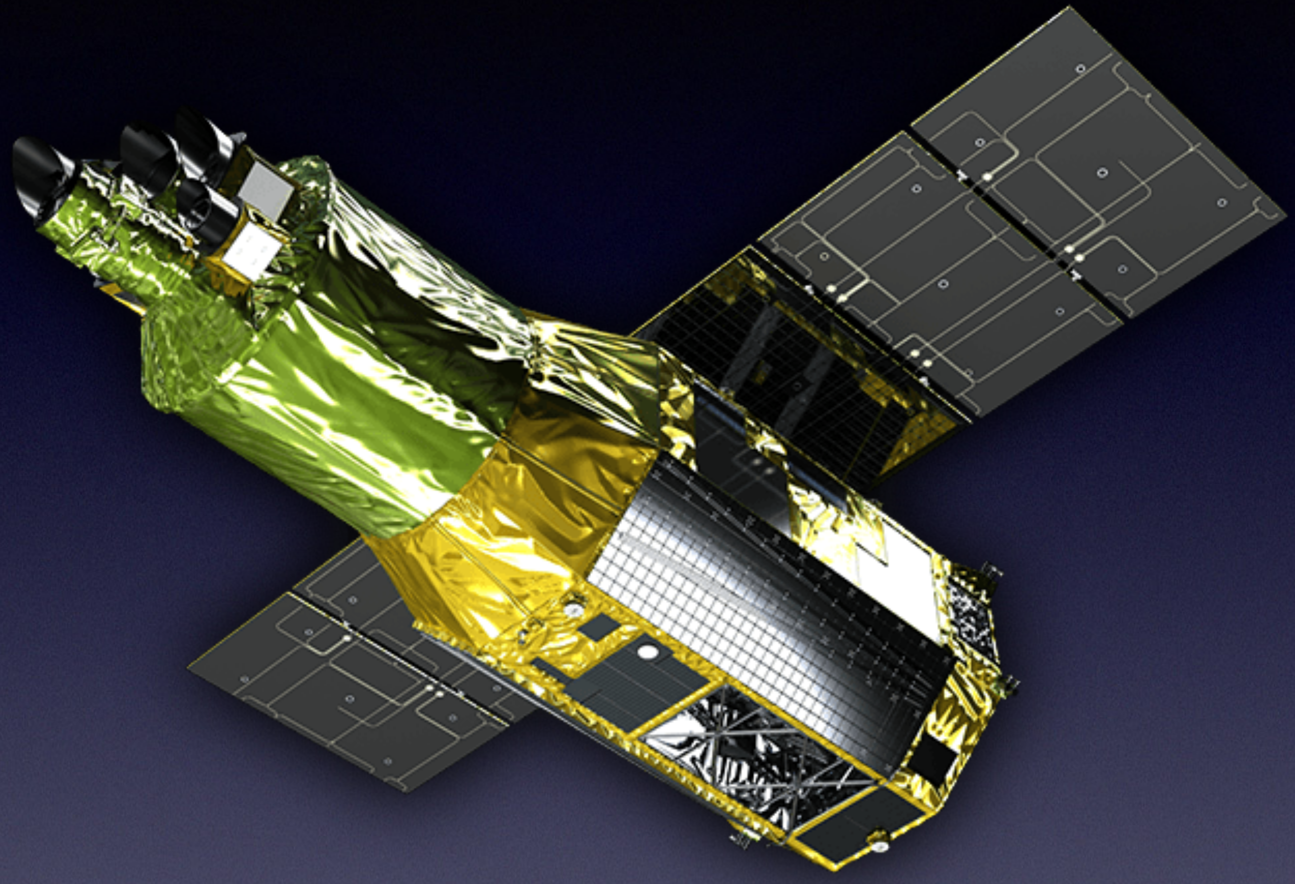
Laboratory Astrophysics Needs for *XRISM* and Beyond

XRISM X-Ray Imaging and Spectroscopy Mission



Brian Williams (NASA/GSFC)

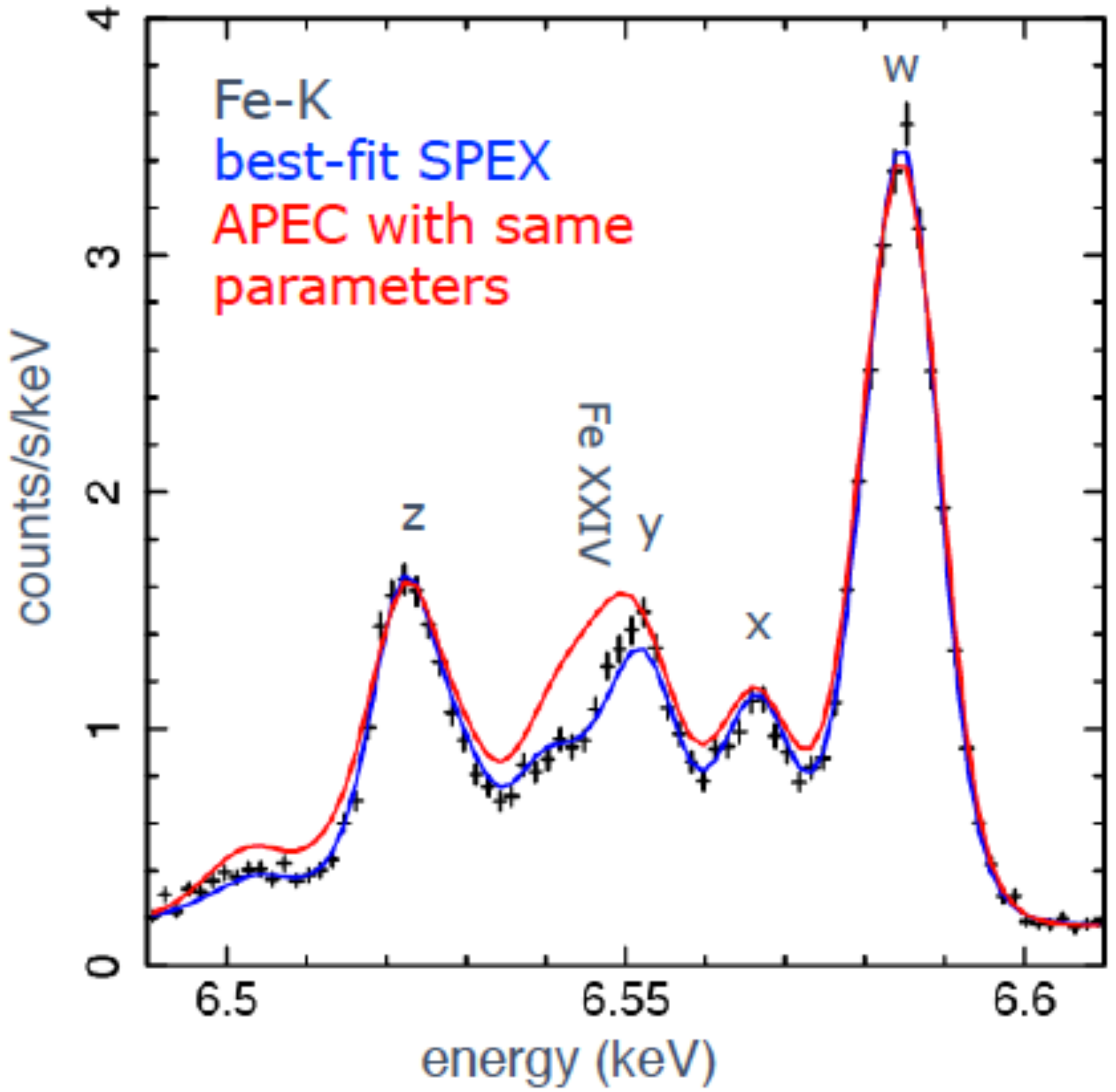
On behalf of Tim Kallman and many others in the
“XRISM Laboratory Astrophysics Working Group”

Background

- *Hitomi* confirmed what many people already knew… the existing atomic databases, codes, and laboratory measurements are insufficient to handle the "next generation" of X-ray spectroscopy
- *XRISM* scheduled for launch in 2022; can't solve all these problems by then, but can at least identify highest priorities and begin to make progress
- Founded "Laboratory Astrophysics Working Group," a team within XRISM project to study this
- Submitted two white papers to Astro2020 Decadal Survey last week

Current people: **Tim Kallman (Chair, NASA GSFC), Jelle Kaastra (Vice-chair, SRON)**, Greg Brown (LLNL), Lia Corrales (U. Michigan), Elisa Costantini (SRON), Renata Cumbee (NASA GSFC), Megan Eckart (LLNL), Teru Enoto (Kyoto), Edmund Hodges-Kluck (NASA GSFC), Liyi Gu (Riken), Kazunori Ishibashi (Nagoya), Maurice Leutenegger (NASA GSFC), Michael Loewenstein (NASA GSFC), Shinya Nakashima (Riken), Scott Porter (NASA GSFC), Makoto Sawada (NASA GSFC), Randall Smith (SAO), Brian Williams (NASA GSFC), Tahir Yaqoob (NASA GSFC)

Problems to be solved



- state-of-art calculations can differ by up to 70% @ 4 keV
- Fe XXIV inner-shell radiative/Auger rates and branching ratios differ by up to 50%.
- As a result, Fe abundance differ by 16%.
- Similar difference in a few H-like excitations.

H/He/Li-like are the simplest systems!

