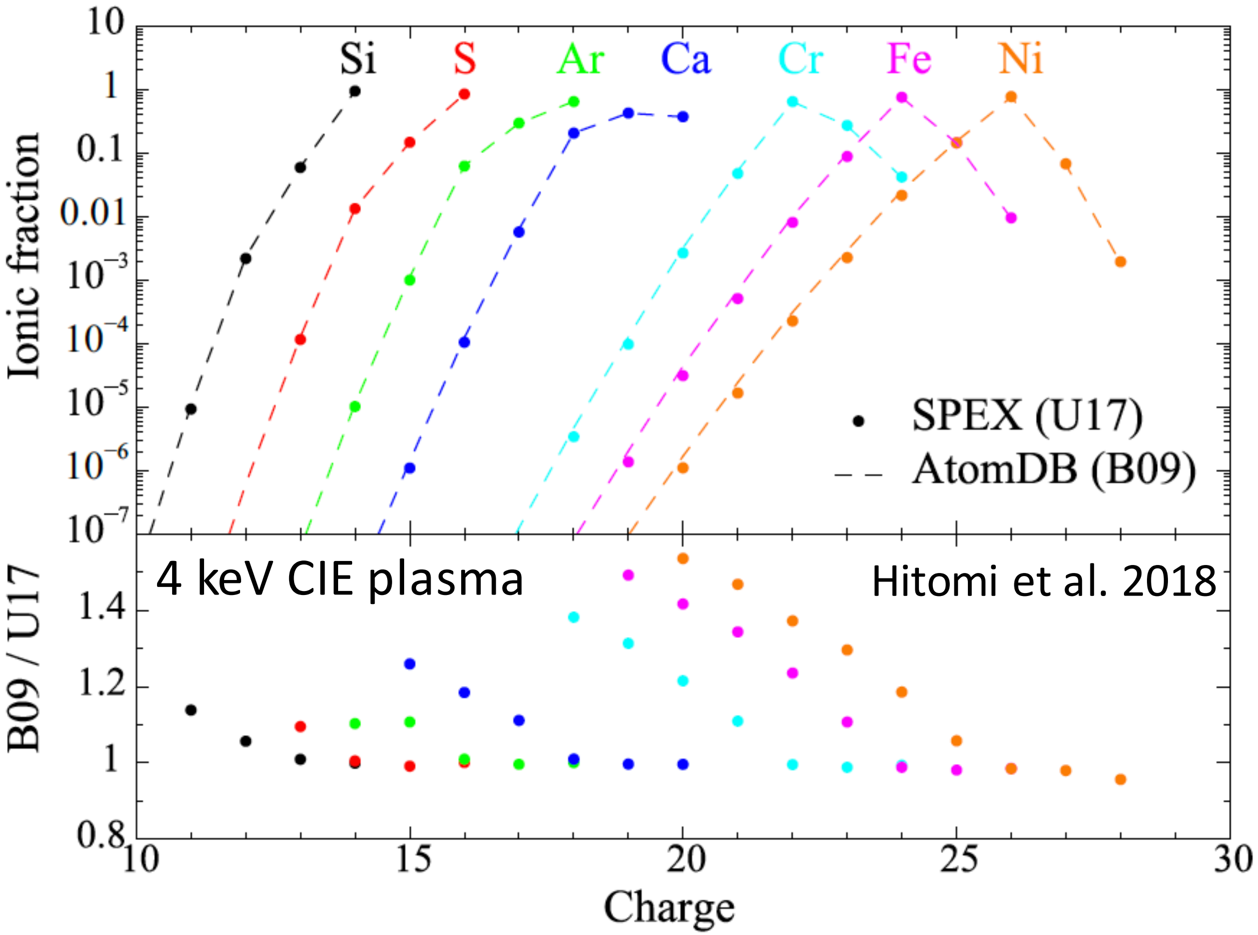


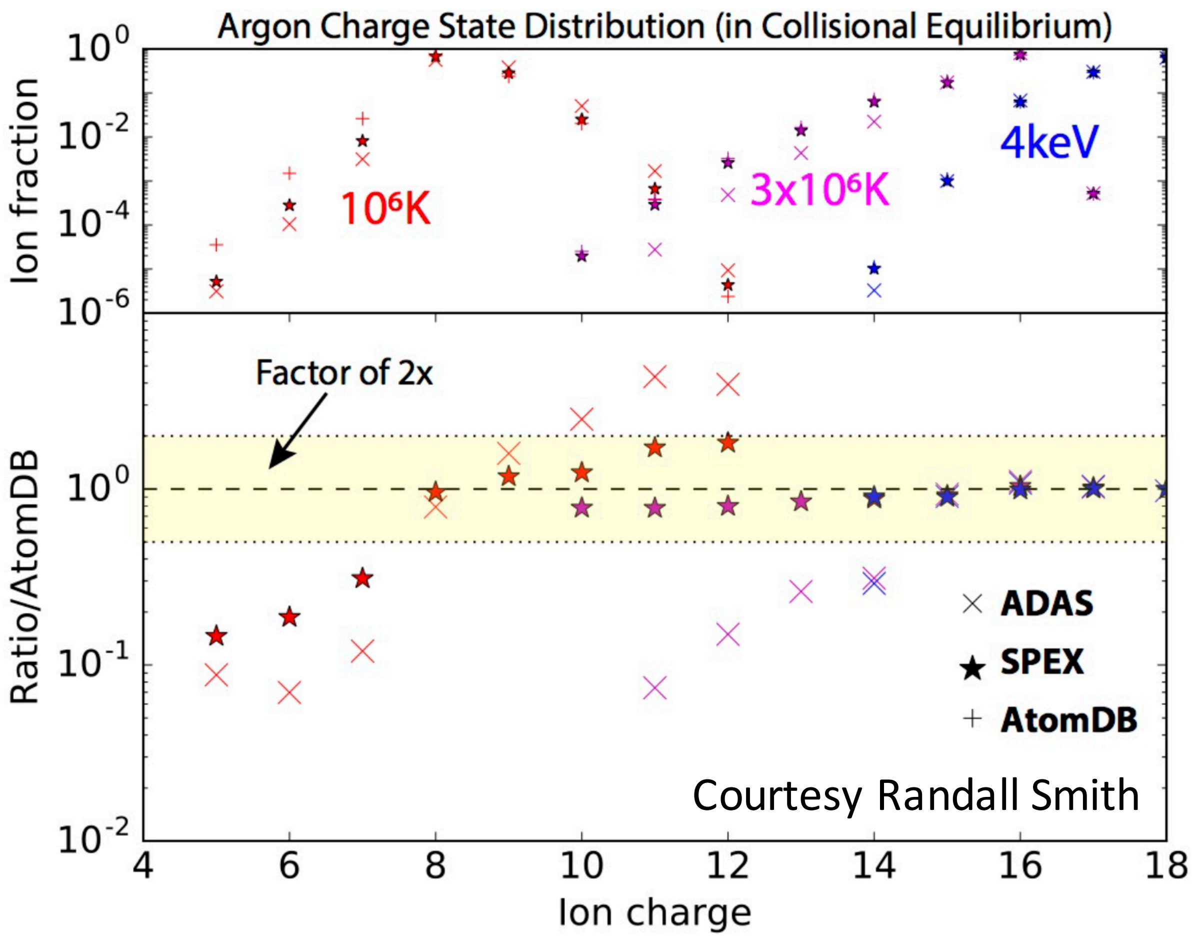


Mernier et al. 18

Improvements in the spectral resolution and atomic model allow the most precise Ni/Fe measurement in clusters (Hitomi et al. *Nature*)

