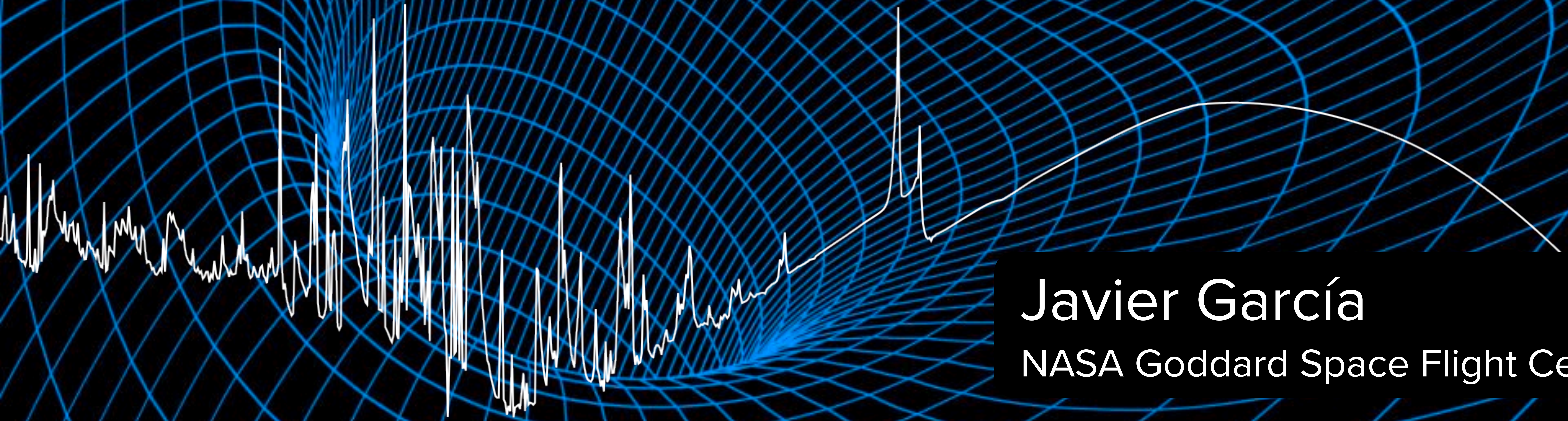
Atomic Physics: Issues, Diagnostics, and Uncertainties



Javier García

NASA Goddard Space Flight Center

Second XRISM Community Workshop

UMD—Jan 19, 2024

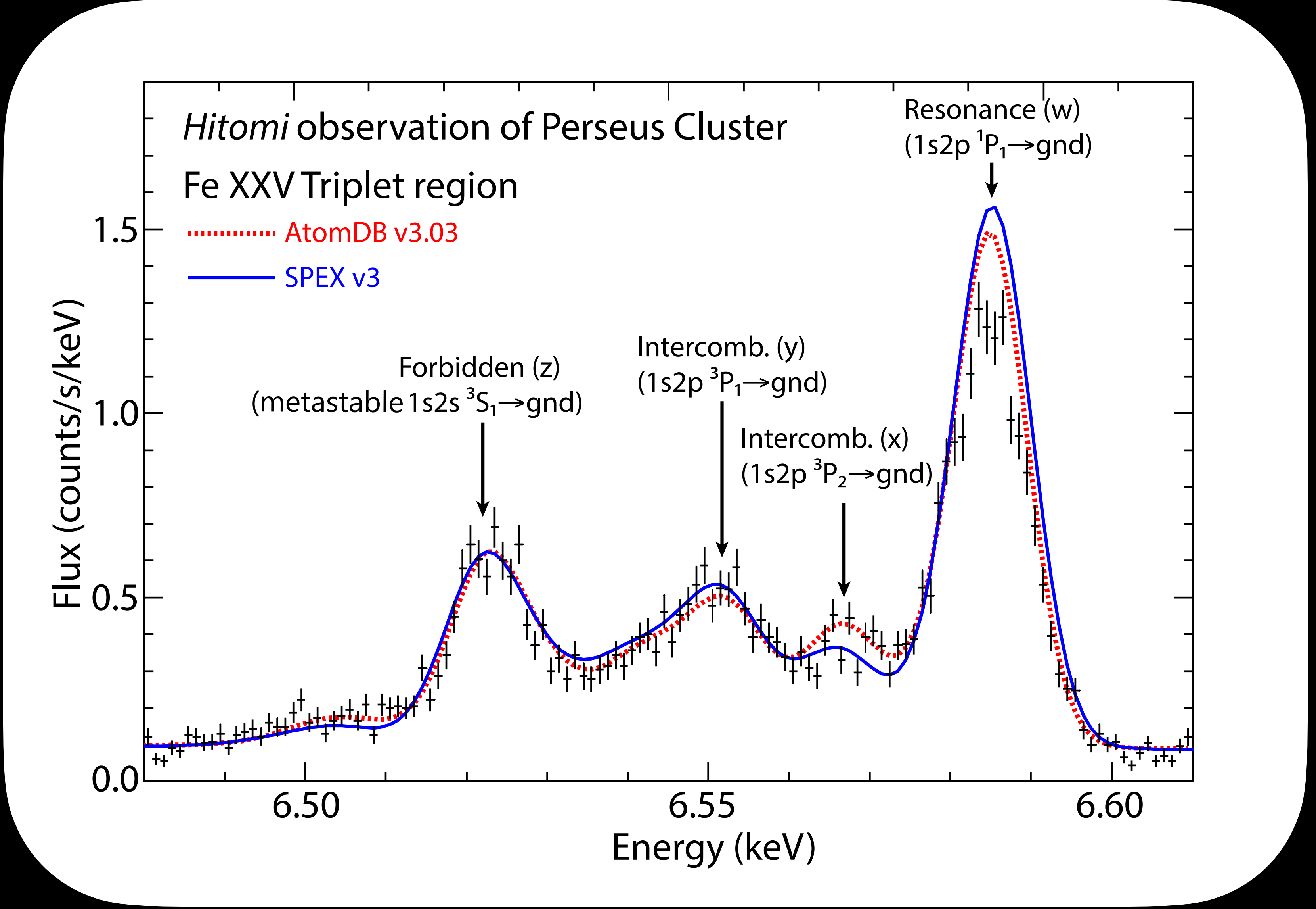
*With inputs and slides from Ralf Ballhausen and others

On the relevance of Lab Astro (X-rays)

Fundamental quantities are not married to any particular mission, but have long term applicability to a large number of problems

Astro 2020 Decadal White Papers:
Betancourt-Martinez+21, Kallman+21, Smith+21

Funding increase for both experiments and computational atomic physics



Training new generation of Lab Astro scientists

Upcoming missions will impose strong and immediate requirements for updated parameters and models

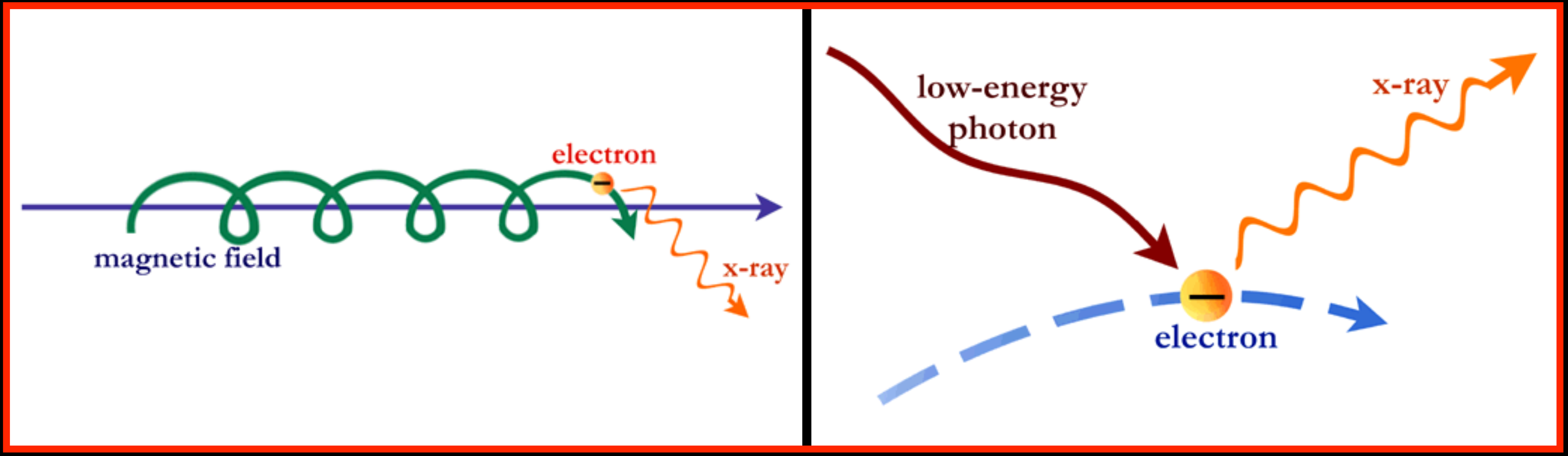
XRISM, IXPE, eXTP, Athena, Lynx, LEM, Arcus, HEX-P, StrobeX