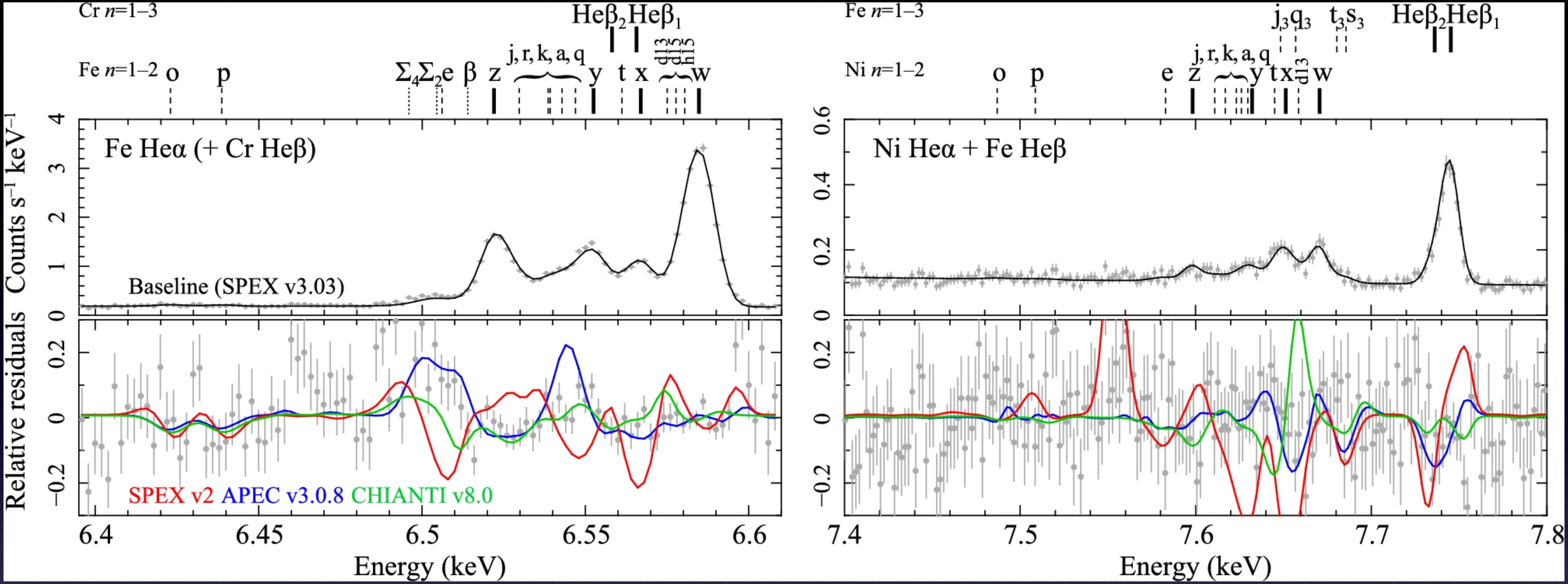
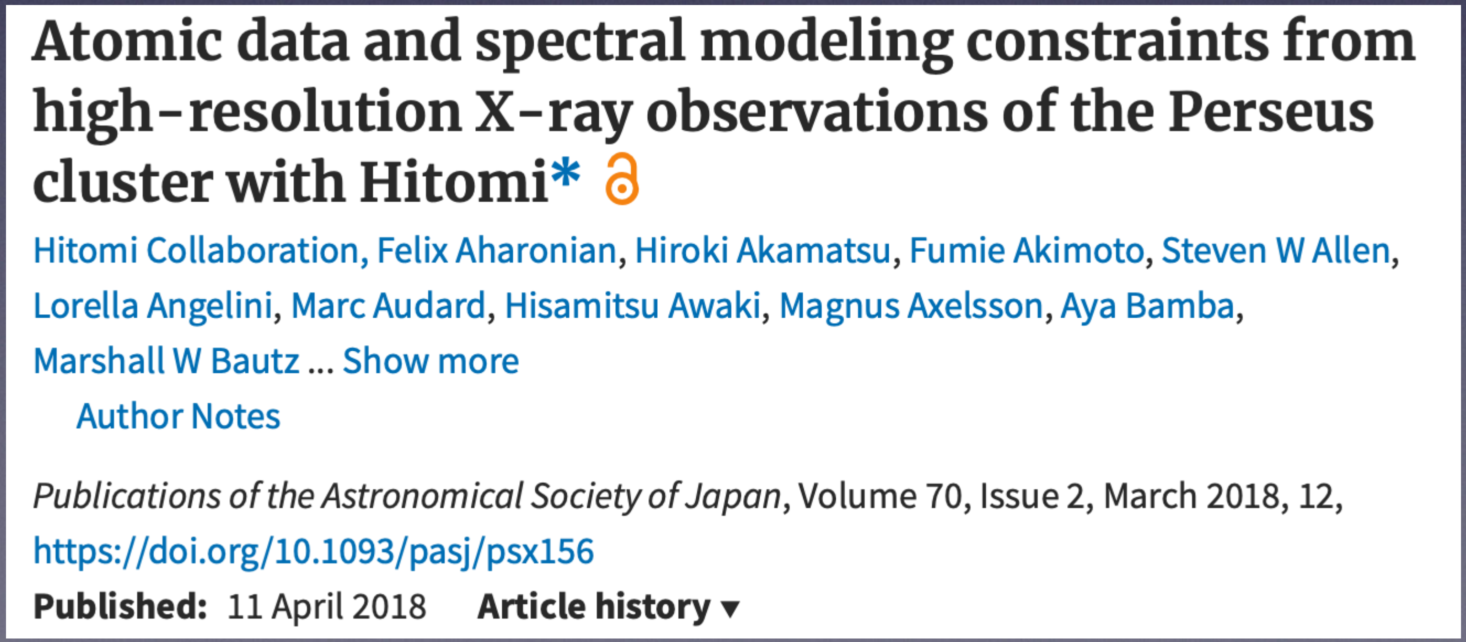


Figure 1 from this paper



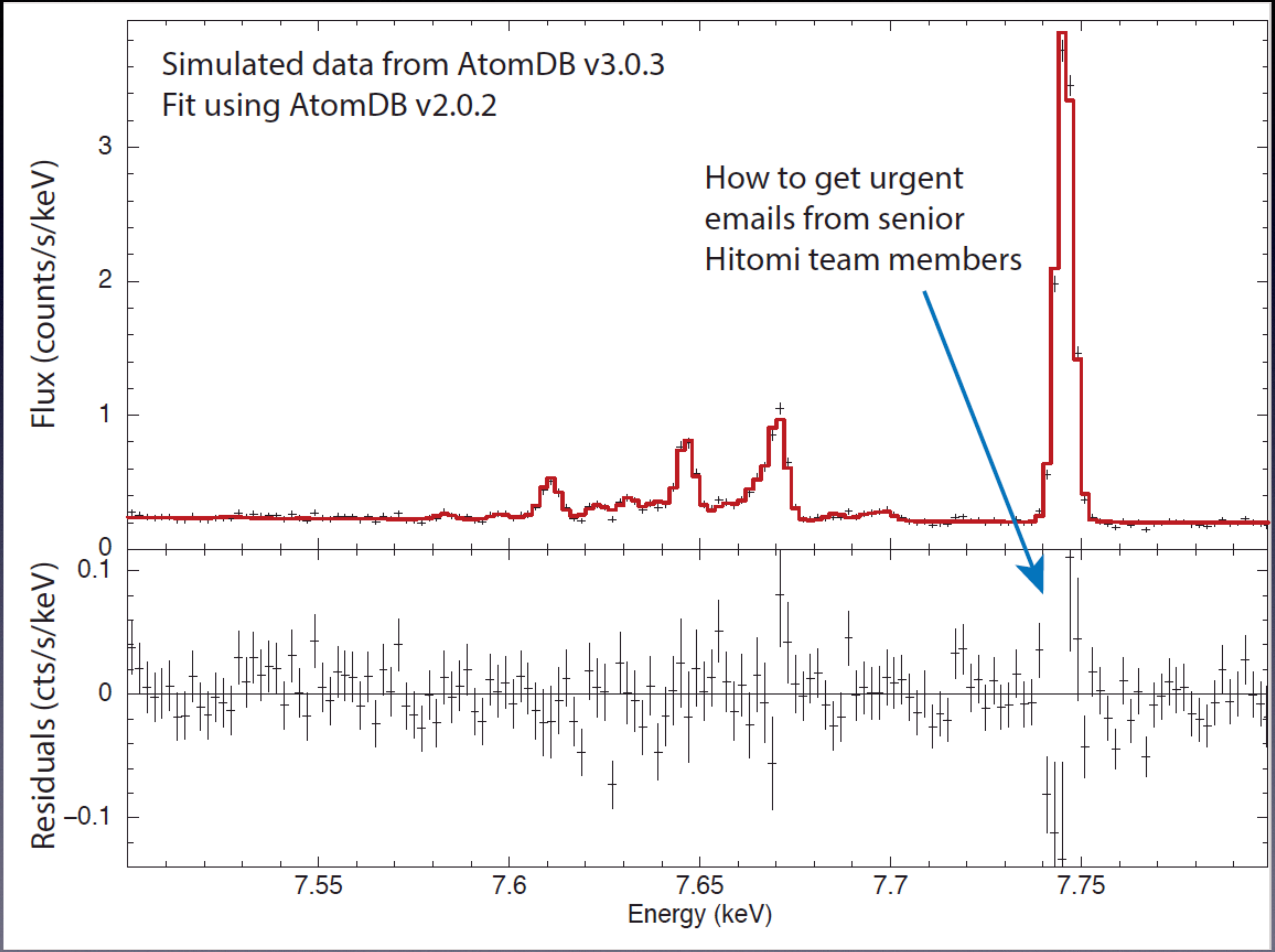
Atomic data and spectral modeling constraints from high-resolution X-ray observations of the Perseus cluster with Hitomi*

Hitomi Collaboration, Felix Aharonian, Hiroki Akamatsu, Fumie Akimoto, Steven W Allen, Lorella Angelini, Marc Audard, Hisamitsu Awaki, Magnus Axelsson, Aya Bamba, Marshall W Bautz ... Show more