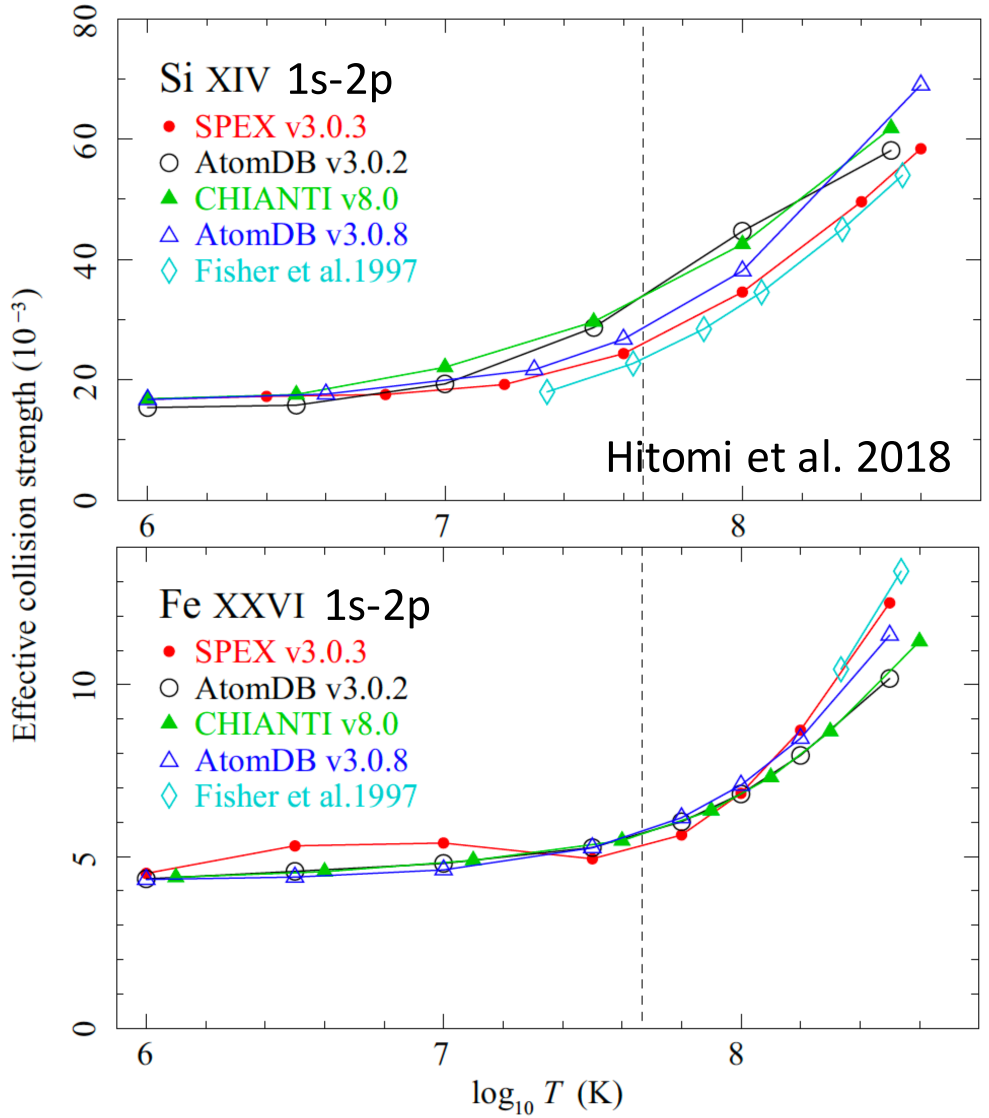
Ionization balance error

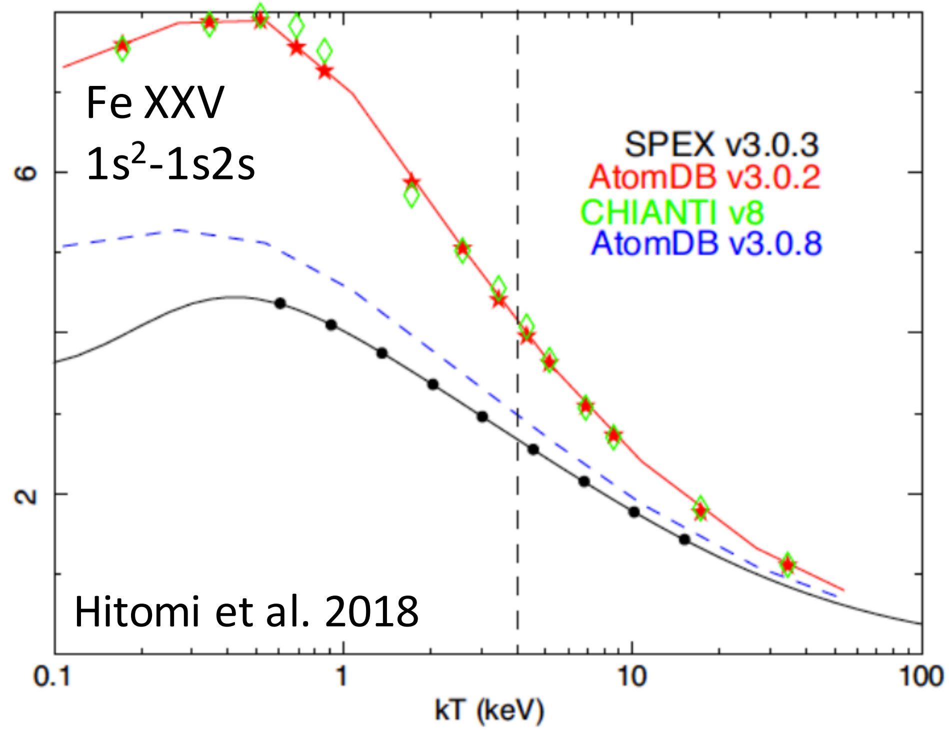




- Ion concentration becomes uncertain at off-peak ionization states

Collisional excitation: Fe K

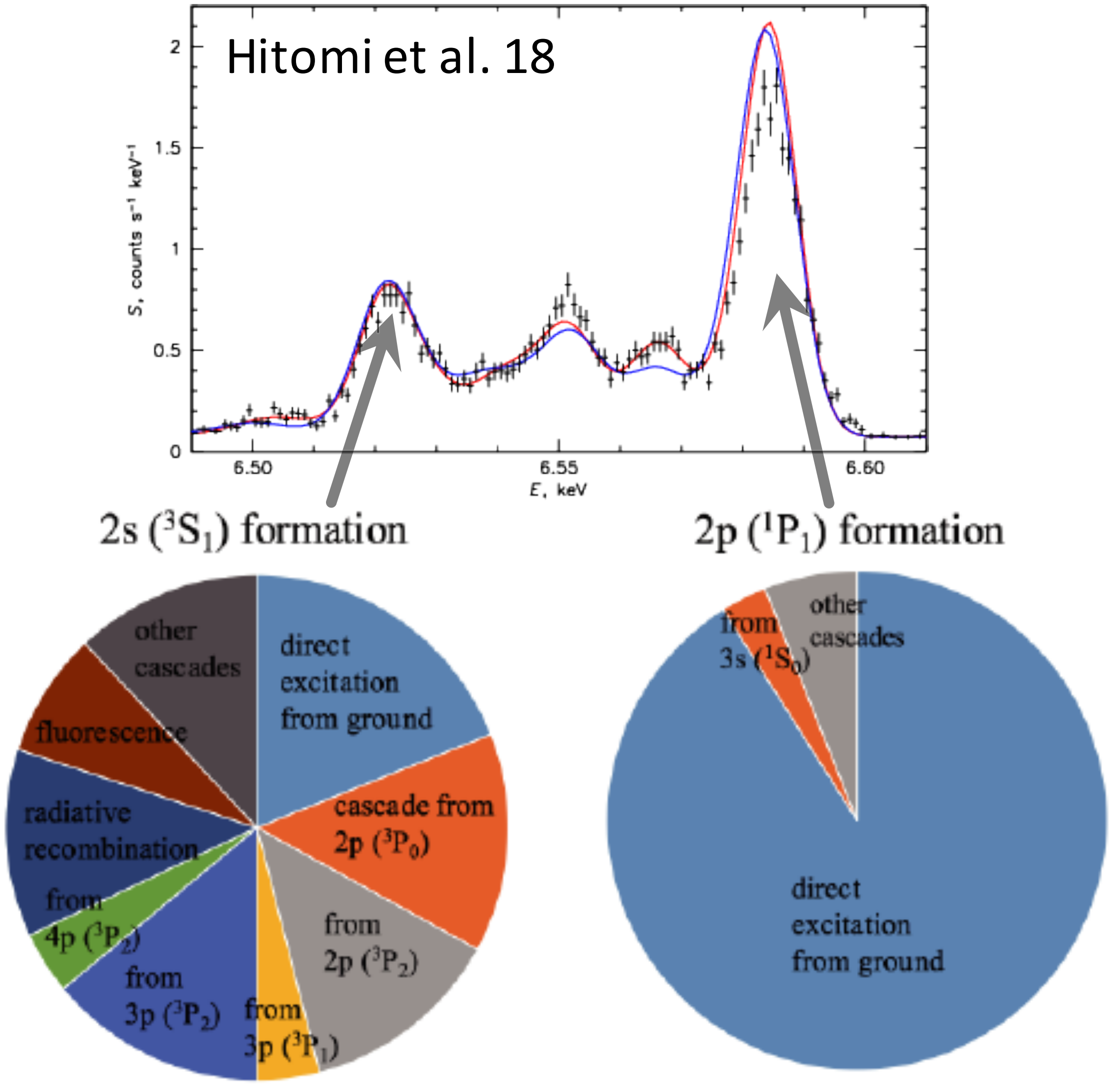




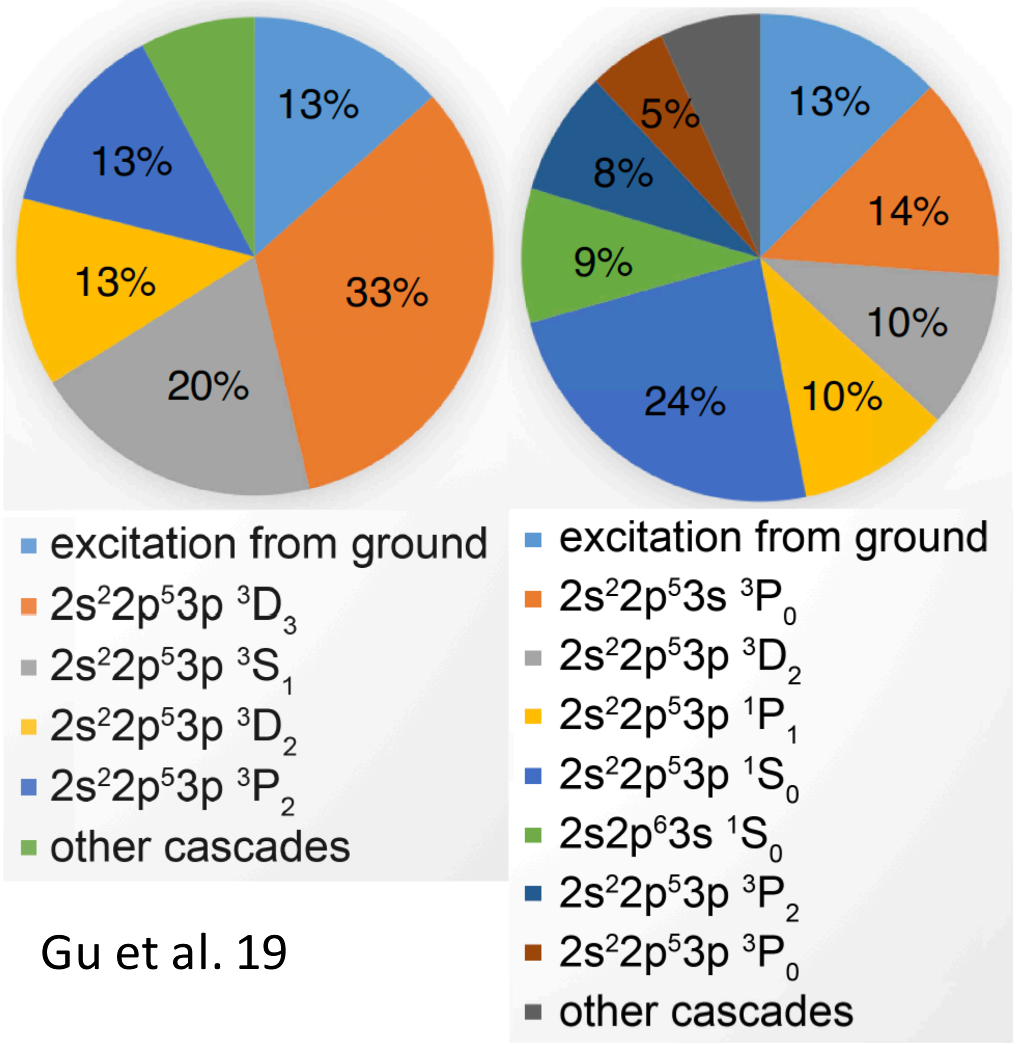
- 30% difference in Si 1s-2p collision strength → ~30% error in abundance
- For Fe XXV 1s-2s transition, issues on radiative damping correction

Sensitivity of line emissivity to atomic uncertainties

Fe XXV w and z lines



Fe XVII M2 (17.09Å) and 3G (17.05Å) lines



Gu et al. 19

Solution to the problem

a) Use multiple codes (AtomDB, SPEX, Chianti, Cloudy, etc)