X-ray Emission Mechanisms

Continuum

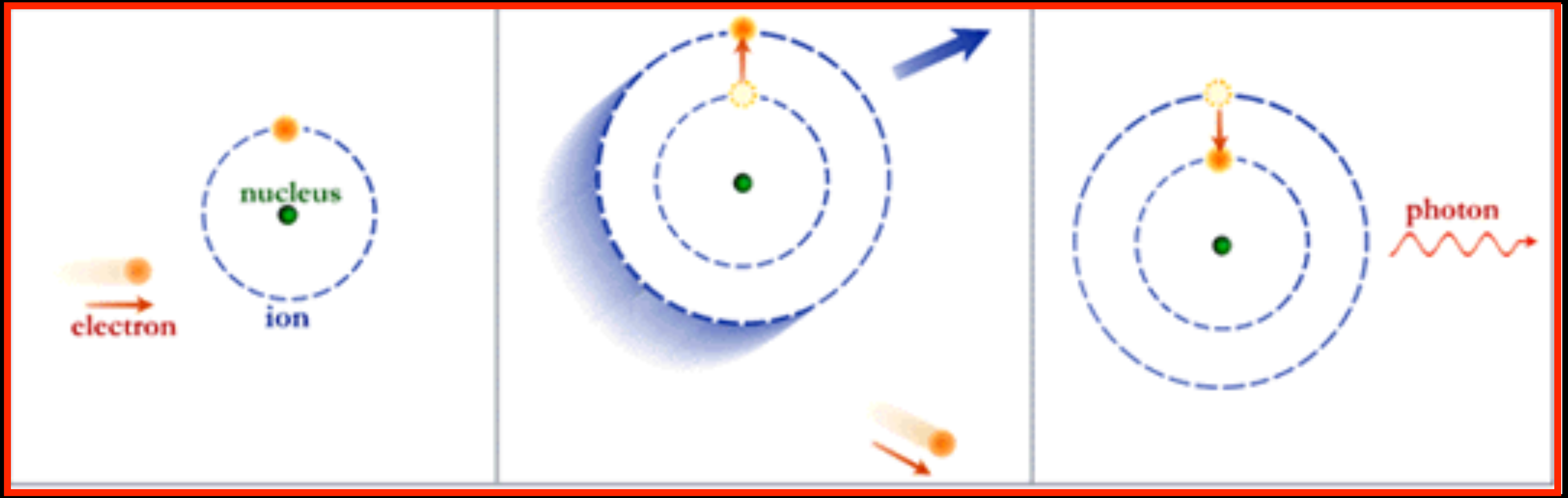
Black-Body
Bremsstrahlung (free-free)

Cyclotron & Synchrotron
Inverse Compton Scattering



Lines

Bound-Bound
Fluorescence
Charge Exchange
Cyclotron
Exotic Physics (?)



X-ray Emission Mechanisms

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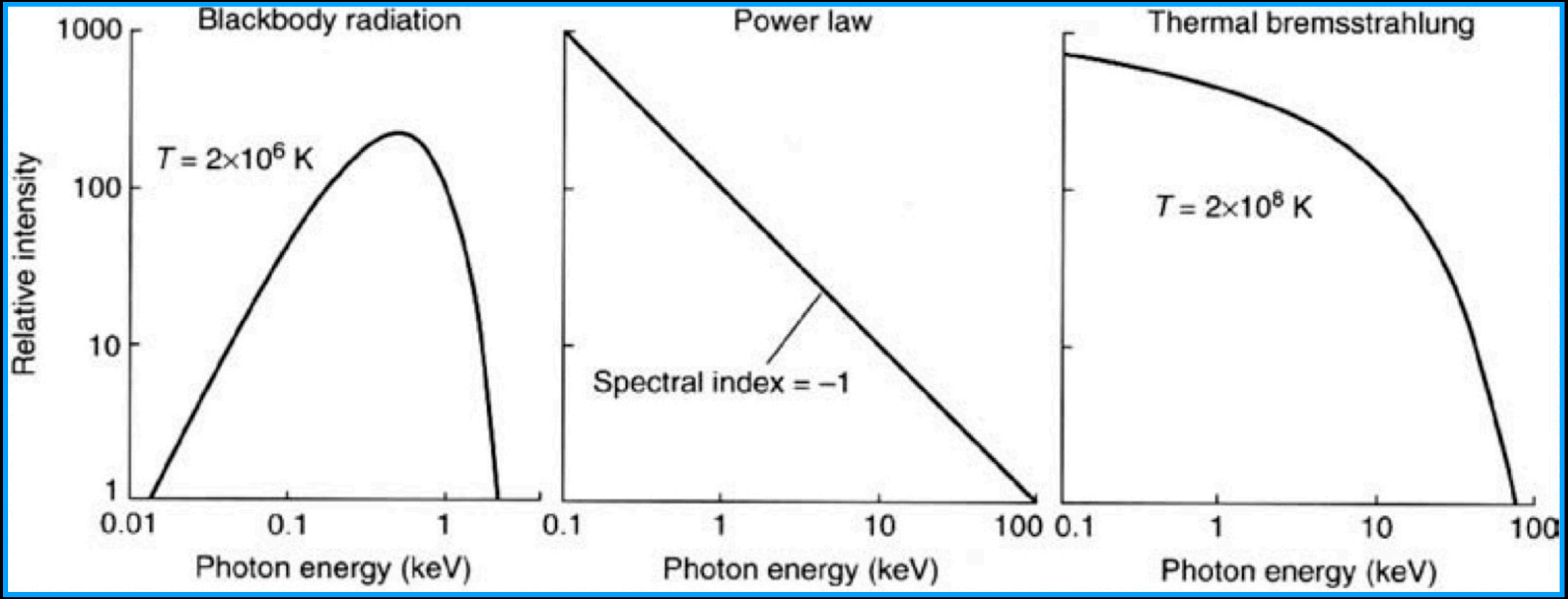
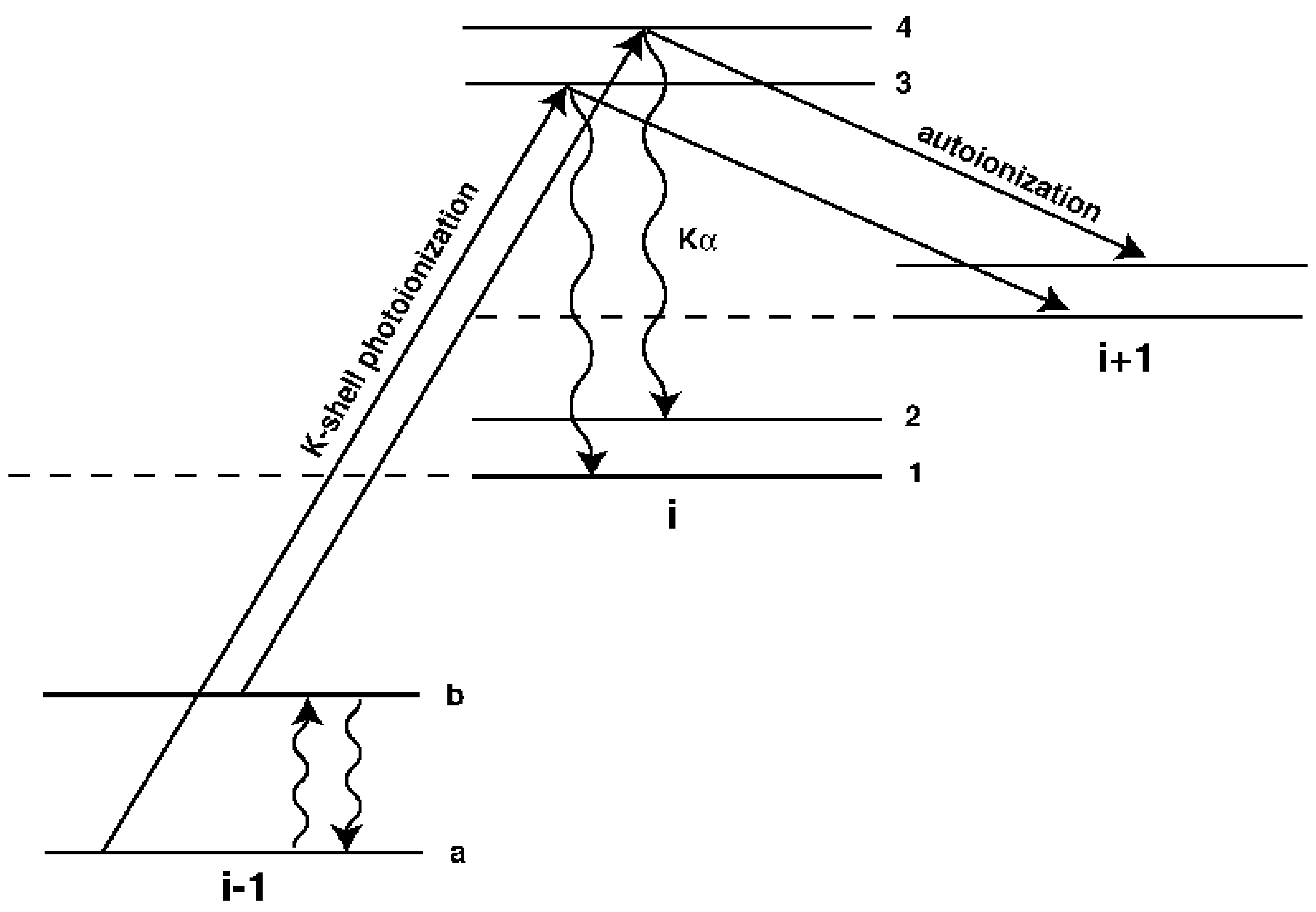