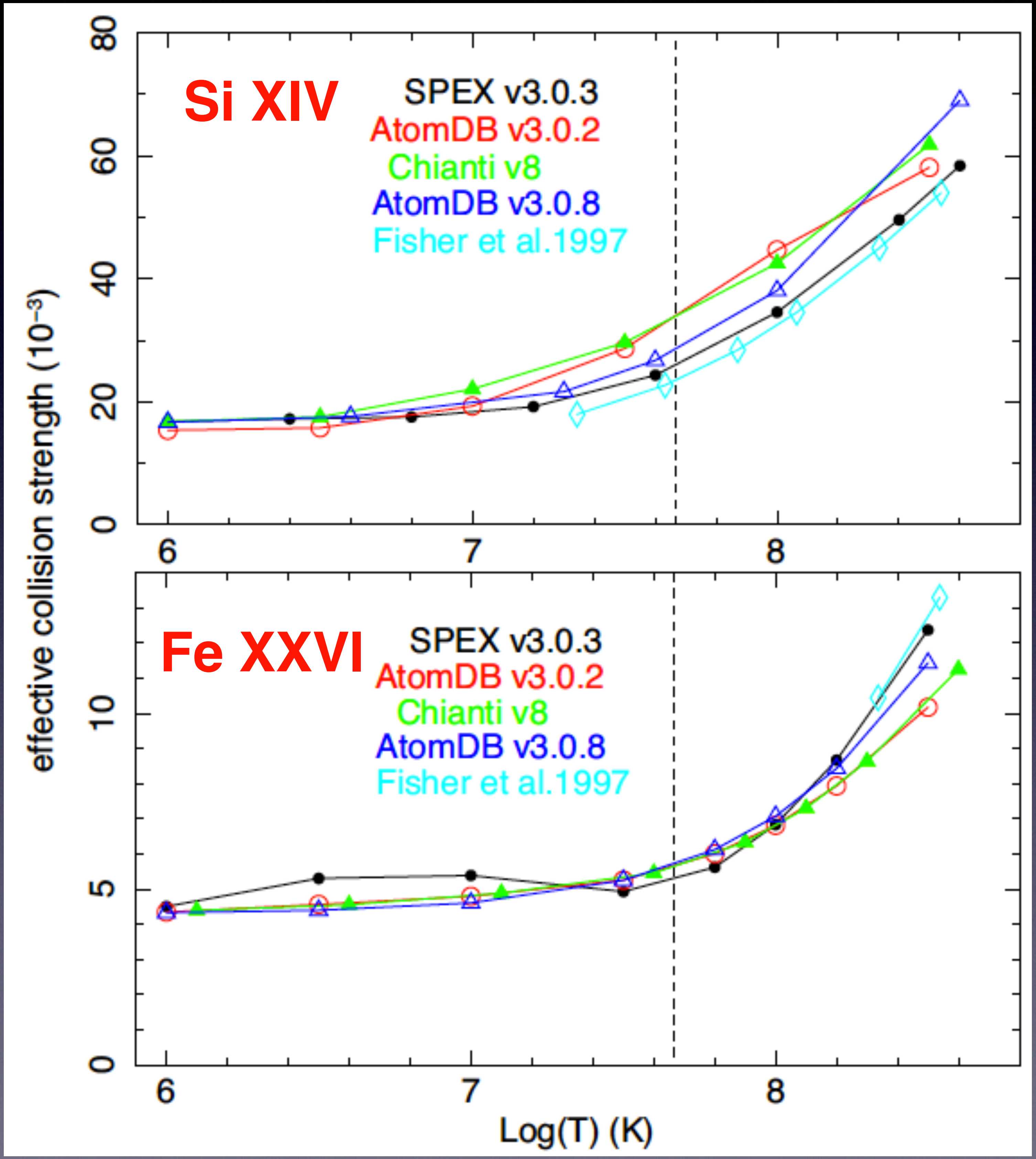
Author Notes

Publications of the Astronomical Society of Japan, Volume 70, Issue 2, March 2018, 12, https://doi.org/10.1093/pasj/psx156

Published: 11 April 2018 **Article history ▾**

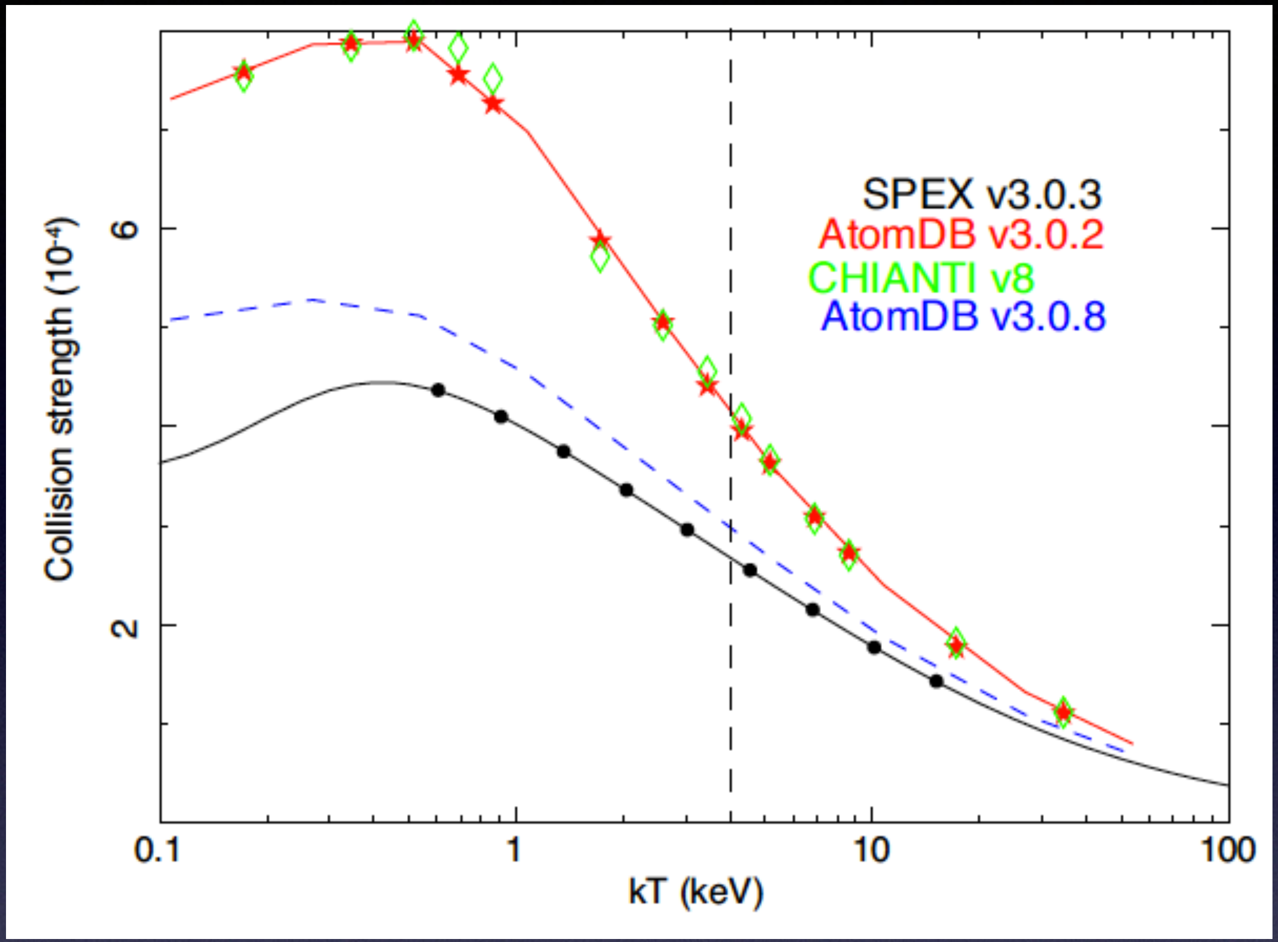

Simulated data from AtomDB v3.0.3
Fit using AtomDB v2.0.2
How to get urgent emails from senior Hitomi team members
Flux (counts/s/keV)
3
2
1
0
Residuals (cts/s/keV)
0.1
0
−0.1
7.55
7.6
7.65
7.7
7.75
Energy (keV)