Example: Hitomi perseus spectrum with multiple sets of atomic database

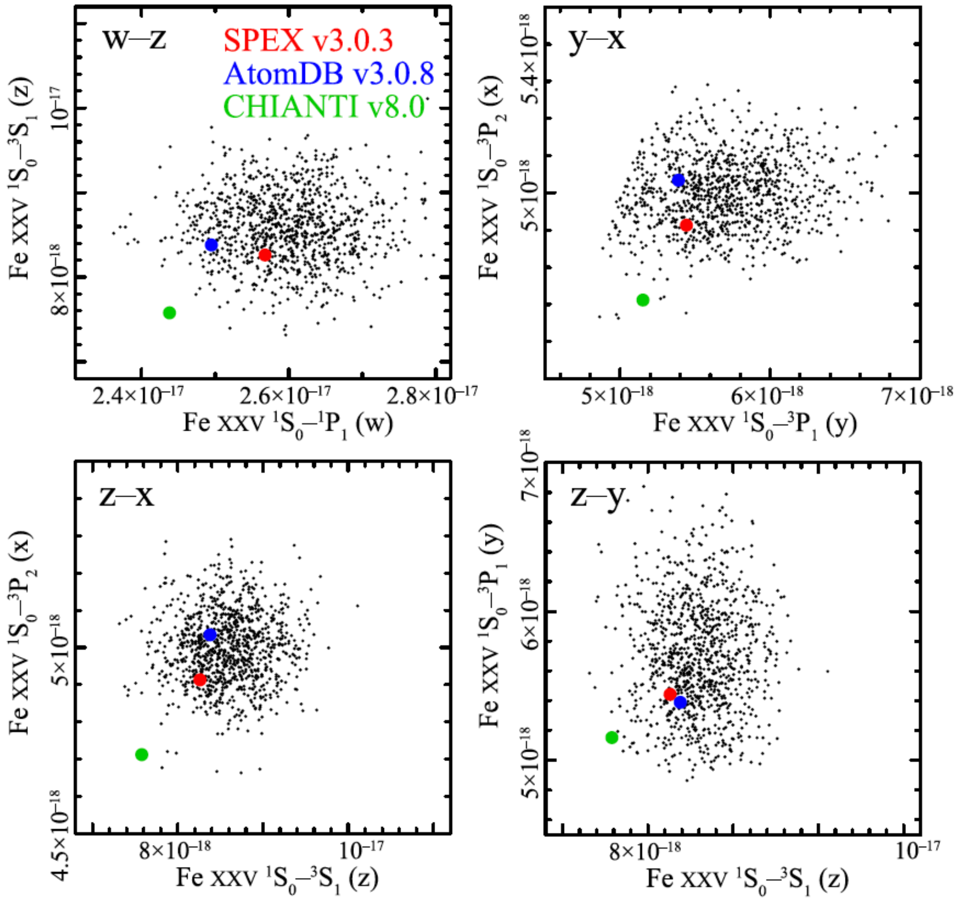
Model	C_{stat}	Y†	kT†	σ_v†	Abundance (solar)‡								$N_{H,hot}$†	cz†
		(10^{73} m^{-3})	(keV)	(km s^{-1})	Si	S	Ar	Ca	Cr	Mn	Fe	Ni	(10^{24} m^{-2})	(km s^{-1})
Baseline	4926.03§	3.73	3.969	156	0.91	0.94	0.83	0.88	0.70	0.74	0.827	0.76	18.8	5264
Stat. error	—	0.01	0.017	3	0.05	0.03	0.04	0.04	0.10	0.15	0.008	0.05	1.3	2
Plasma codes (section 4):														
SPEX v2	1125.06	0.03	0.031	**14**	−0.13	**−0.14**	−0.05	−0.08	—	—	**−0.026**	0.11	−0.8	−6
SPEX v3.00	2372.33	**−0.08**	**0.263**	**12**	0.03	0.09	0.10	0.06	−0.11	−0.12	**−0.243**	**−0.28**	**−18.8**	−2
APEC v3.0.2	670.06	**0.07**	−0.039	**−13**	**−0.24**	**−0.21**	**−0.15**	**−0.13**	−0.24	−0.39	**−0.047**	**−0.17**	−2.7	1
APEC v3.0.8	22.27	0.03	**0.071**	**−16**	−0.10	−0.07	−0.05	−0.07	0.01	−0.05	**−0.134**	−0.05	**−7.6**	−6