X-ray Emission Mechanisms

Lines

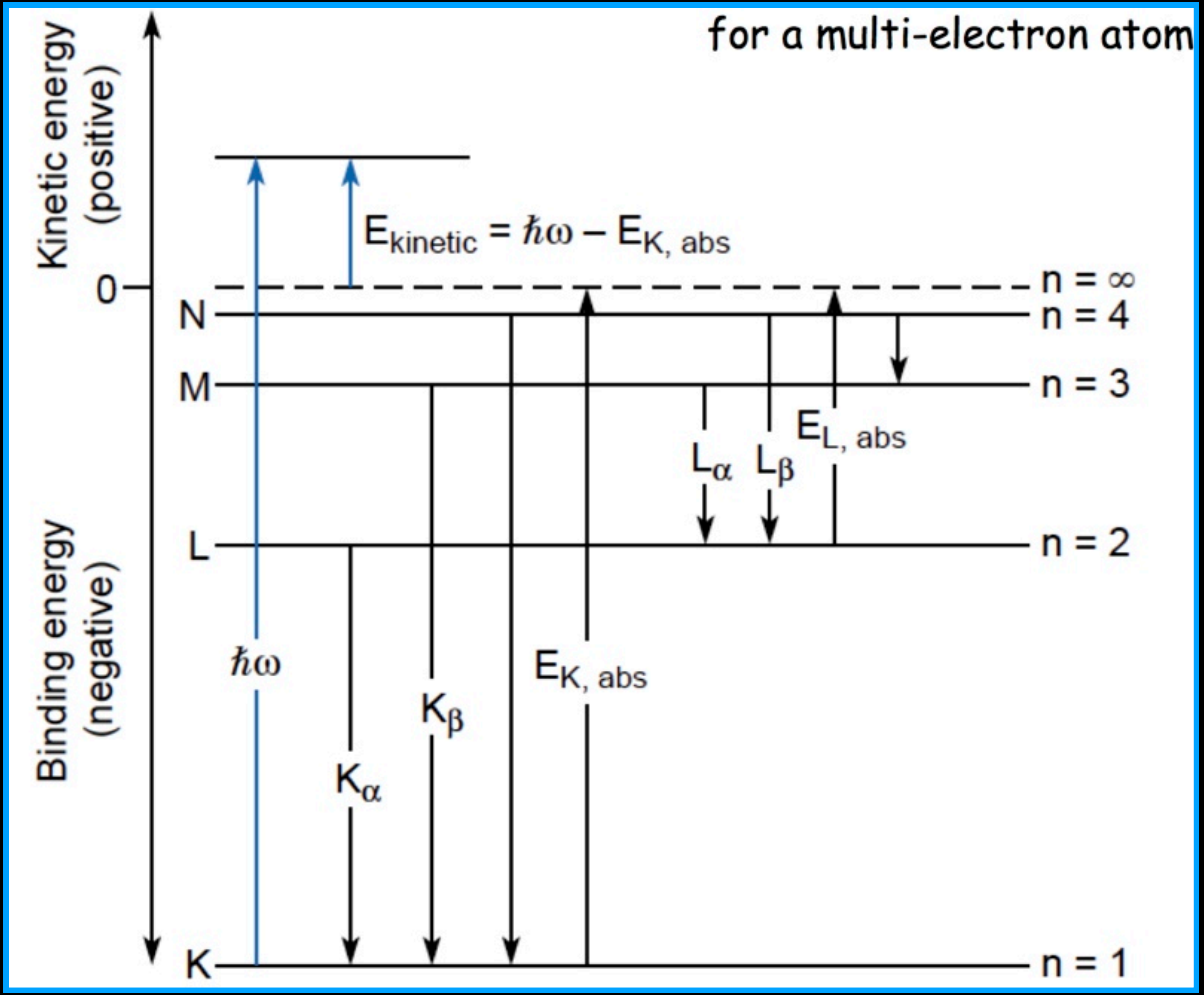


Liedahl+Torres05

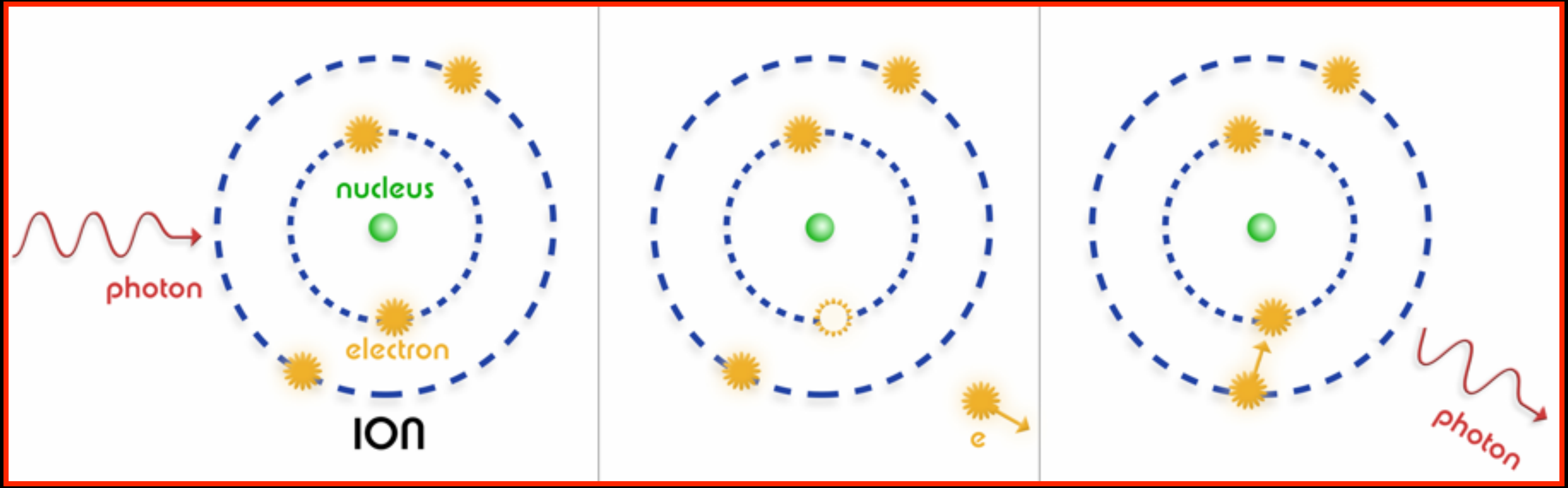
The X-ray band ($\sim$ 0.1 – 10 keV) covers the emission and absorption produced by the inner-shell transitions of the astrophysically abundant ions (C $\rightarrow$ Ni).

- **Line positions** provide information about the gas composition (identification), as well as about its dynamics (redshifts, gas outflows)
- **Line intensities** provide information about the column of the absorbing material (including ions), constrains on the ionization degree of the gas ($\xi = L/nR^2$), temperature and density
- **Line shapes** provide information about the thermal and turbulent motions of the gas, and can also probe relativistic effects near strong gravitational fields

X-ray Emission Lines



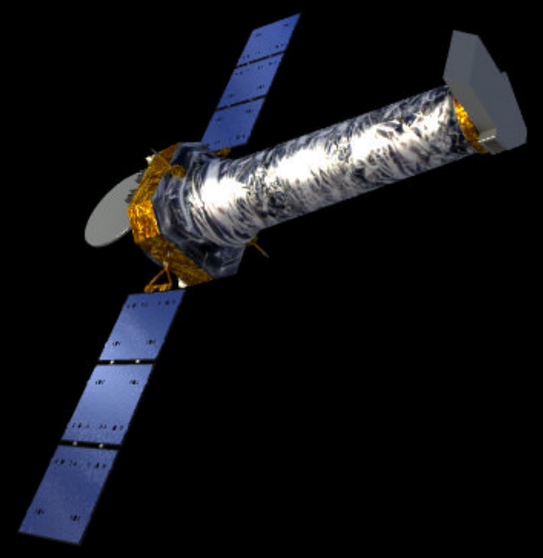
K-shell Fluorescence



- Needs L-shell electrons
- Photoionization, then either 2p → 1s radiative transition or Auger ionization
- Fluorescence yield ~ Z^4, appreciable for a high-Z element
- Such a process is an important contributor to iron K emission

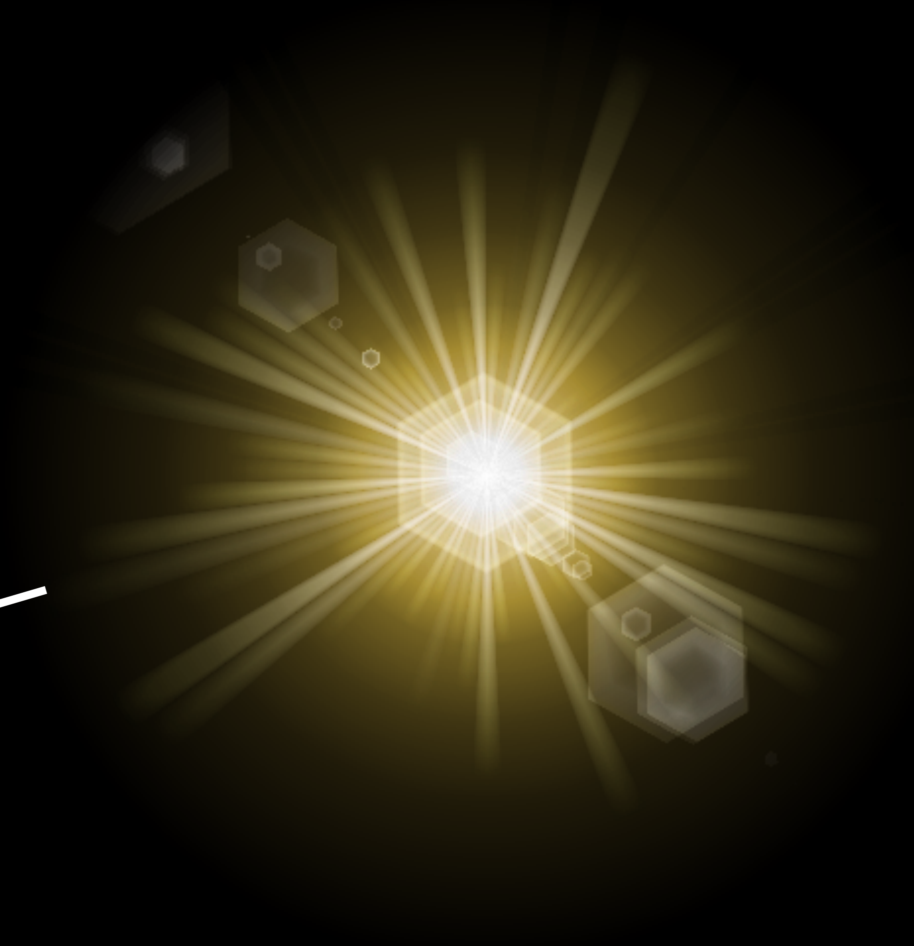
Astrophysical Plasmas

Collisional

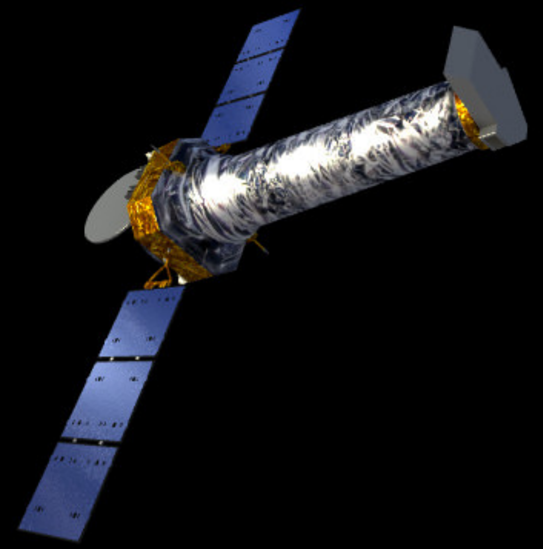


T, n, abundances

kT ~ Ionization energy of the ions in the plasma



Photoionized



n (or P), abundances

kT << Ionization energy of the ions in the plasma

T is not a free parameter!