Atomic Data: H-like ions

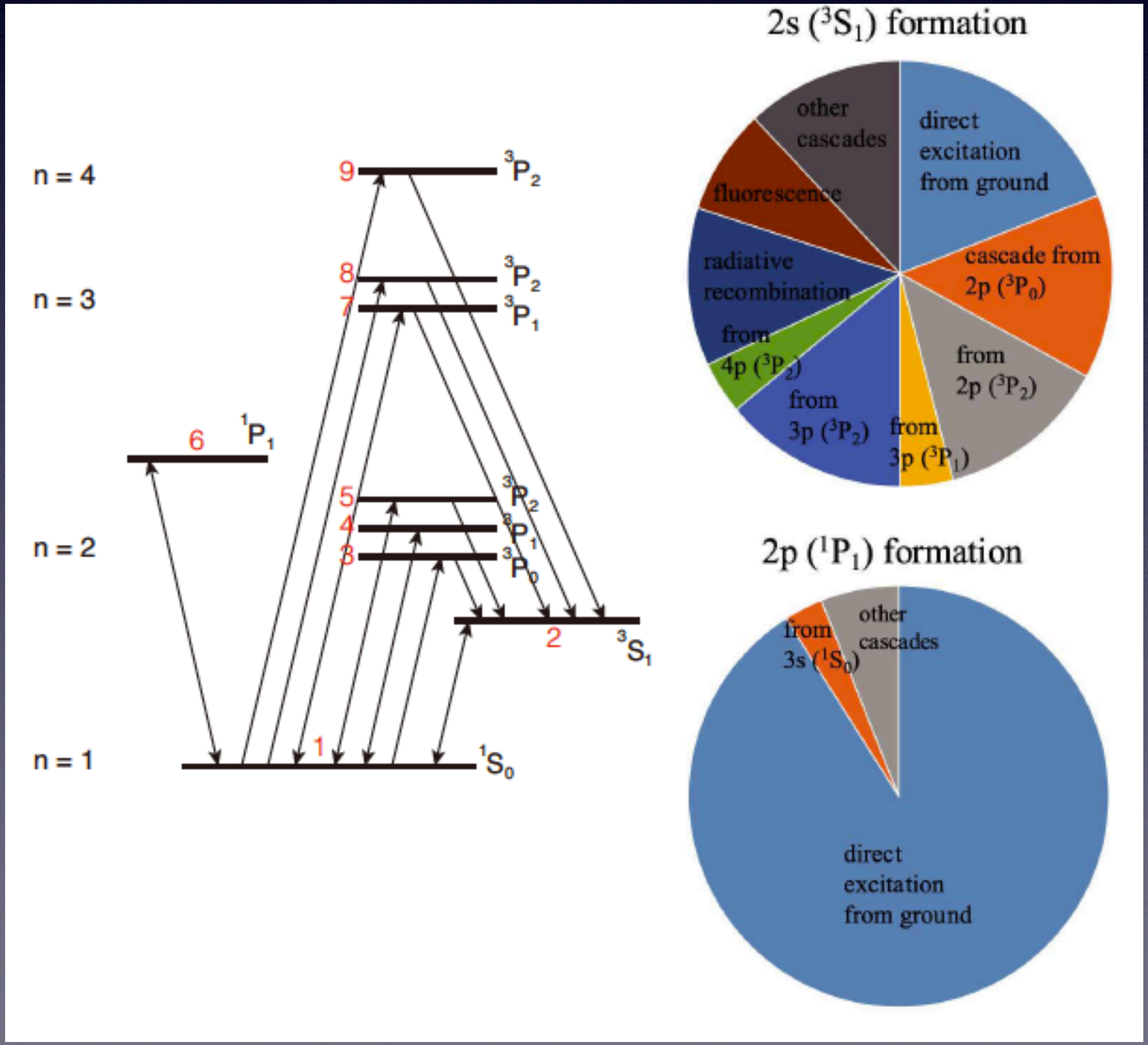


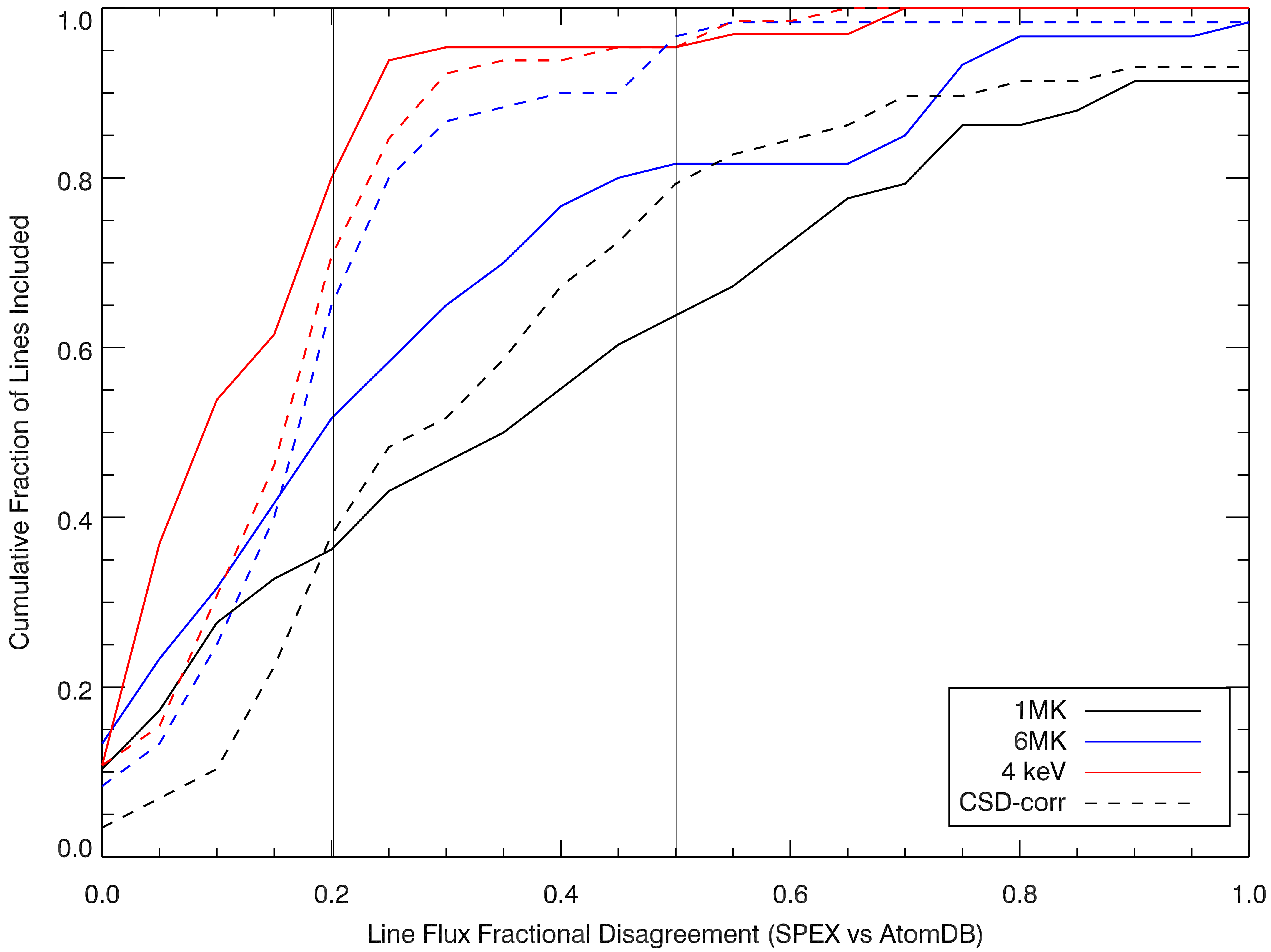
For Si XIV, leads to 30% difference line flux -> 30% difference deduced abundance

Atomic Data: He-like ions



This is with only 2 electrons!




Cumulative Fraction of Lines Included
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0
Line Flux Fractional Disagreement (SPEX vs AtomDB)
1MK
6MK
4 keV
CSD-corr