CHIANTI v8.0	327.44	0.01	0.002	4	**−0.17**	**−0.12**	**0.14**	−0.08	—	—	0.011	−0.04	−1.8	**8**
Cloudy v13.04	21416.07	**0.74**	**−0.370**	−7	**−0.54**	**−0.52**	**−0.53**	**−0.46**	**−0.43**	−0.15	**−0.399**	0.14	**−18.8**	**−8**

Hitomi et al. 2018

Be aware: sometimes codes agree better than their true uncertainty (e.g., defined by laboratory measurements)

Solution to the problem

b) Study connection between spectral diagnostics with atomic data (excitation/ionization/recombination/etc)



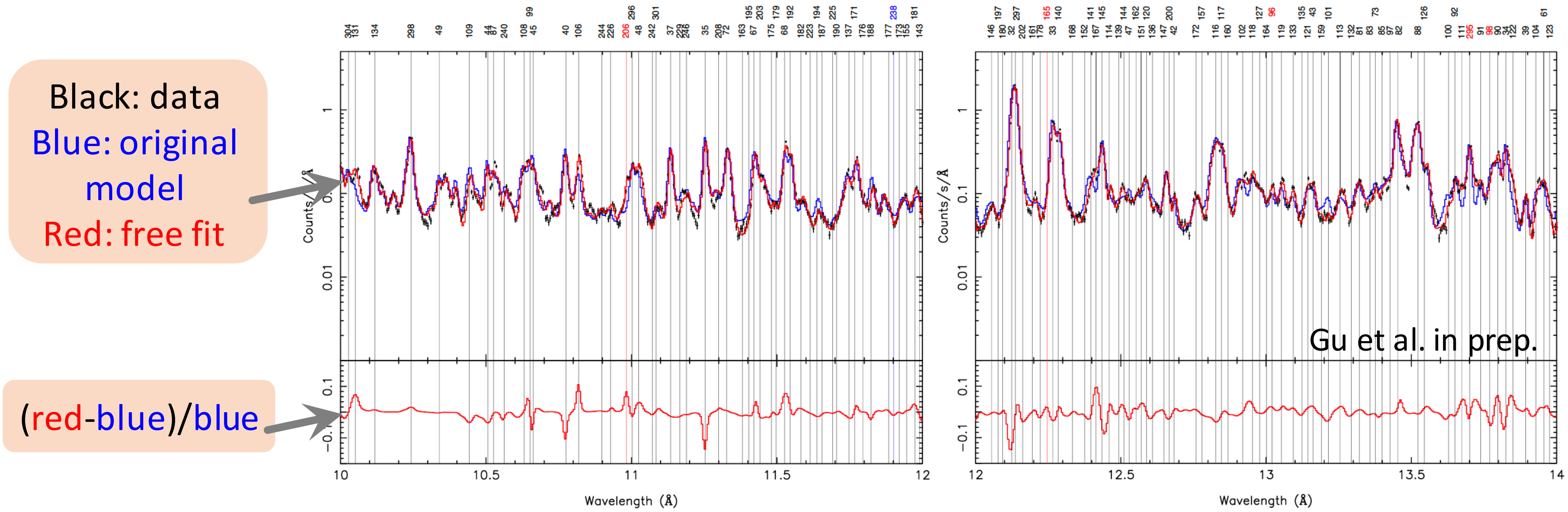
Hitomi et al. 2018

- Monte Carlo of Fe XXV w,x,y,z lines for 4 keV plasma based on empirical atomic data error
- Often lack sufficient information to get ‘empirical atomic error’
- AtomDB team is working on the correlated uncertainties in the fundamental atomic data (e.g., collision strength) as well as a tool for estimating sensitivity of line/line ratio to atomic uncertainties