Plasma Codes and Databases

Understanding a plasma requires a physical model. For these, a large number of atomic lines are needed (hundreds or more). Modern plasma codes have made of the hard work, compiling millions of transitions!

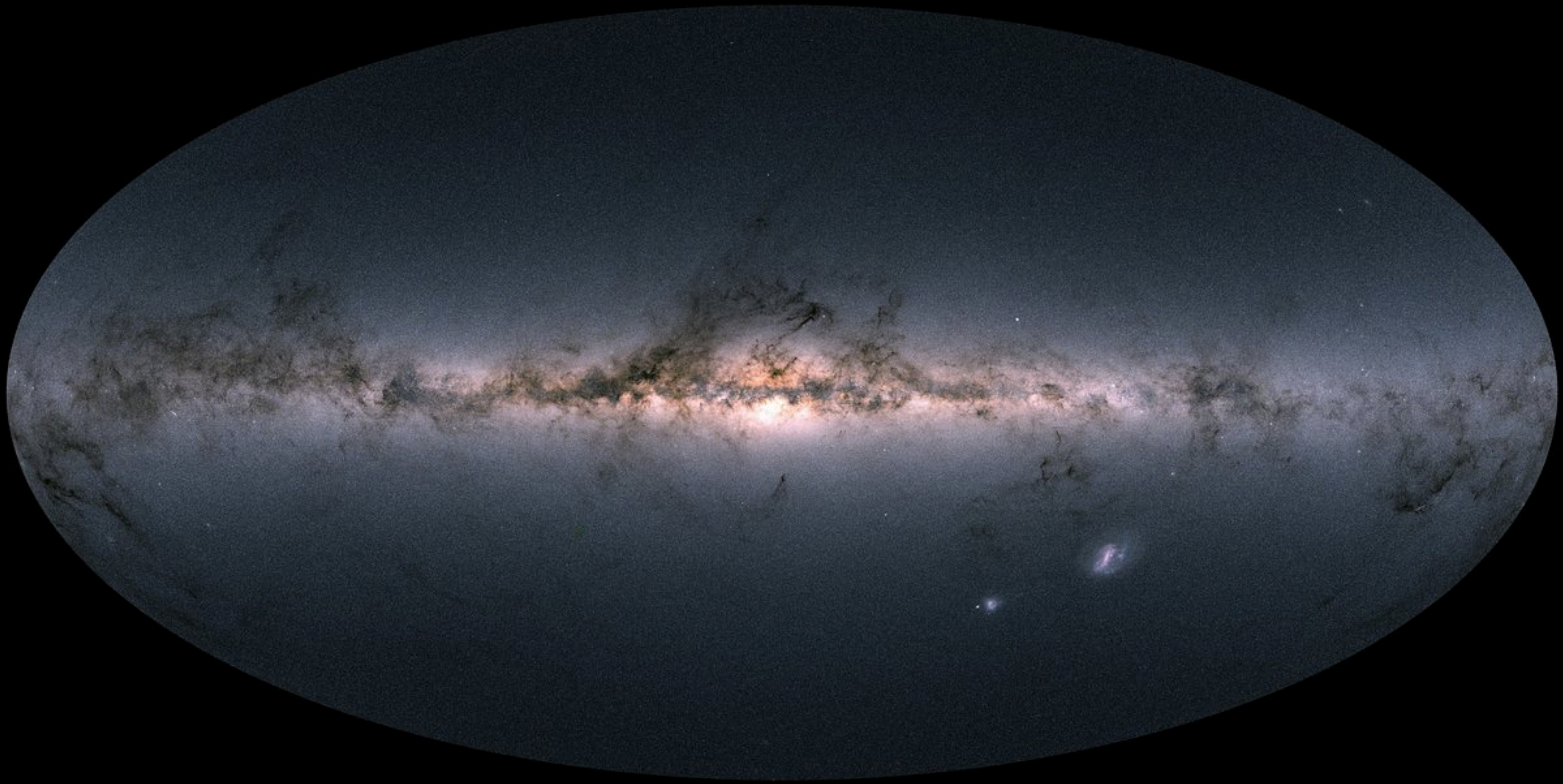
Collisional

SPEX/CIE	(Kaastra+03)	http://www.sron.nl/spex
Chianti	(Del Zanna+21)	http://chiantidatabase.org
AtomDB	(Foster+12)	http://atomdb.org

Photoionized

Cloudy	(Ferland+17)	http://www.nublado.org
XSTAR	(Kallman+Bautista01)	https://heasarc.gsfc.nasa.gov/xstar/xstar
SPEX/PIE	(Kaastra+03)	http://www.sron.nl/spex
Moccasin	(Ercolano+03)	https://mocassin.nebulousresearch.org
Titan	(Dumont+00)	??

The Interstellar Medium (ISM)



Credit: ESA/Gaia/DPAC, CC BY-SA 3.0 IGO

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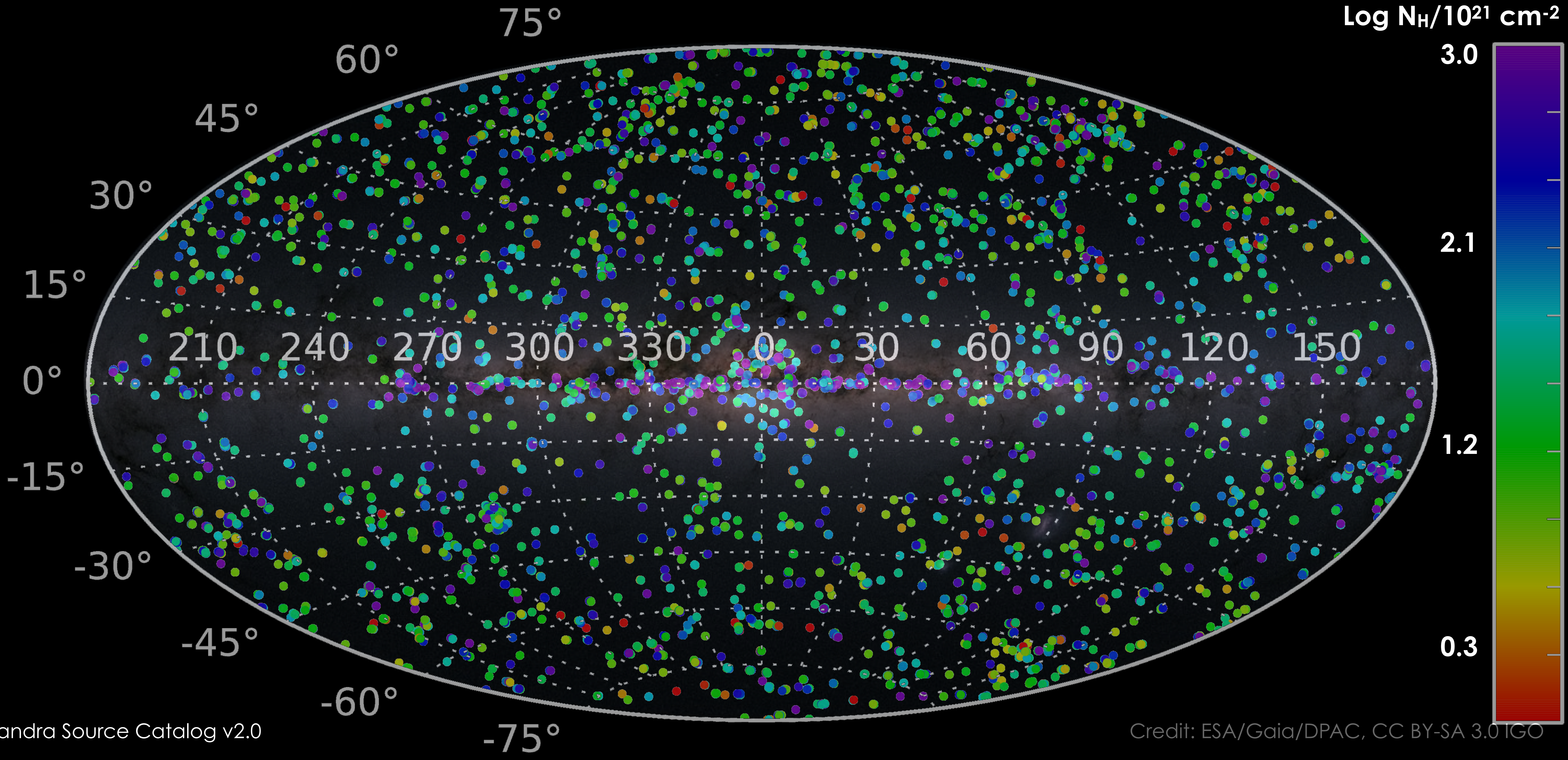


Chandra Source Catalog v2.0

Credit: ESA/Gaia/DPAC, CC BY-SA 3.0 IGO

Absorption in the ISM

Observations of absorption lines in the ISM are a driver for the improvement of atomic data and model accuracy.