Impact of charge-state distributions

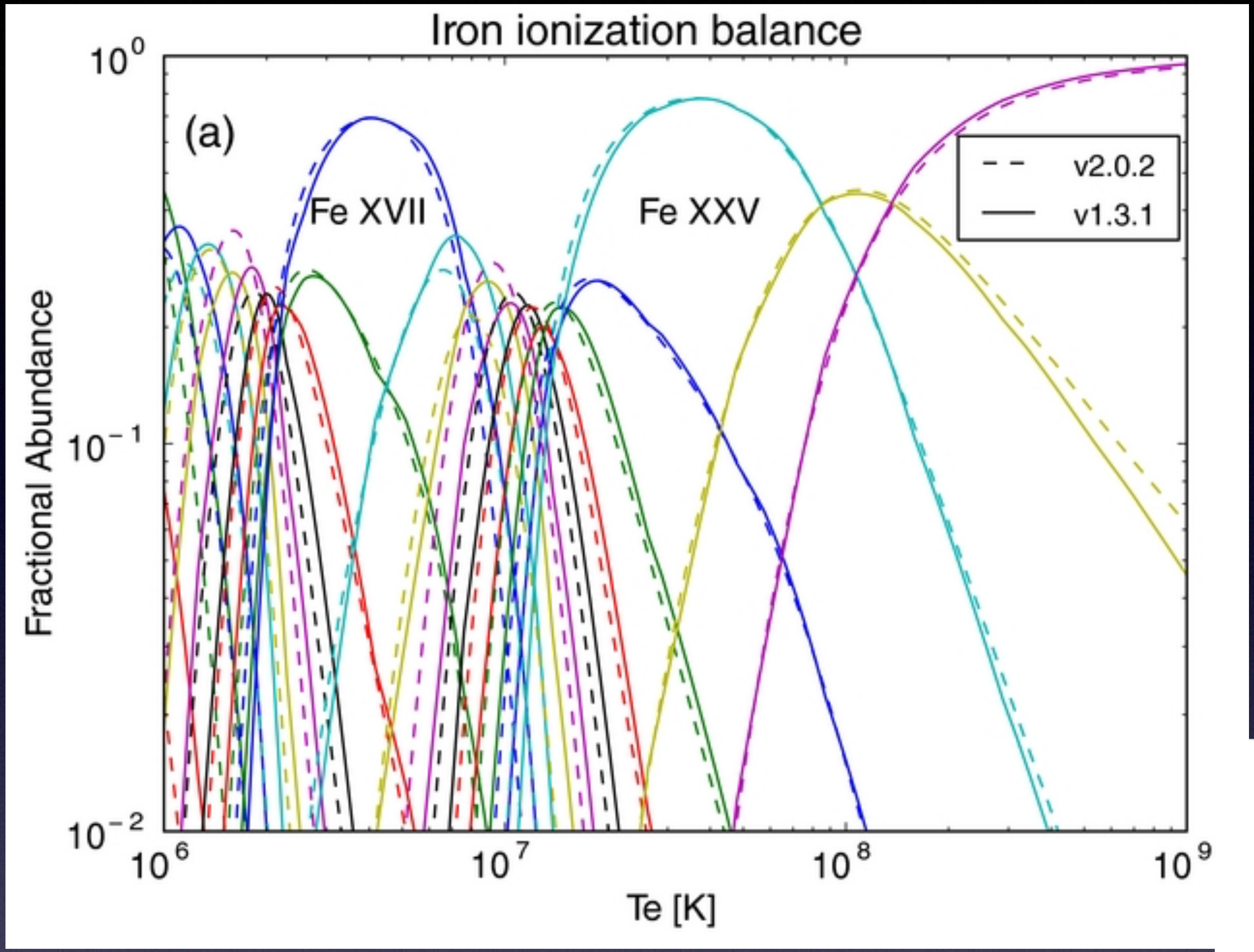
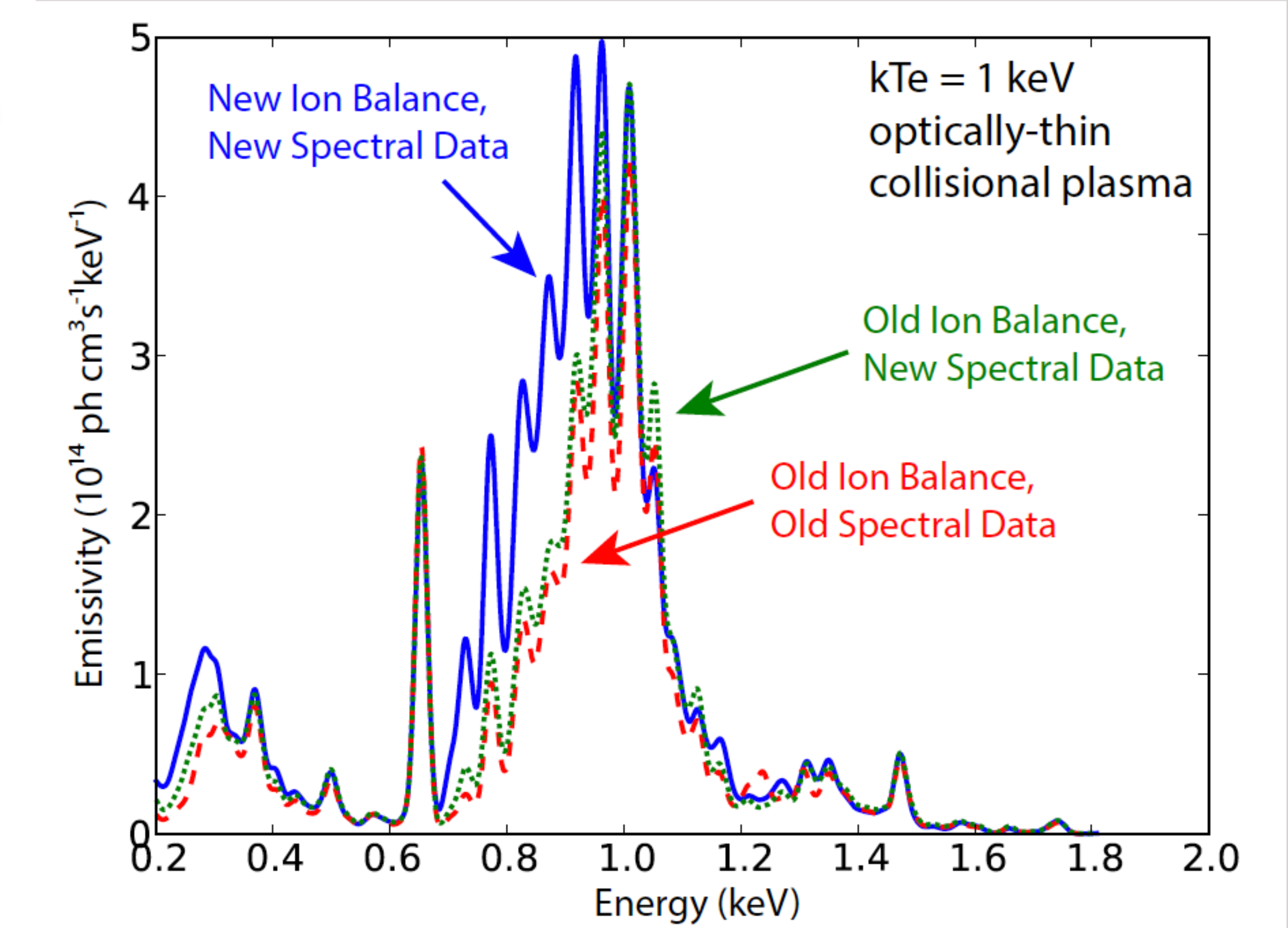
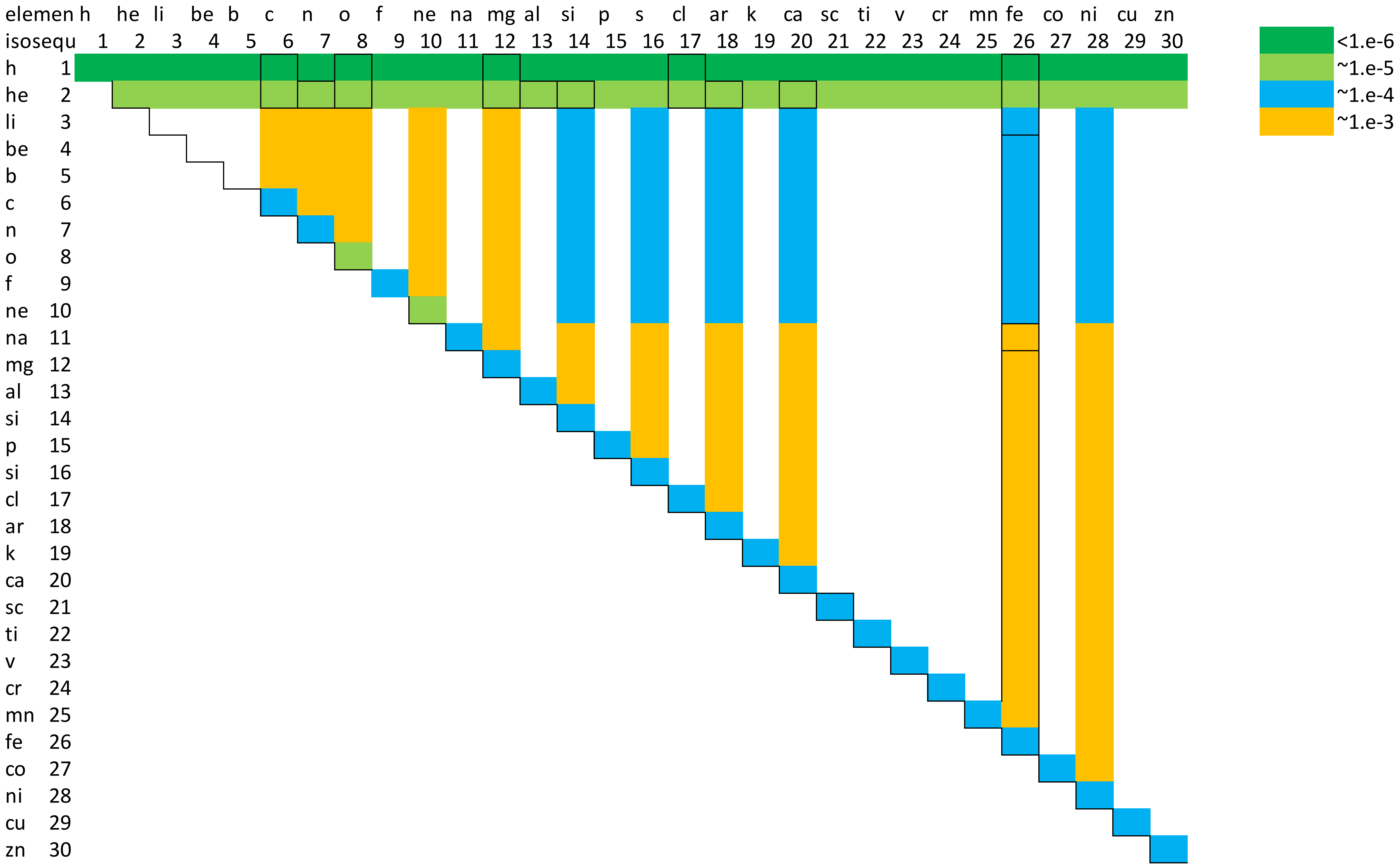


Figure 3 from Foster et al. (2012)





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zn	30																														🟦