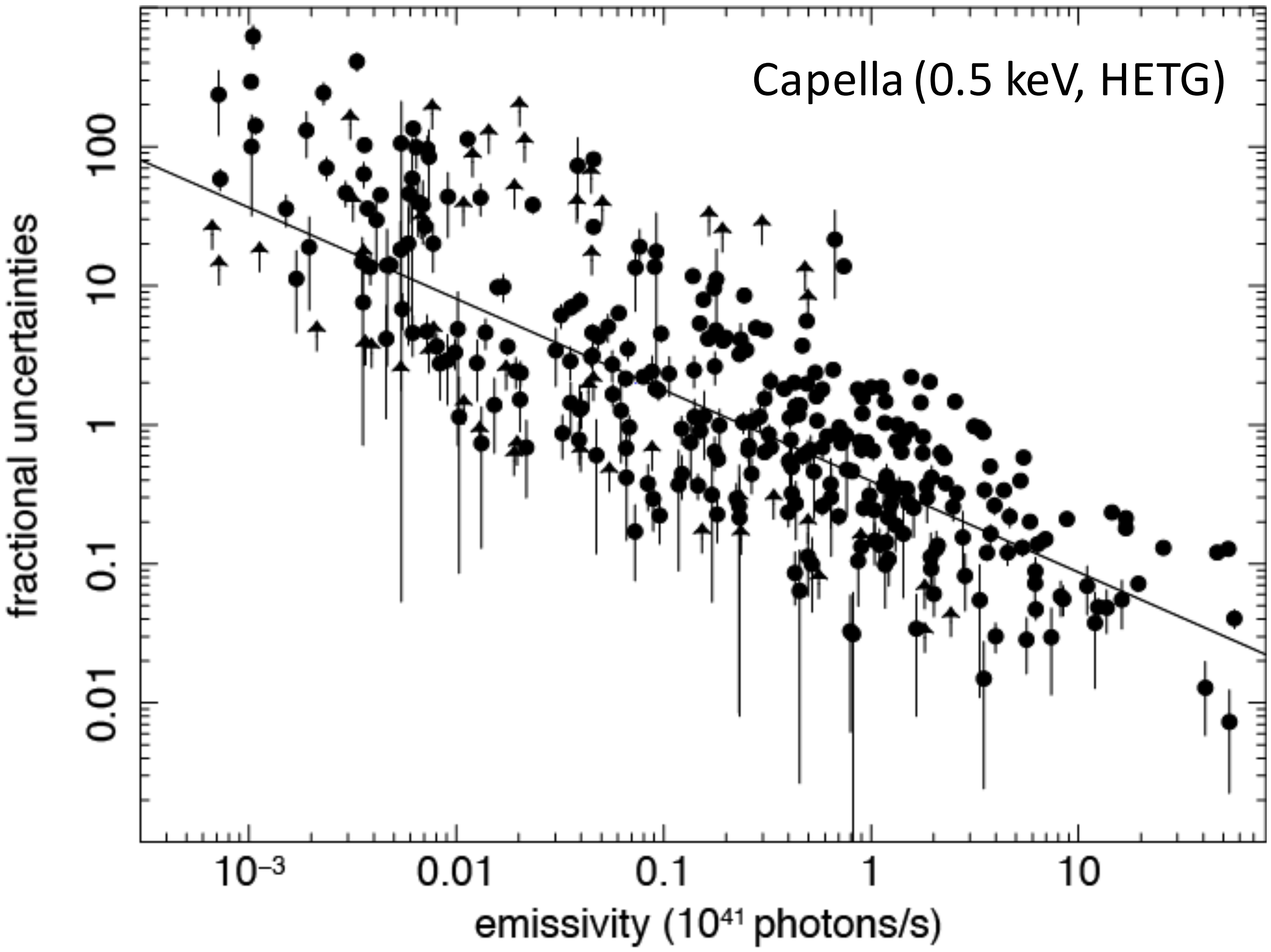
Solution to the problem

c) A practical approach: assuming ideal instrumental calibration and astrophysical modeling, spectral model error should equal to **the error needed to obtain ideal fit of astrophysical spectrum**

Exercise: allow model line emissivity free to fit the stacked Capella HETG spectrum
Original model: 18 CIE + astrophysical and instrumental corrections (Gu et al. 20)