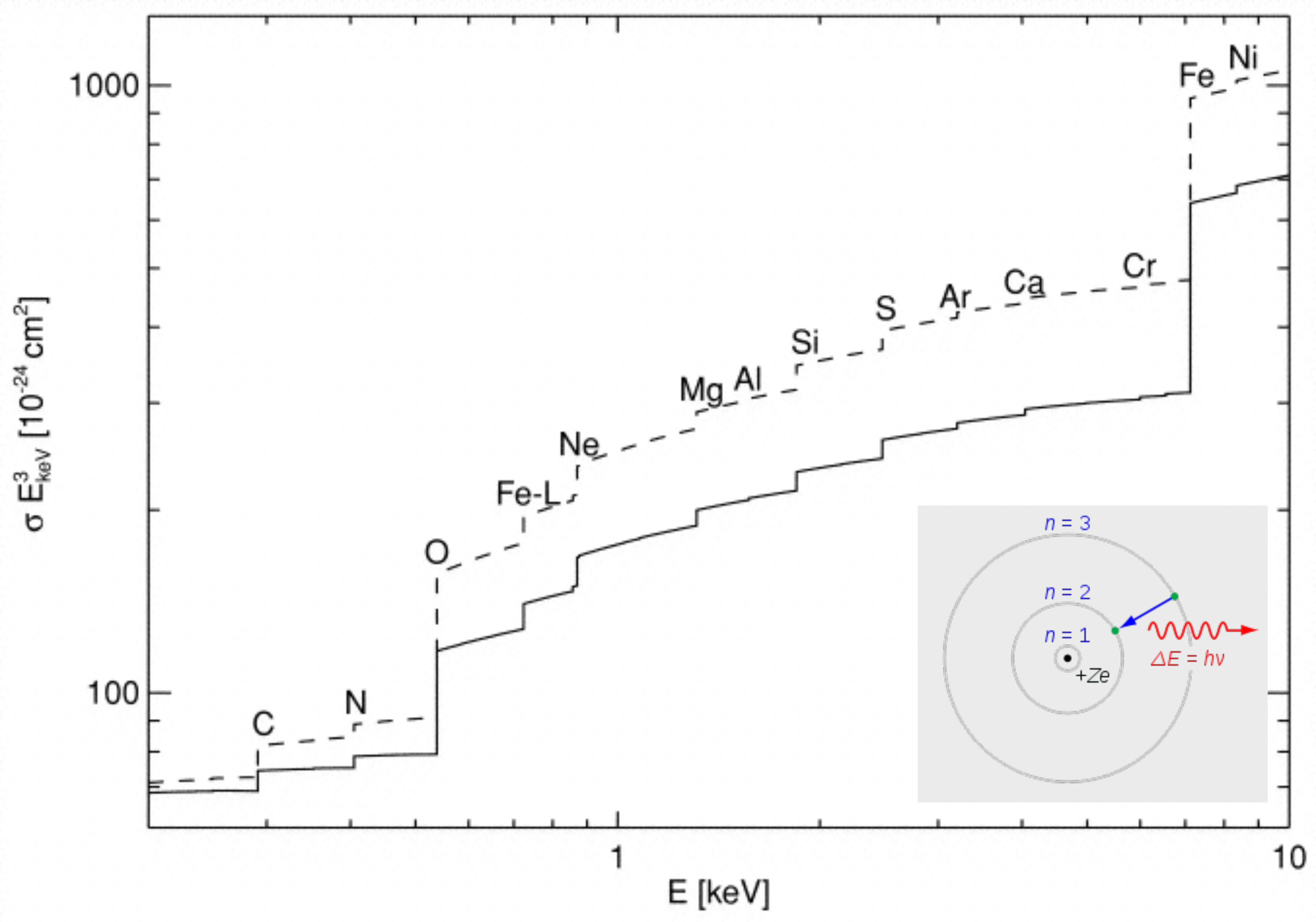
Simple absorption model:

$$F_{\mathrm{Obs}} = F_0 \, e^{-\tau(E)}$$

$$\tau(E) = \sum_i \sigma_i(E) \, N_i$$

$\tau(E)$: Total optical depth
$\sigma_i(E)$: Photoionization cross
N_i : Ion column density

Thus, the goal is to compute the photoionization cross section for all ions



Wilms et al. (2000)

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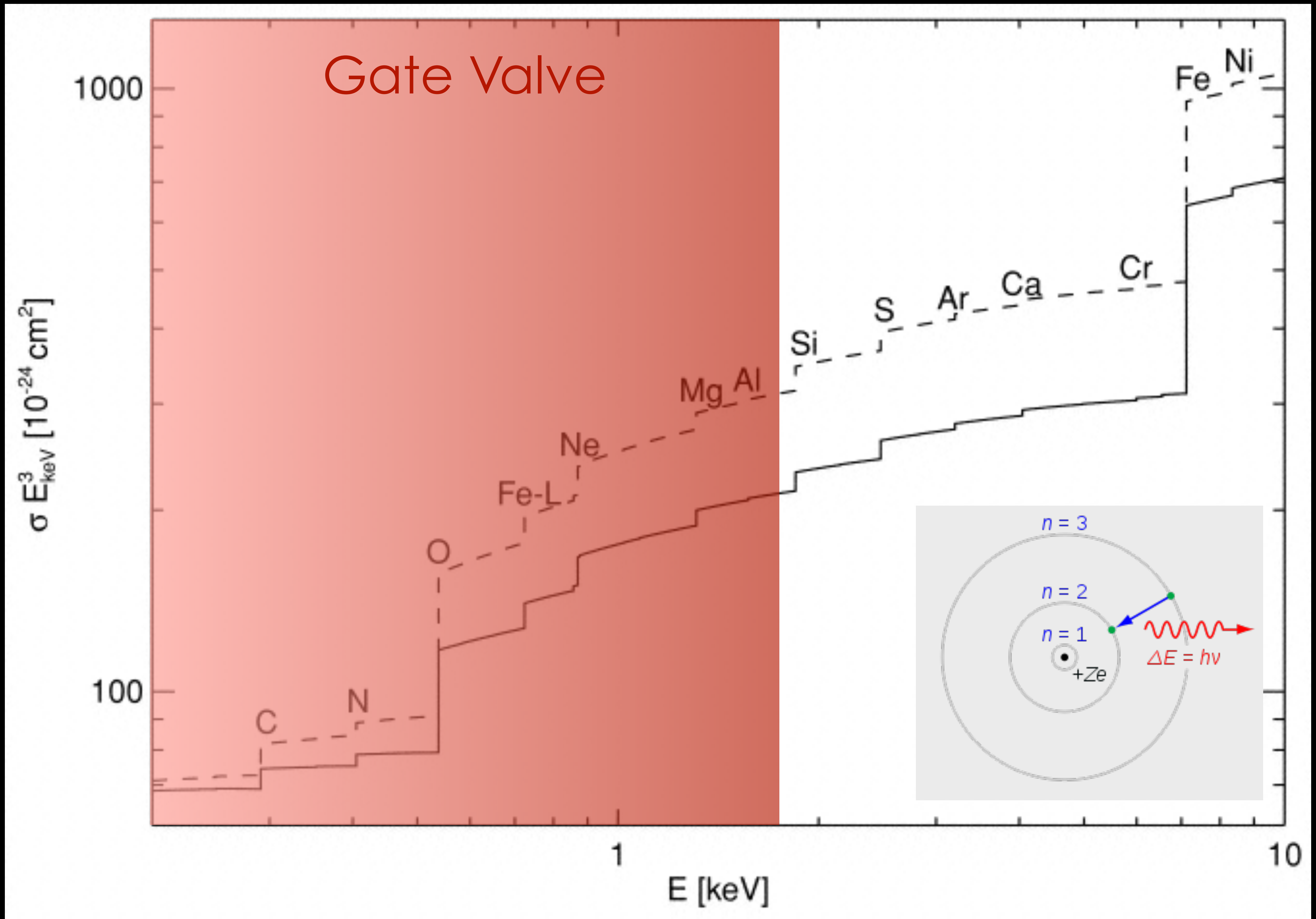