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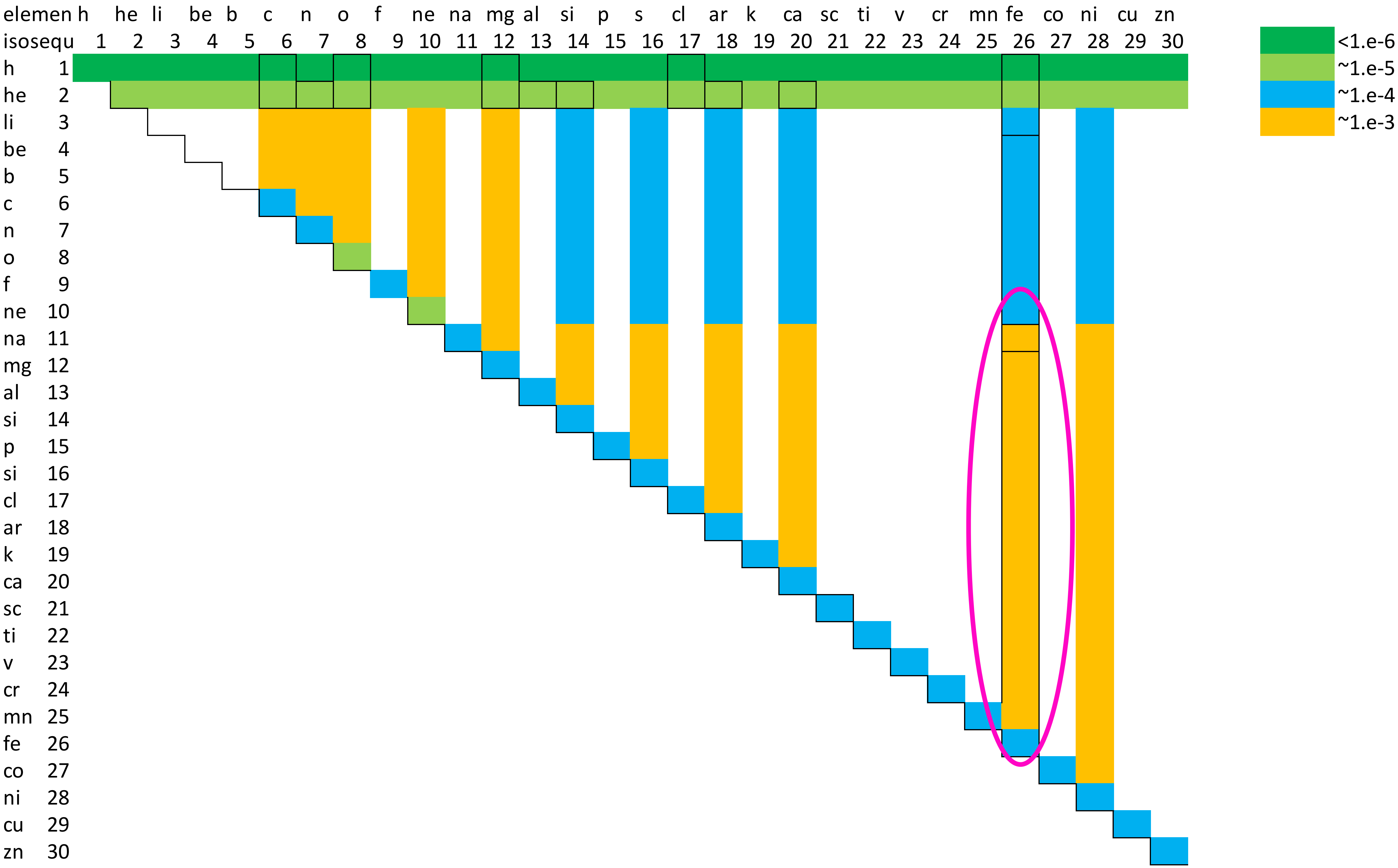
Accuracy of transition energies for K and L-shell lines



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be	4						🟧	🟧	🟧		🟧		🟧		🟦		🟦		🟦		🟦						🟦		🟦		
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ni	28																												🟦		
cu	29																													🟦	
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Accuracy of transition energies for K and L-shell lines

What do we need?

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A precise and accurate determination of:

- wavelengths for common transitions
- charge state distributions
- absorption cross sections
- collisional and radiative rates
- line widths
- energy edges and shapes
- line fluxes

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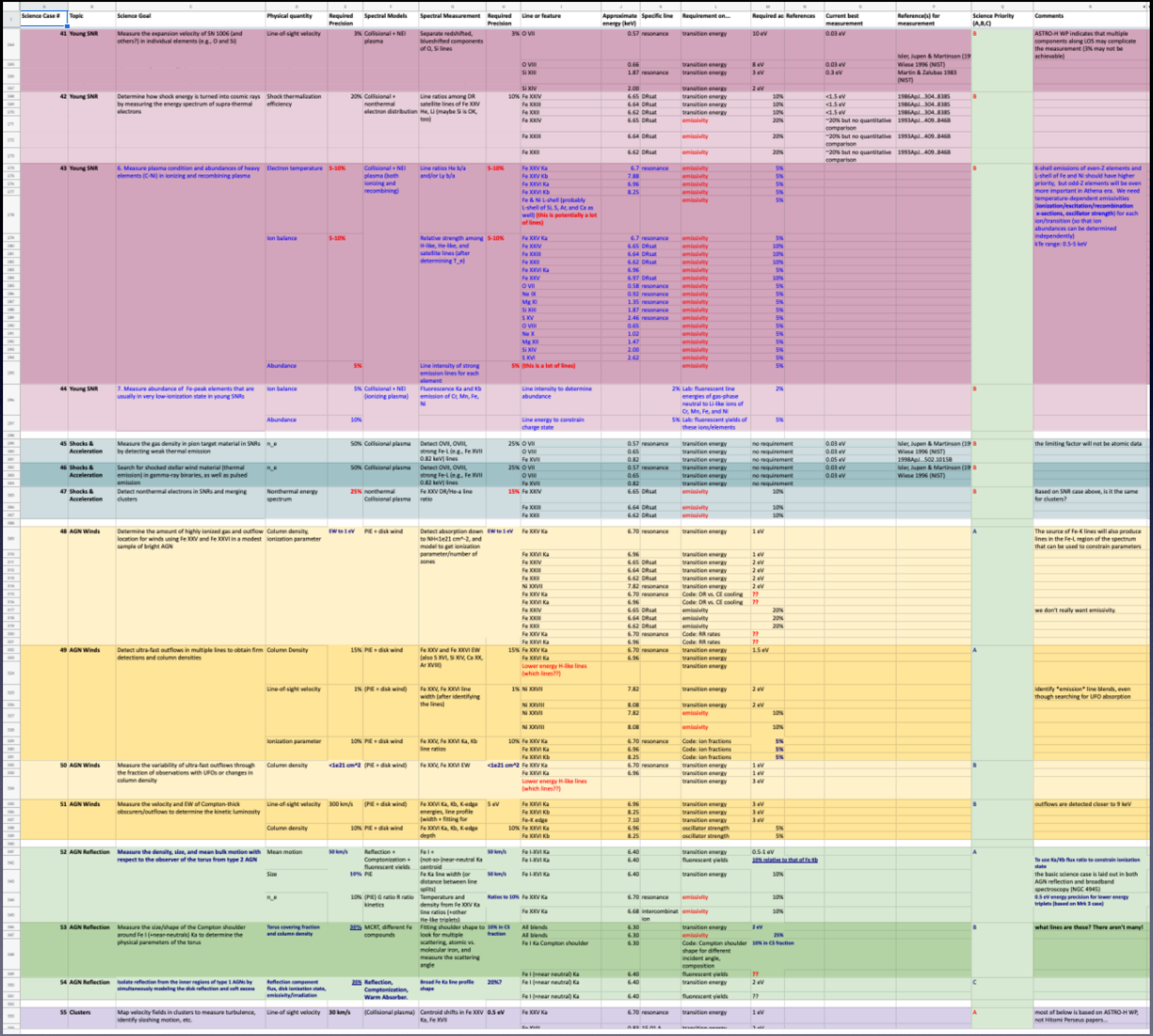
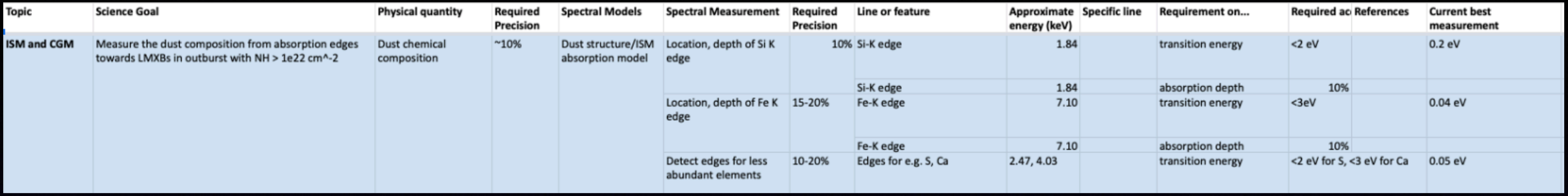
- **line fluxes**
- ***plus estimates of uncertainties on all of these quantities***

The goal for the coming years should be to reach the point where our scientific progress is limited by observational uncertainties, not laboratory ones.

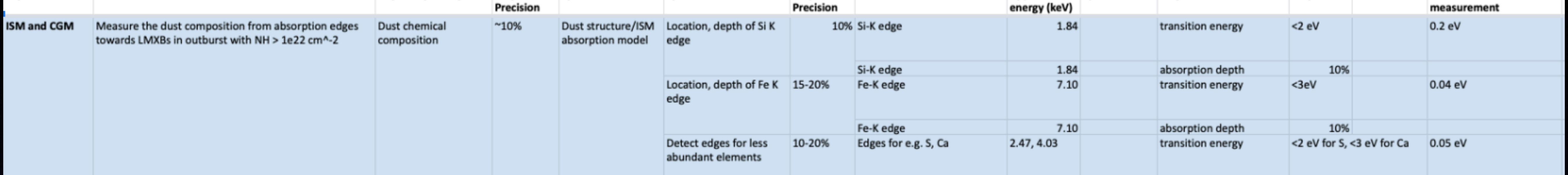
XRISM Project convened Lab Astro WG in late 2018 to assess current state of field. Started by crowd-sourcing project out to XRISM Science Team to determine most important measurements XRISM will make, and what is required for these.