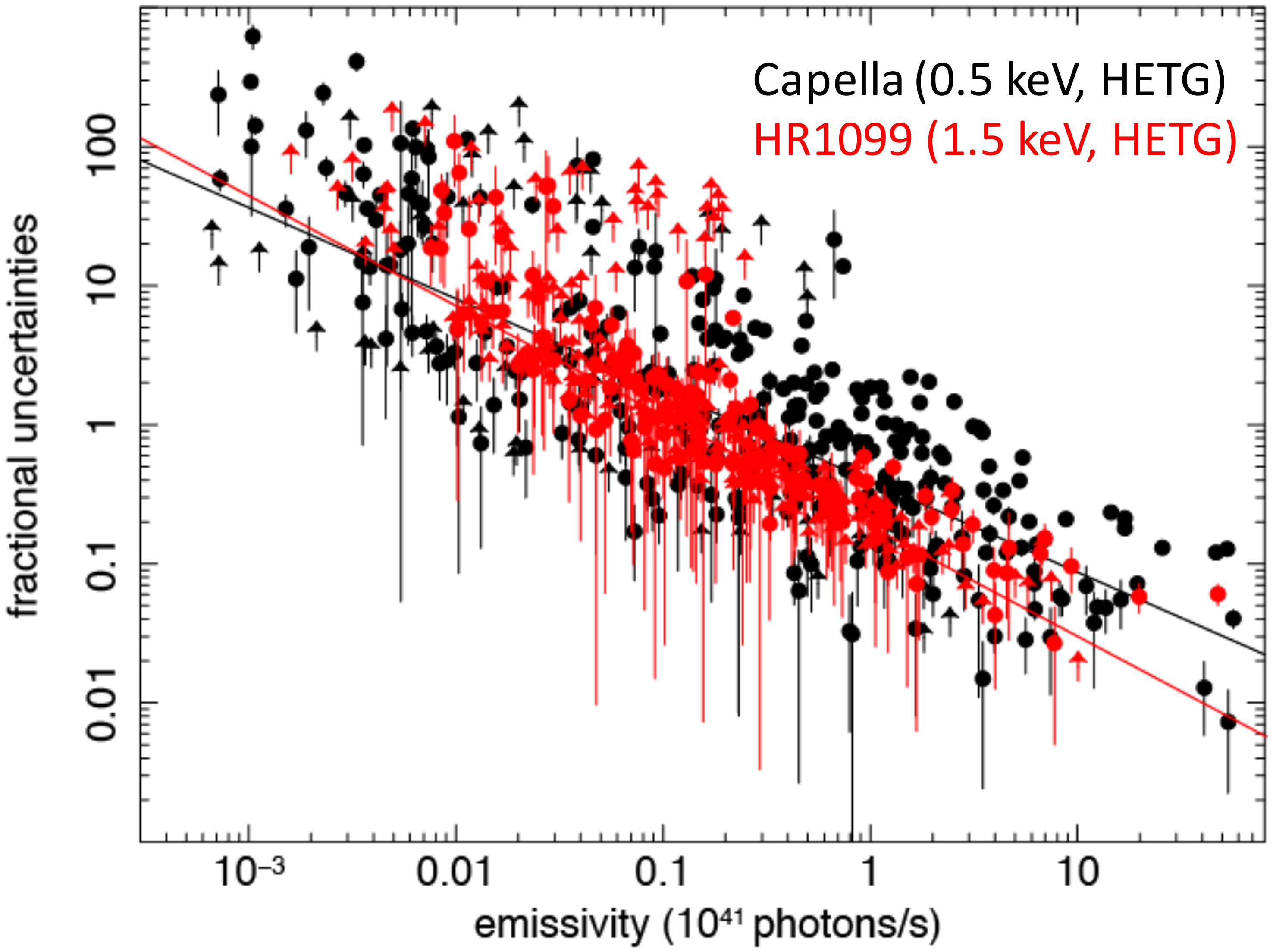


Capella exercise



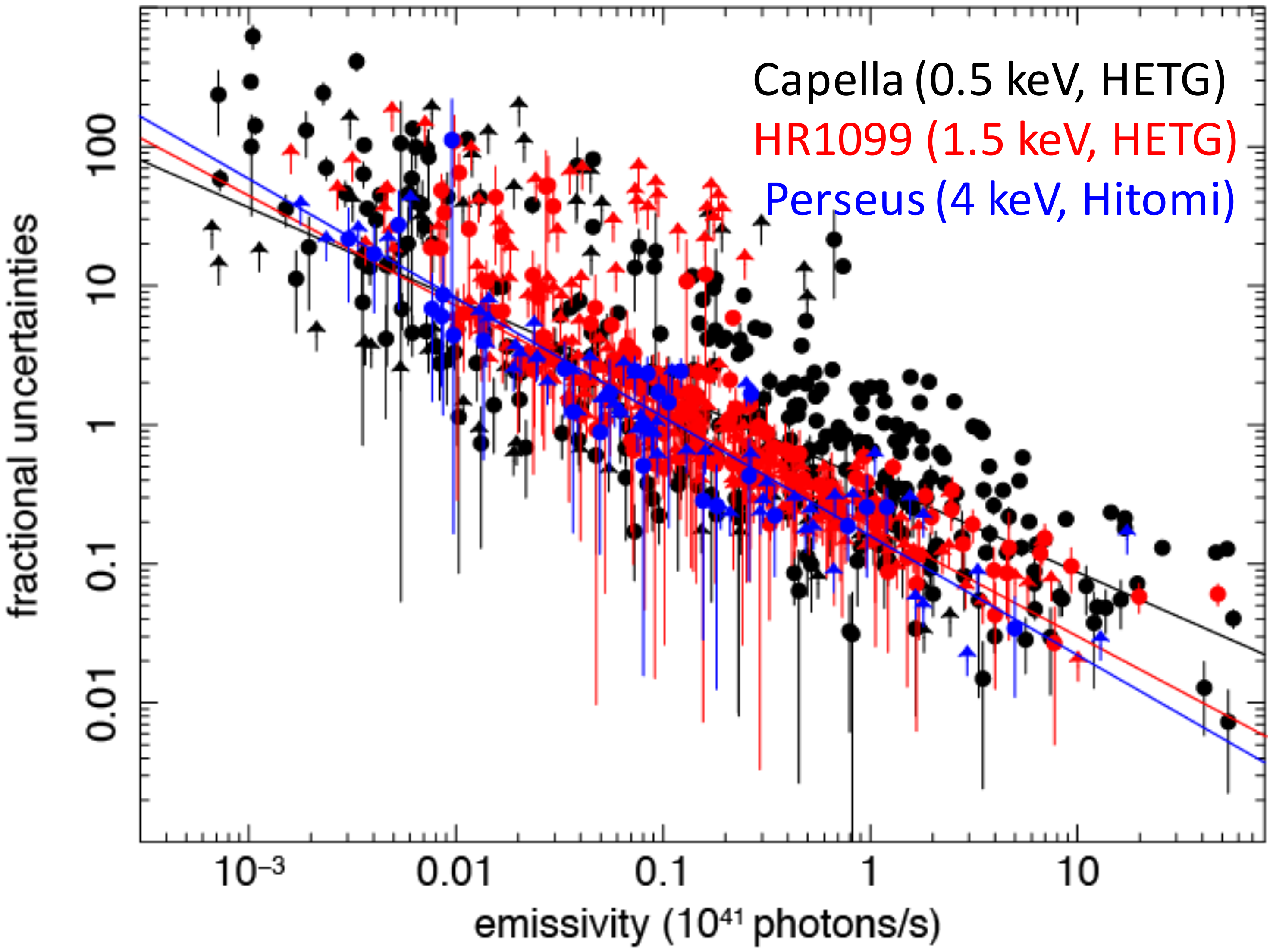
- Changes in line emissivities = expected model uncertainties (E) plotted against the emissivity (I)