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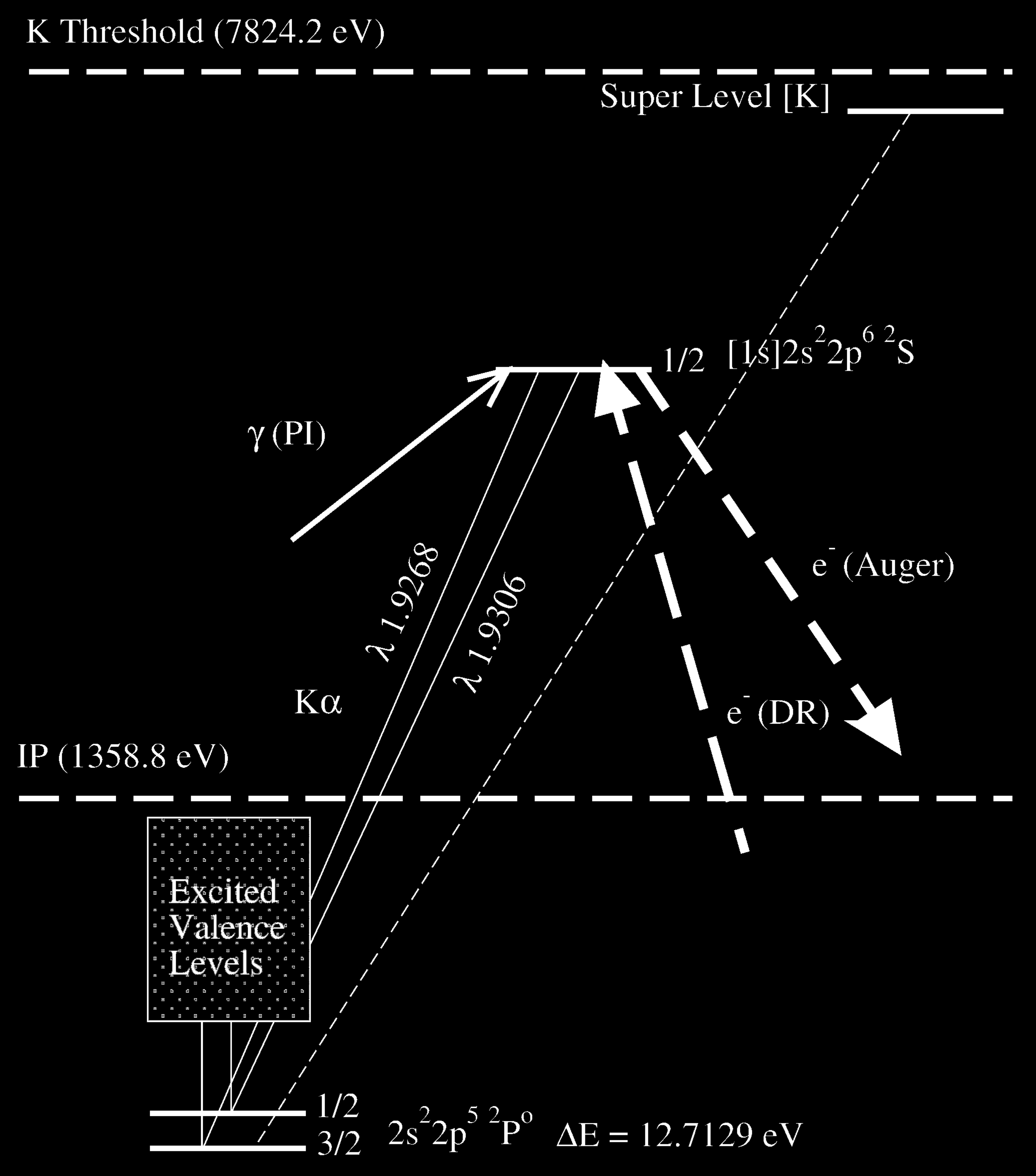
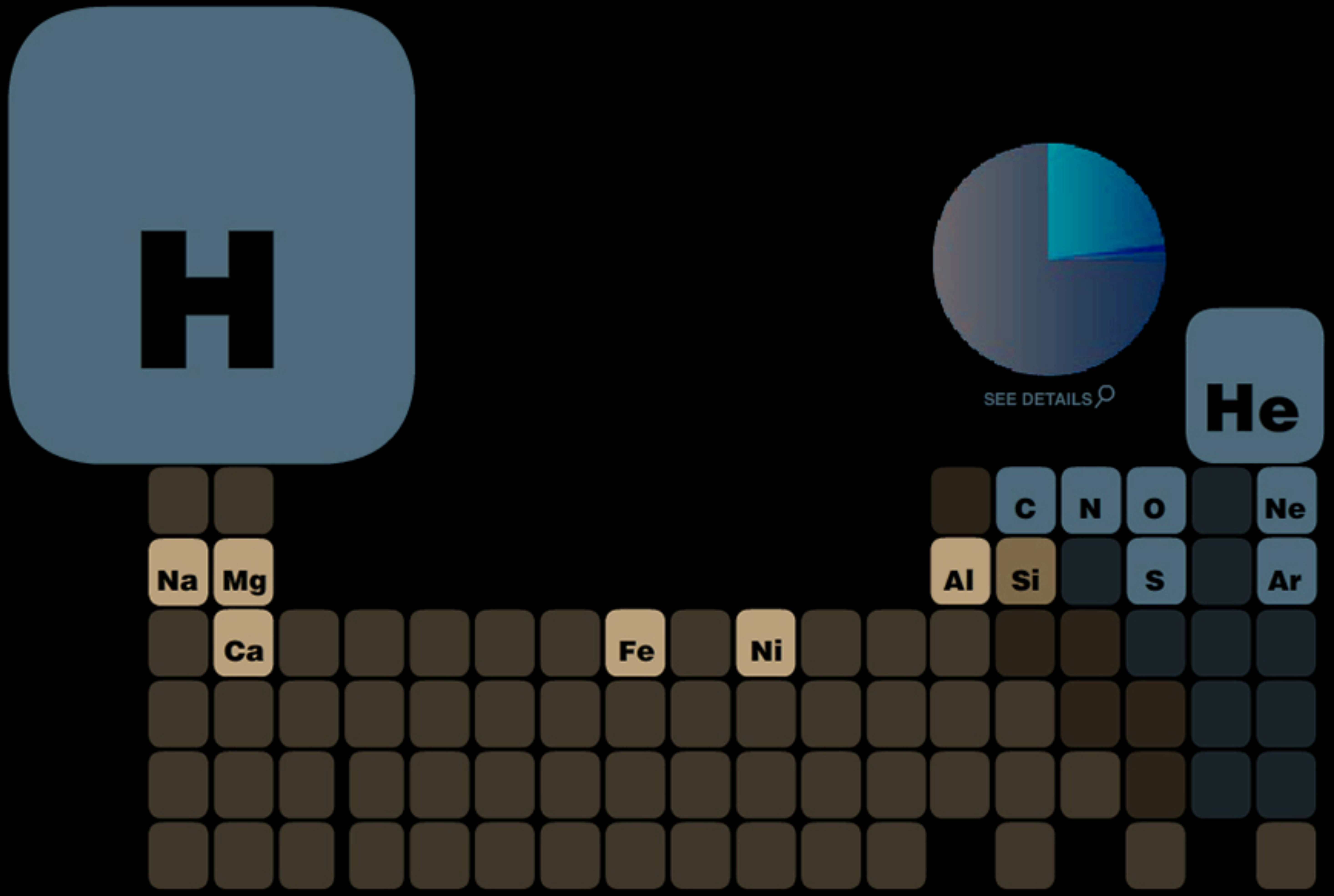
Inner-shell Photo-Ionization





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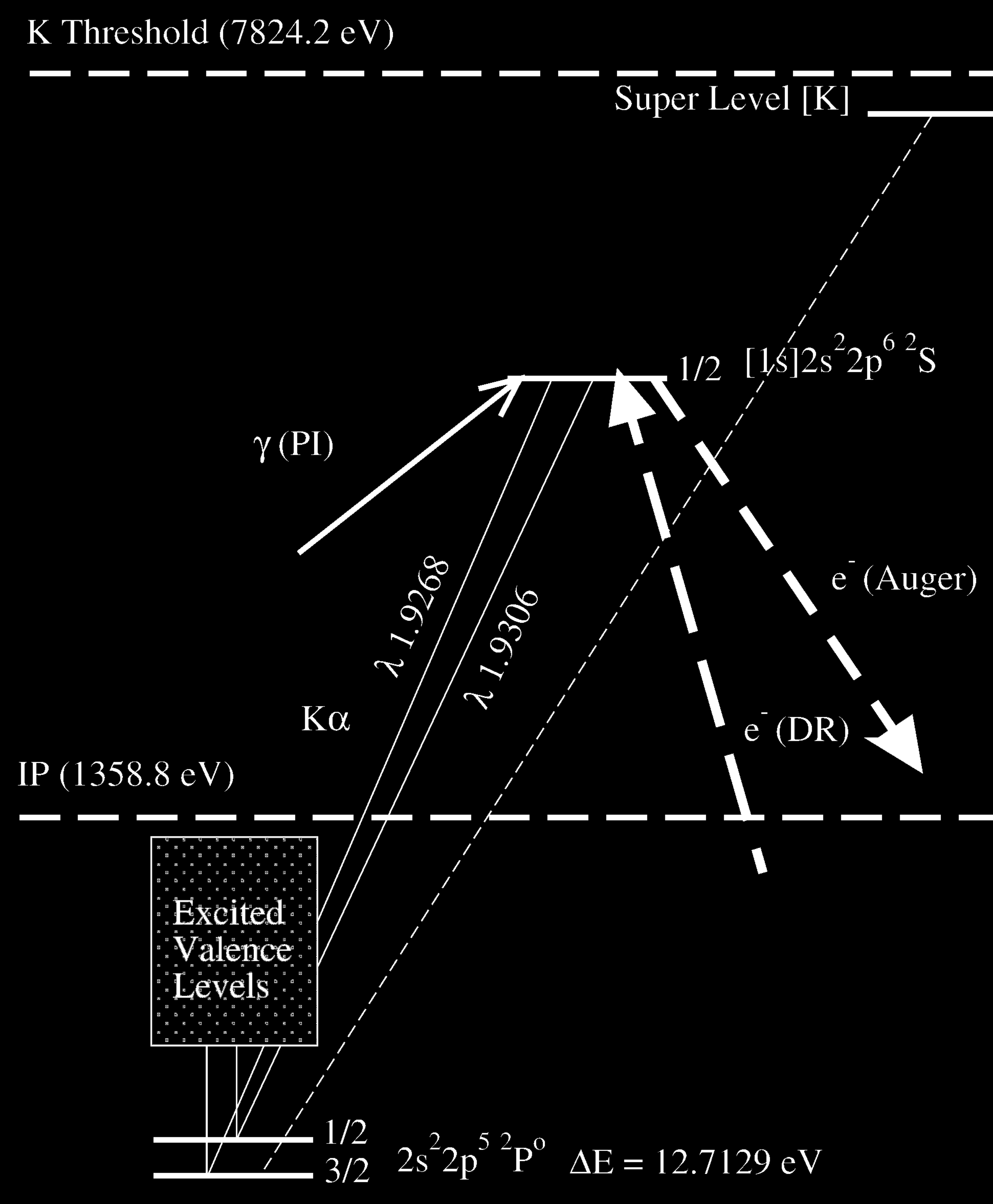