Science Case #	Topic	Science Goal	Physical quantity	Required Precision	Spectral Models	Spectral Measurement	Required Precision	Line or feature	Approximate energy (keV)	Specific line	Requirement on...	Required ac	References	Current best measurement	Reference(s) for measurement	Science Priority (A,B,C)	Comments
41	Young SNR	Measure the expansion velocity of SN 1006 (and others?) in individual elements (e.g., O and Si)	Line-of-sight velocity	3%	Collisional + NEI plasma	Separate redshifted, blueshifted components of O, Si lines	3%	O VII	0.57	resonance	transition energy	10 eV		0.03 eV	Isler, Jupen & Martinson (19	B	ASTRO-H WP indicates that multiple components along LOS may complicate the measurement (3% may not be achievable)
								O VIII	0.66		transition energy	8 eV		0.03 eV	Wiese 1996 (NIST)		
								Si XIII	1.87	resonance	transition energy	3 eV		0.3 eV	Martin & Zalubas 1983 (NIST)		
								Si XIV	2.00		transition energy	2 eV					
42	Young SNR	Determine how shock energy is turned into cosmic rays by measuring the energy spectrum of supra-thermal electrons	Shock thermalization efficiency	20%	Collisional + nonthermal electron distribution	Line ratios among DR satellite lines of Fe XXV He, Li (maybe Si is OK, too)	10%	Fe XXIV	6.65	DRsat	transition energy	10%		<1.5 eV	1986ApJ...304..838S	B	
								Fe XXIII	6.64	DRsat	transition energy	10%		<1.5 eV	1986ApJ...304..838S		
								Fe XXII	6.62	DRsat	transition energy	10%		<1.5 eV	1986ApJ...304..838S		
								Fe XXIV	6.65	DRsat	emissivity	20%		~20% but no quantitative comparison	1993ApJ...409..846B		
								Fe XXIII	6.64	DRsat	emissivity	20%		~20% but no quantitative comparison	1993ApJ...409..846B		
								Fe XXII	6.62	DRsat	emissivity	20%		~20% but no quantitative comparison	1993ApJ...409..846B		
43	Young SNR	6. Measure plasma condition and abundances of heavy elements (C-Ni) in ionizing and recombining plasma	Electron temperature	5-10%	Collisional + NEI plasma (both ionizing and recombining)	Line ratios He b/a and/or Ly b/a	5-10%	Fe XXV Ka	6.7	resonance	emissivity	5%				B	K-shell emissions of even-Z elements and L-shell of Fe and Ni should have higher priority, but odd-Z elements will be even more important in Athena era. We need temperature-dependent emissivities **(ionization/excitation/recombination x-sections, oscillator strength)** for each ion/transition (so that ion abundances can be determined independently) kTe range: 0.5-5 keV
								Fe XXV Kb	7.88		emissivity	5%					
								Fe XXVI Ka	6.96		emissivity	5%					
								Fe XXVI Kb	8.25		emissivity	5%					
								Fe & Ni L-shell (probably L-shell of Si, S, Ar, and Ca as well) **(this is potentially a lot of lines)**			emissivity	5%					
			Ion balance	5-10%		Relative strength among H-like, He-like, and satellite lines (after determining T_e)	5-10%	Fe XXV Ka	6.7	resonance	emissivity	5%					
								Fe XXIV	6.65	DRsat	emissivity	10%					
								Fe XXIII	6.64	DRsat	emissivity	10%					
								Fe XXII	6.62	DRsat	emissivity	10%					
								Fe XXVI Ka	6.96		emissivity	5%					
								Fe XXV	6.97	DRsat	emissivity	10%					
								O VII	0.58	resonance	emissivity	5%					
								Ne IX	0.92	resonance	emissivity	5%					
								Mg XI	1.35	resonance	emissivity	5%					
								Si XIII	1.87	resonance	emissivity	5%					
								S XV	2.46	resonance	emissivity	5%					
								O VIII	0.65		emissivity	5%					
								Ne X	1.02		emissivity	5%					
								Mg XII	1.47		emissivity	5%					
								Si XIV	2.00		emissivity	5%					
								S XVI	2.62		emissivity	5%					
			Abundance	5%		Line intensity of strong emission lines for each element	5%	**(this is a lot of lines)**			emissivity	5%					
44	Young SNR	7. Measure abundance of Fe-peak elements that are usually in very low-ionization state in young SNRs	Ion balance	5%	Collisional + NEI (ionizing plasma)	Fluorescence Ka and Kb emission of Cr, Mn, Fe, Ni		Line intensity to determine abundance		2%	Lab: fluorescent line energies of gas-phase neutral to Li-like ions of Cr, Mn, Fe, and Ni	2%				B	
			Abundance	10%				Line energy to constrain charge state		5%	Lab: fluorescent yields of these ions/elements	5%					
45	Shocks & Acceleration	Measure the gas density in pion target material in SNRs by detecting weak thermal emission	n_e	50%	Collisional plasma	Detect OVII, OVIII, strong Fe-L (e.g., Fe XVII 0.82 keV) lines	25%	O VII	0.57	resonance	transition energy	no requirement		0.03 eV	Isler, Jupen & Martinson (19	B	the limiting factor will not be atomic data
								O VIII	0.65		transition energy	no requirement		0.03 eV	Wiese 1996 (NIST)		
								Fe XVII	0.82		transition energy	no requirement		0.05 eV	1998ApJ...502.1015B		
46	Shocks & Acceleration	Search for shocked stellar wind material (thermal emission) in gamma-ray binaries, as well as pulsed emission	n_e	50%	Collisional plasma	Detect OVII, OVIII, strong Fe-L (e.g., Fe XVII 0.82 keV) lines	25%	O VII	0.57	resonance	transition energy	no requirement		0.03 eV	Isler, Jupen & Martinson (19	B	
								O VIII	0.65		transition energy	no requirement		0.03 eV	Wiese 1996 (NIST)		
								Fe XVII	0.82		transition energy	no requirement					
47	Shocks & Acceleration	Detect nonthermal electrons in SNRs and merging clusters	Nonthermal energy spectrum	25%	nonthermal Collisional plasma	Fe XXV DR/He-a line ratio	15%	Fe XXIV	6.65	DRsat	emissivity	10%				B	Based on SNR case above, is it the same for clusters?
								Fe XXIII	6.64	DRsat	emissivity	10%					
								Fe XXII	6.62	DRsat	emissivity	10%					
48	AGN Winds	Determine the amount of highly ionized gas and outflow location for winds using Fe XXV and Fe XXVI in a modest sample of bright AGN	Column density, ionization parameter	EW to 1 eV	PIE + disk wind	Detect absorption down to NH<1e21 cm^-2, and model to get ionization parameter/number of zones	EW to 1 eV	Fe XXV Ka	6.70	resonance	transition energy	1 eV				A	The source of Fe-K lines will also produce lines in the Fe-L region of the spectrum that can be used to constrain parameters
								Fe XXVI Ka	6.96		transition energy	1 eV					
								Fe XXIV	6.65	DRsat	transition energy	2 eV					
								Fe XXIII	6.64	DRsat	transition energy	2 eV					
								Fe XXII	6.62	DRsat	transition energy	2 eV					
								Ni XXVII	7.82	resonance	transition energy	2 eV					
								Fe XXV Ka	6.70	resonance	Code: DR vs. CE cooling	??					
								Fe XXVI Ka	6.96		Code: DR vs. CE cooling	??					
								Fe XXIV	6.65	DRsat	emissivity	20%					we don't really want emissivity.
								Fe XXIII	6.64	DRsat	emissivity	20%					
								Fe XXII	6.62	DRsat	emissivity	20%					
								Fe XXV Ka	6.70	resonance	Code: RR rates	??					
								Fe XXVI Ka	6.96		Code: RR rates	??					
49	AGN Winds	Detect ultra-fast outflows in multiple lines to obtain firm detections and column densities	Column Density	15%	PIE + disk wind	Fe XXV and Fe XXVI EW (also S XVI, Si XIV, Ca XX, Ar XVIII)	15%	Fe XXV Ka	6.70	resonance	transition energy	1.5 eV				A	
								Fe XXVI Ka	6.96		transition energy						
								Lower energy H-like lines (which lines??)			transition energy						
			Line-of-sight velocity	1%	(PIE + disk wind)	Fe XXV, Fe XXVI line width (after identifying the lines)	1%	Ni XXVII	7.82		transition energy	2 eV					identify *emission* line blends, even though searching for UFO absorption
								Ni XXVIII	8.08		transition energy	2 eV					
								Ni XXVII	7.82		emissivity	10%					
								Ni XXVIII	8.08		emissivity	10%					
			Ionization parameter	10%	PIE + disk wind	Fe XXV, Fe XXVI Ka, Kb line ratios	10%	Fe XXV Ka	6.70	resonance	Code: ion fractions	5%					
								Fe XXVI Ka	6.96		Code: ion fractions	5%					
								Fe XXVI Kb	8.25		Code: ion fractions	5%					
50	AGN Winds	Measure the variability of ultra-fast outflows through the fraction of observations with UFOs or changes in column density	Column density	<1e21 cm^2	(PIE + disk wind)	Fe XXV, Fe XXVI EW	<1e21 cm^2	Fe XXV Ka	6.70	resonance	transition energy	1 eV				B	
								Fe XXVI Ka	6.96		transition energy	1 eV					
								Lower energy H-like lines (which lines??)			transition energy	3 eV					
51	AGN Winds	Measure the velocity and EW of Compton-thick obscurers/outflows to determine the kinetic luminosity	Line-of-sight velocity	300 km/s	(PIE + disk wind)	Fe XXVI Ka, Kb, K-edge energies, line profile (width + fitting for	5 eV	Fe XXVI Ka	6.96		transition energy	3 eV				B	outflows are detected closer to 9 keV
								Fe XXVI Kb	8.25		transition energy	3 eV					
								Fe-K edge	7.10		transition energy	3 eV					
			Column density	10%	PIE + disk wind	Fe XXVI Ka, Kb, K-edge depth	10%	Fe XXVI Ka	6.96		oscillator strength	5%					
								Fe XXVI Kb	8.25		oscillator strength	5%					
52	AGN Reflection	**Measure the density, size, and mean bulk motion with respect to the observer of the torus from type 2 AGN**	Mean motion	50 km/s	Reflection + Comptonization + fluorescent yields	Fe I + (not-so-)near-neutral Ka centroid	50 km/s	Fe I-XVI Ka	6.40		transition energy	0.5-1 eV				A	
								Fe I-XVI Ka	6.40		fluorescent yields	10% relative to that of Fe Kb					To use Ka/Kb flux ratio to constrain ionization state
			Size	10%	PIE	Fe Ka line width (or distance between line splits)	50 km/s	Fe I-XVI Ka	6.40		transition energy	10%					the basic science case is laid out in both AGN reflection and broadband spectroscopy (NGC 4945)
			n_e	10%	(PIE) G ratio R ratio kinetics	Temperature and density from Fe XXV Ka line ratios (+other He-like triplets)	Ratios to 10%	Fe XXV Ka	6.70	resonance	emissivity	10%					0.5 eV energy precision for lower energy triplets (based on Mrk 3 case)
								Fe XXV Ka	6.68	intercombination	emissivity	10%					
53	AGN Reflection	Measure the size/shape of the Compton shoulder around Fe I (+near-neutrals) Ka to determine the physical parameters of the torus	Torus covering fraction and column density	30%	MCRT, different Fe compounds	Fitting shoulder shape to look for multiple scattering, atomic vs. molecular iron, and measure the scattering angle	10% in CS fraction	All blends	6.30		transition energy	2 eV				B	**what lines are these? There aren't many!**
								All blends	6.30		emissivity	25%					
								Fe I Ka Compton shoulder	6.30		Code: Compton shoulder shape for different incident angle, composition	10% in CS fraction					
								Fe I (+near neutral) Ka	6.40		fluorescent yields	??					
54	AGN Reflection	Isolate reflection from the inner regions of type 1 AGNs by simultaneously modeling the disk reflection and soft excess	Reflection component flux, disk ionization state, emissivity/irradiation	20%	**Reflection, Comptonization, Warm Absorber.**	Broad Fe Ka line profile shape	20%?	Fe I (+near neutral) Ka	6.40		transition energy	2 eV				C	
								Fe I (+near neutral) Ka	6.40		fluorescent yields	??					
55	Clusters	Map velocity fields in clusters to measure turbulence, identify sloshing motion, etc.	Line-of sight velocity	30 km/s	(Collisional plasma)	Centroid shifts in Fe XXV Ka, Fe XVII	0.5 eV	Fe XXV Ka	6.70	resonance	transition energy	1 eV				A	most of below is based on ASTRO-H WP, not Hitomi Perseus papers...