Capella + others



- Changes in line emissivities = expected model uncertainties (E) plotted against the emissivity (I)

An analytic form on uncertainty-emissivity relation

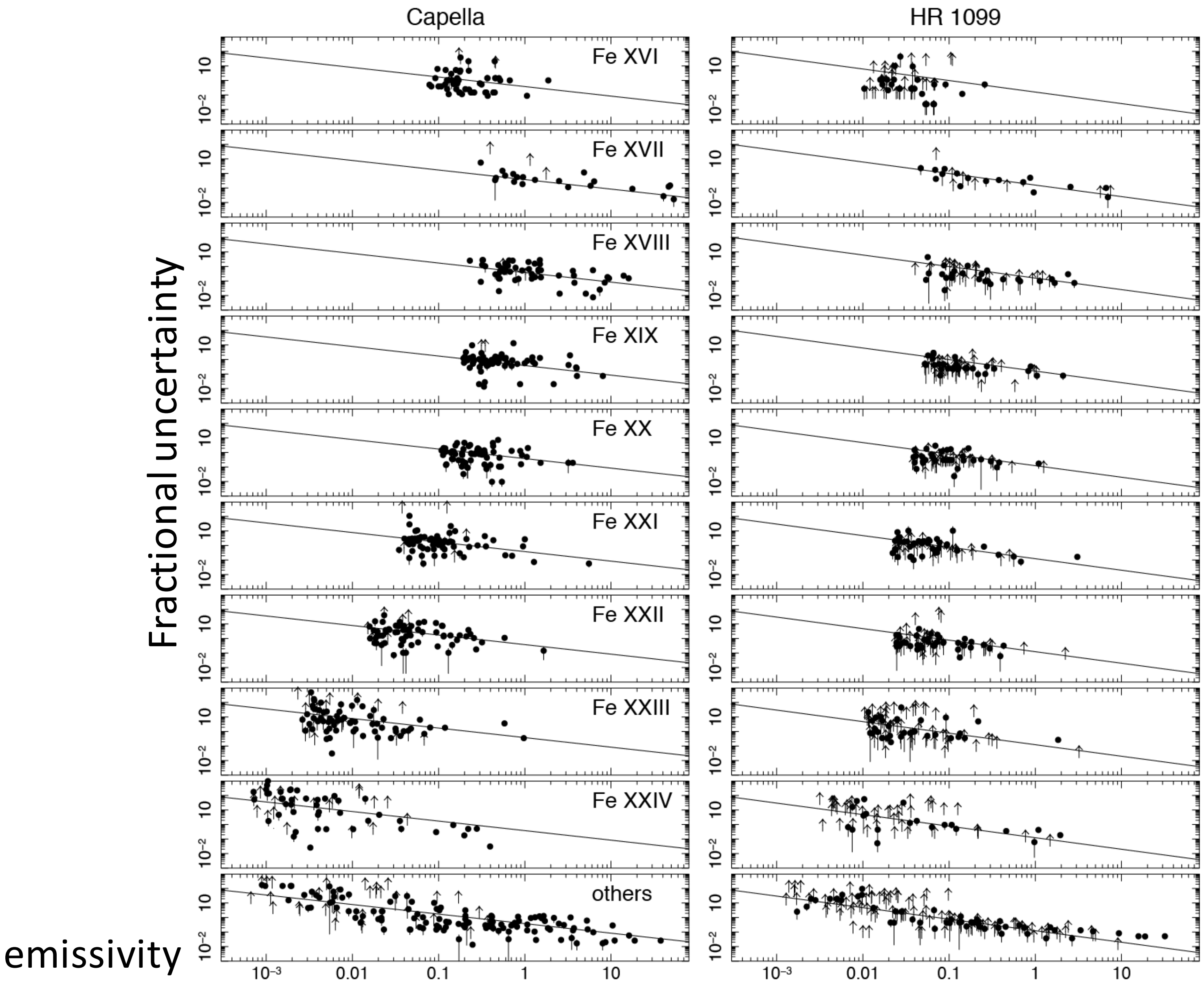


- Changes in line emissivities = expected model uncertainties (E) plotted against the emissivity (I)

- All the observations are in line with an analytic form:

$$E = 0.4 \times \left(\frac{I}{10^{41}\ ph\ s^{-1}}\right)^{-0.7}$$

A universal form?



- This relation is found independent on ion, wavelength, line formation process, object, instrument...
- The calibration and astrophysical effects are minor
- Theoretical solution should be able to reproduce the observed relation
- This relation is easy to implement in codes

Summary

Effort needed to get X-ray spectral models ready for the arrivals of new capabilities from XRISM and Athena

Community requests precise atomic data with *some estimate of uncertainties*

Spectral model error can be obtained from

- Laboratory (instrumental/calibration error, polarization correction error, etc)
- Theory (correlation study, propagation of rate perturbation)
- Observation (observed uncertainty-emissivity relation)

The error could be model-dependent (CIE, PIE), and time-evolving