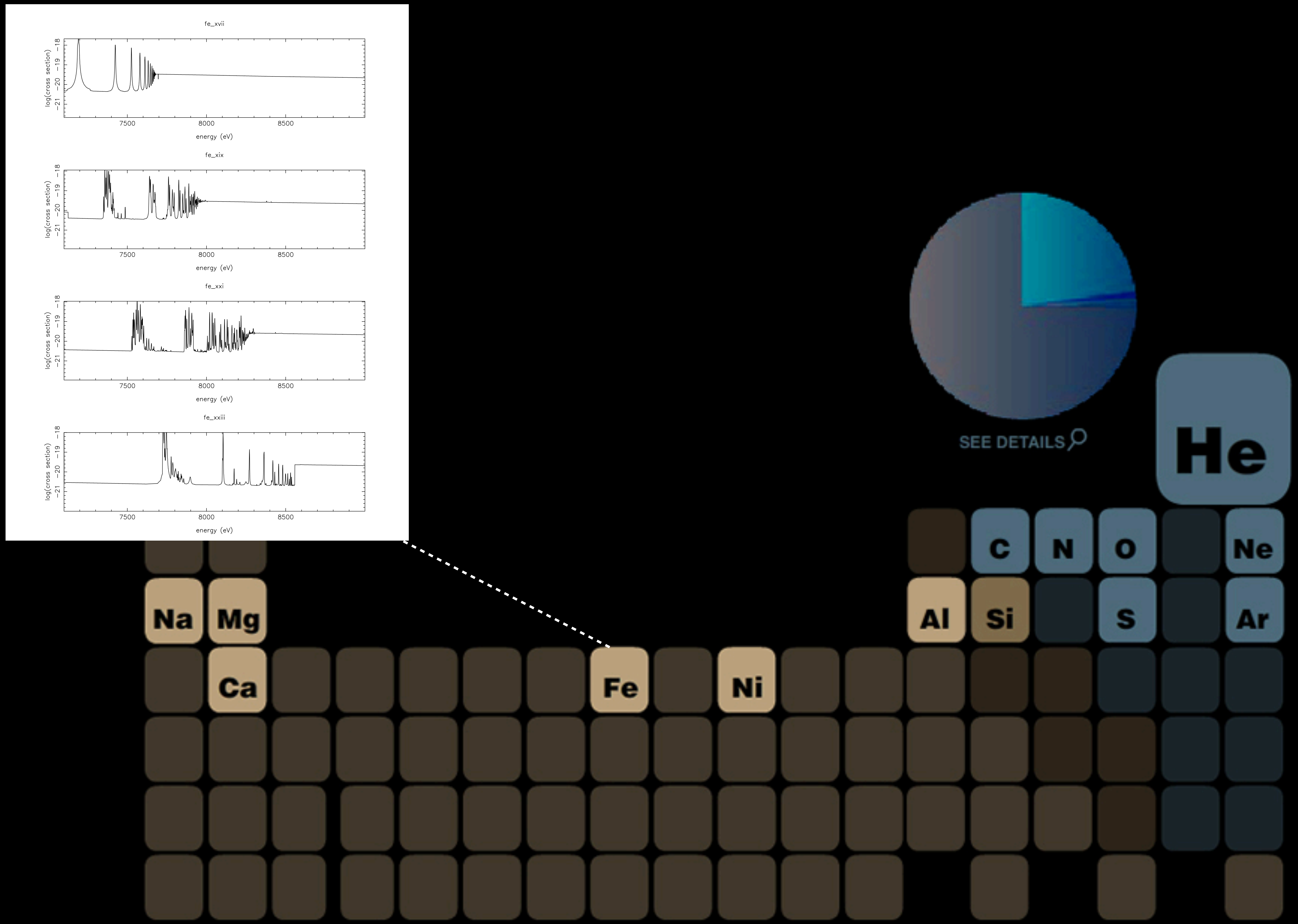

Palmeri+02; Bautista+03; Palmeri+03a,b; Mendoza+04; Kallman+04

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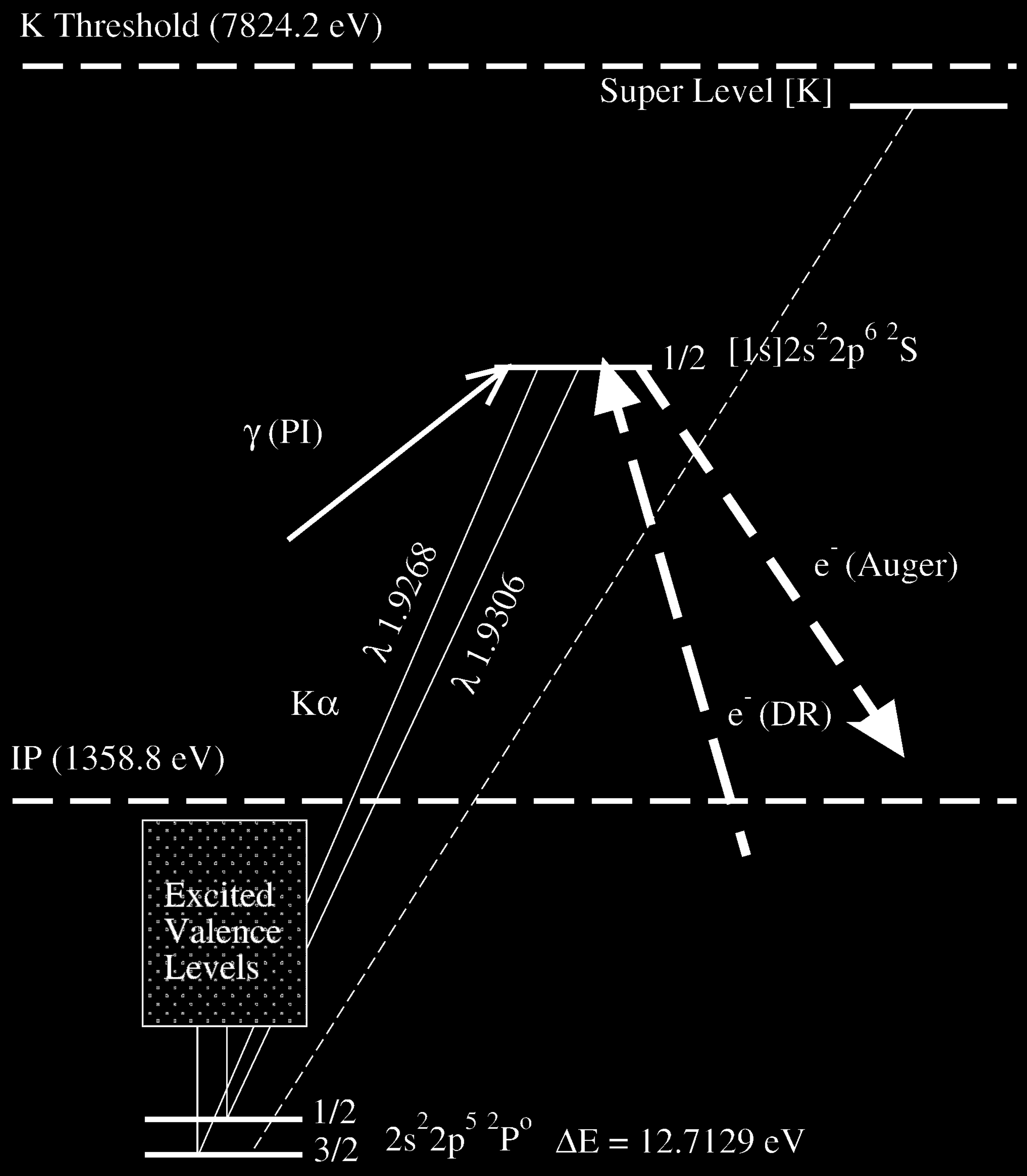