Topic	Science Goal	Physical quantity	Required Precision	Spectral Models	Spectral Measurement	Required Precision	Line or feature	Approximate energy (keV)	Specific line	Requirement on...	Required ac	References	Current best measurement
ISM and CGM	Measure the dust composition from absorption edges towards LMXBs in outburst with NH > 1e22 cm^-2	Dust chemical composition	~10%	Dust structure/ISM absorption model	Location, depth of Si K edge	10%	Si-K edge	1.84		transition energy	<2 eV		0.2 eV
							Si-K edge	1.84		absorption depth	10%		
					Location, depth of Fe K edge	15-20%	Fe-K edge	7.10		transition energy	<3eV		0.04 eV
							Fe-K edge	7.10		absorption depth	10%		
					Detect edges for less abundant elements	10-20%	Edges for e.g. S, Ca	2.47, 4.03		transition energy	<2 eV for S, <3 eV for Ca		0.05 eV



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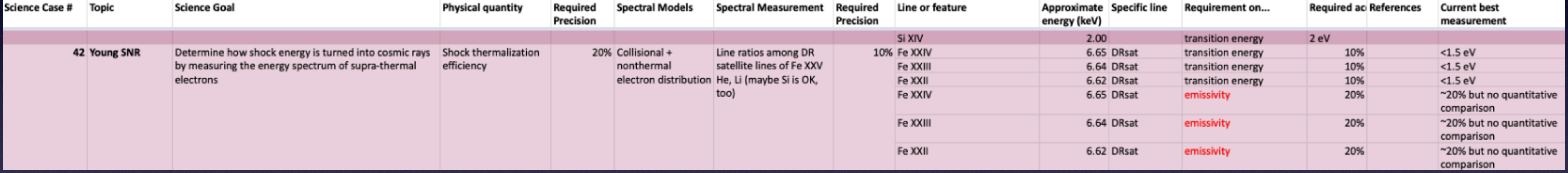

Science Case #	Topic	Science Goal	Physical quantity	Required Precision	Spectral Models	Spectral Measurement	Required Precision	Line or feature	Approximate energy (keV)	Specific line	Requirement on...	Required ac	References	Current best measurement
								Si XIV	2.00		transition energy	2 eV		
42	**Young SNR**	Determine how shock energy is turned into cosmic rays by measuring the energy spectrum of supra-thermal electrons	Shock thermalization efficiency	20%	Collisional + nonthermal electron distribution	Line ratios among DR satellite lines of Fe XXV He, Li (maybe Si is OK, too)	10%	Fe XXIV	6.65	DRsat	transition energy	10%		<1.5 eV
								Fe XXIII	6.64	DRsat	transition energy	10%		<1.5 eV
								Fe XXII	6.62	DRsat	transition energy	10%		<1.5 eV
								Fe XXIV	6.65	DRsat	emissivity	20%		~20% but no quantitative comparison
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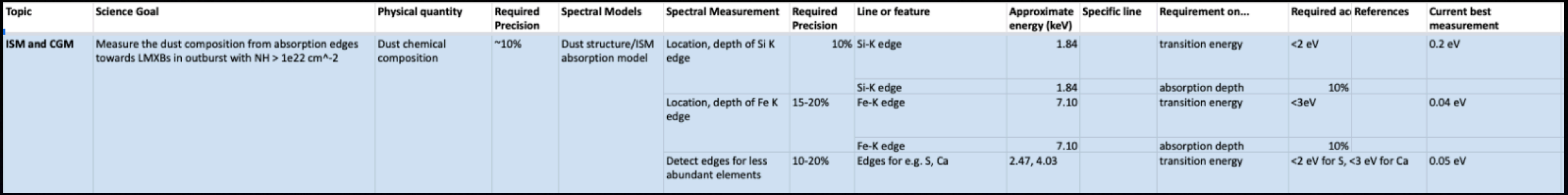

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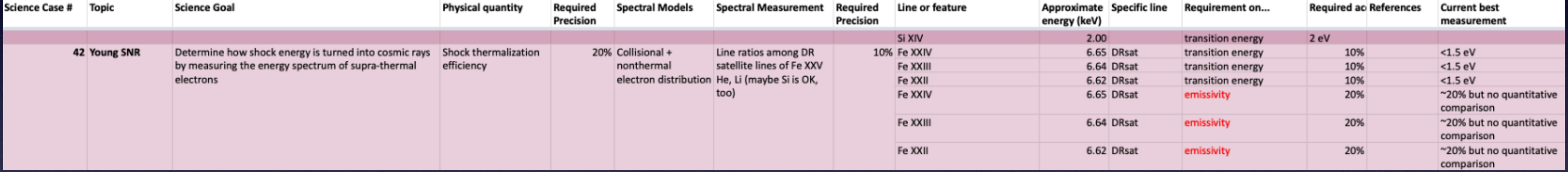

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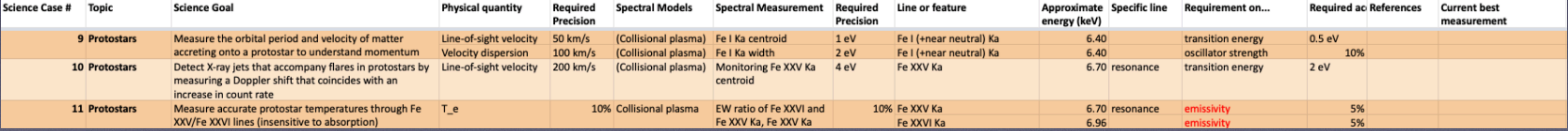

Science Case #	Topic	Science Goal	Physical quantity	Required Precision	Spectral Models	Spectral Measurement	Required Precision	Line or feature	Approximate energy (keV)	Specific line	Requirement on...	Required ac	References	Current best measurement
9	**Protostars**	Measure the orbital period and velocity of matter accreting onto a protostar to understand momentum	Line-of-sight velocity	50 km/s	(Collisional plasma)	Fe I Ka centroid	1 eV	Fe I (+near neutral) Ka	6.40		transition energy	0.5 eV		
			Velocity dispersion	100 km/s	(Collisional plasma)	Fe I Ka width	2 eV	Fe I (+near neutral) Ka	6.40		oscillator strength	10%		
10	**Protostars**	Detect X-ray jets that accompany flares in protostars by measuring a Doppler shift that coincides with an increase in count rate	Line-of-sight velocity	200 km/s	(Collisional plasma)	Monitoring Fe XXV Ka centroid	4 eV	Fe XXV Ka	6.70	resonance	transition energy	2 eV		
11	**Protostars**	Measure accurate protostar temperatures through Fe XXV/Fe XXVI lines (insensitive to absorption)	T_e	10%	Collisional plasma	EW ratio of Fe XXVI and Fe XXV Ka, Fe XXV Ka	10%	Fe XXV Ka	6.70	resonance	emissivity	5%		
								Fe XXVI Ka	6.96		emissivity	5%		

Lab Astro WG just (on July 10th) submitted two companion white papers to Astro2020 Decadal Survey

“Laboratory Astrophysics Needs for X-ray Calorimeter Observatories”
Lead author: Tim Kallman; focus: science above 2 keV

“Laboratory Astrophysics Needs for X-ray Grating Spectrometers”
Lead author: Randall Smith; focus: science below 2 keV

(US-based) Conclusions: Current lab astro funding comes form NASA APRA program. Supports ~25 programs per year (for three years each). We propose a modest increase in funding of $1.5M/year. This will support ~4 lab groups ($250K/year) using existing facilities, as well as place one new EBIT at a light source ($2M). Also support ~5 grad students or postdocs doing theoretical work