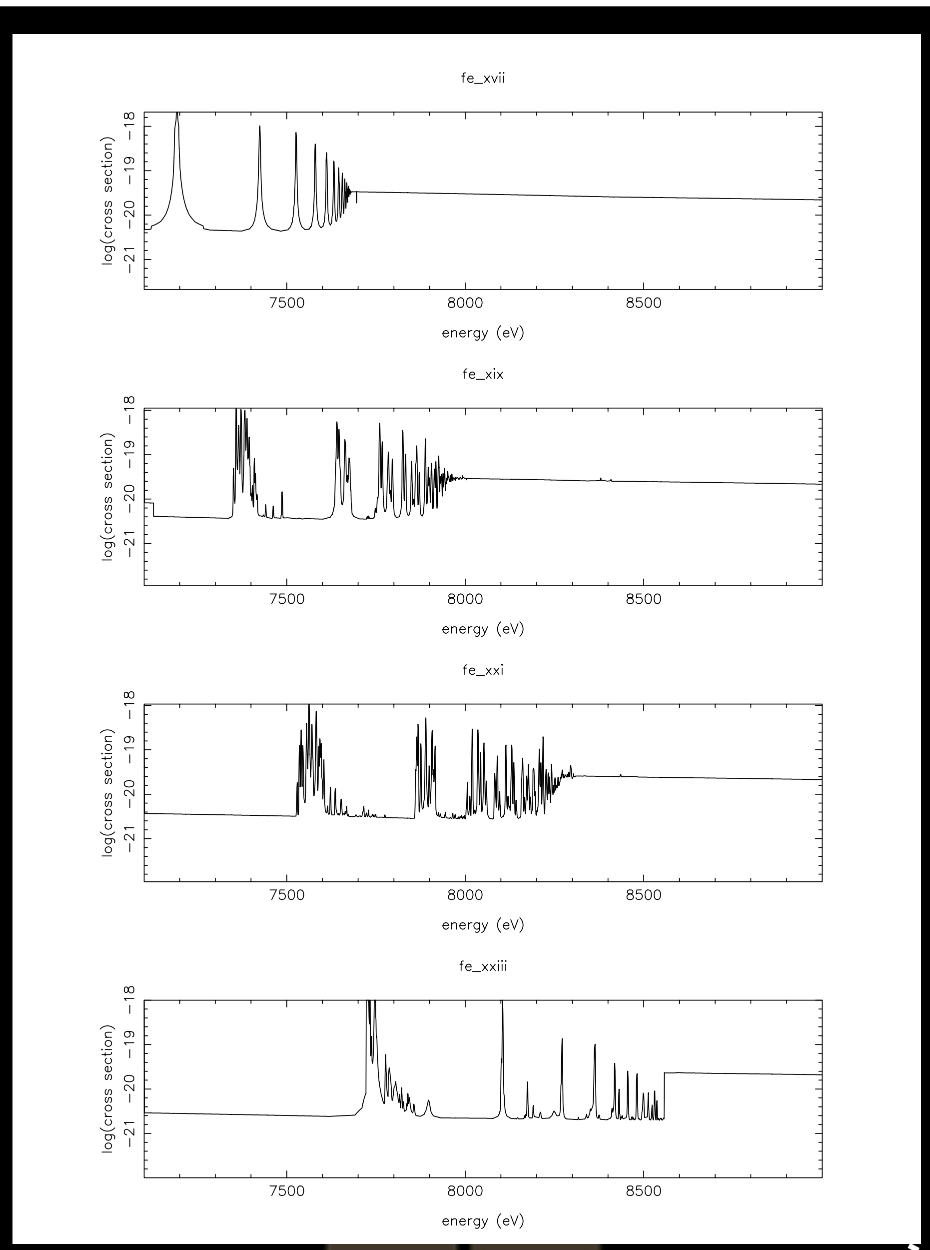

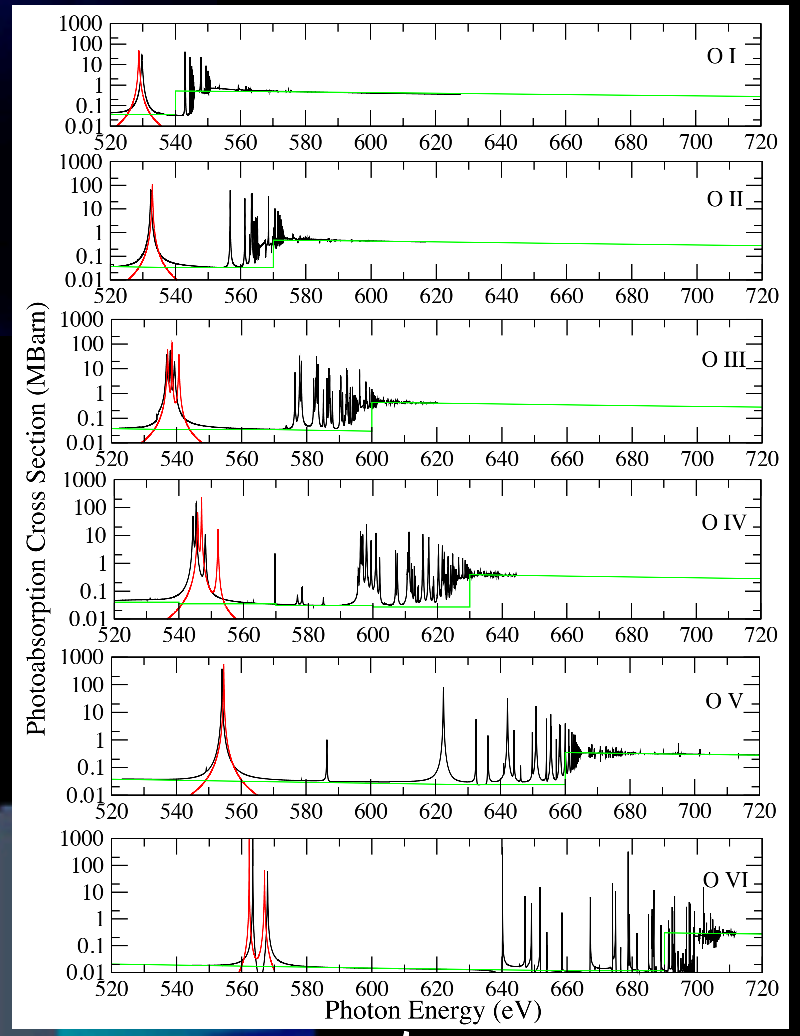

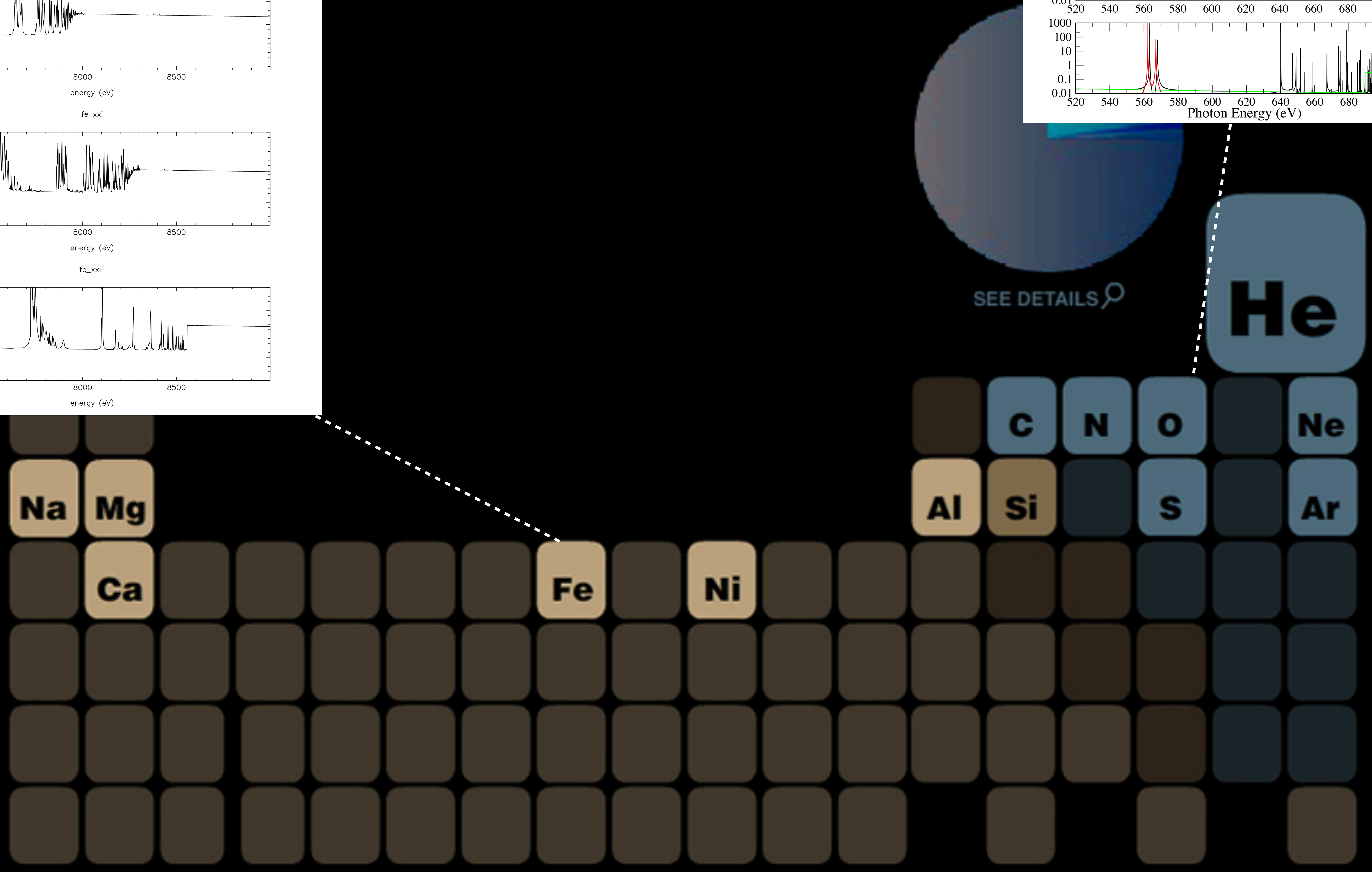

Palmeri+02; Bautista+03; Palmeri+03a,b; Mendoza+04; Kallman+04

García+05; Gorczyca+13;

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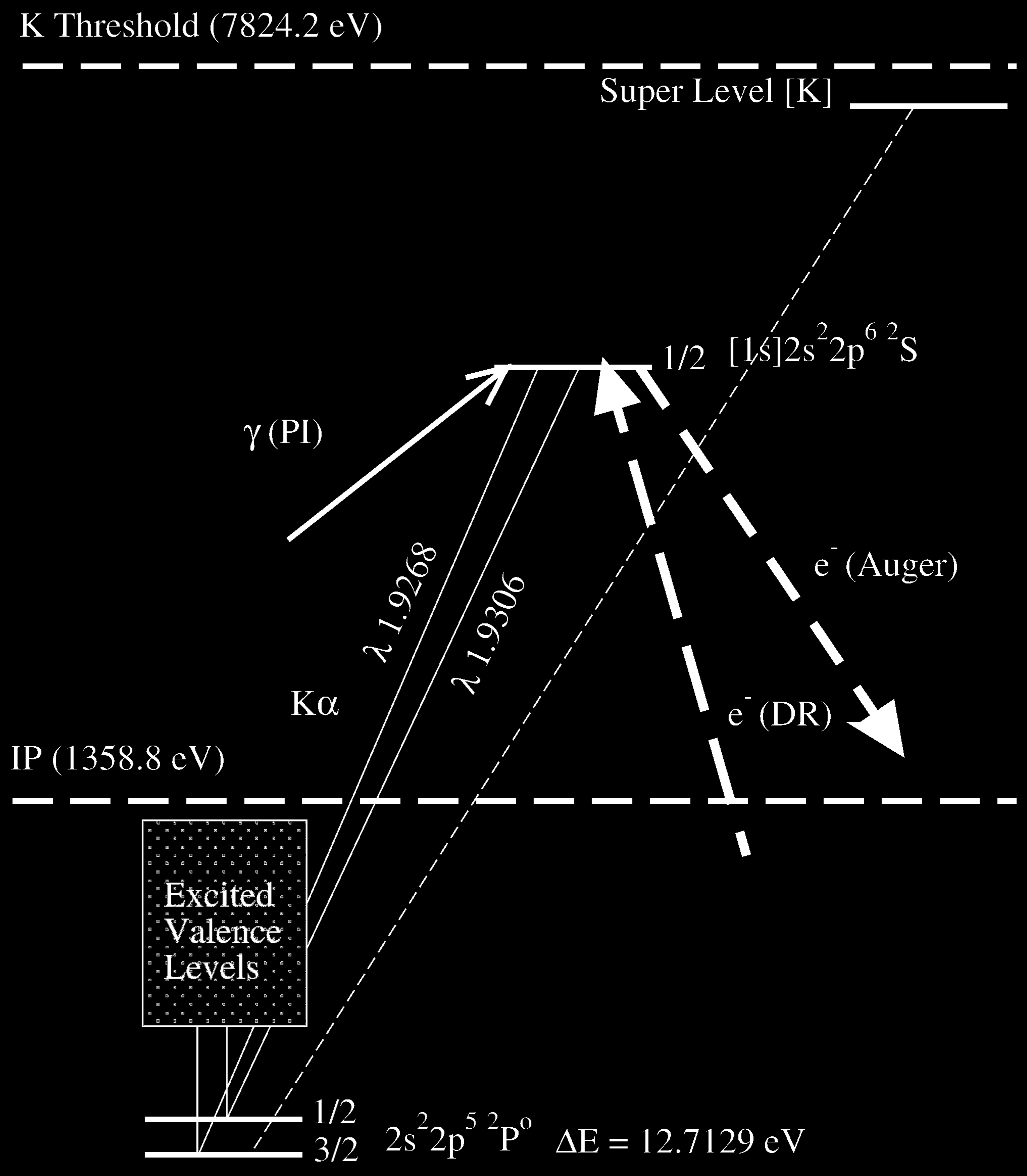

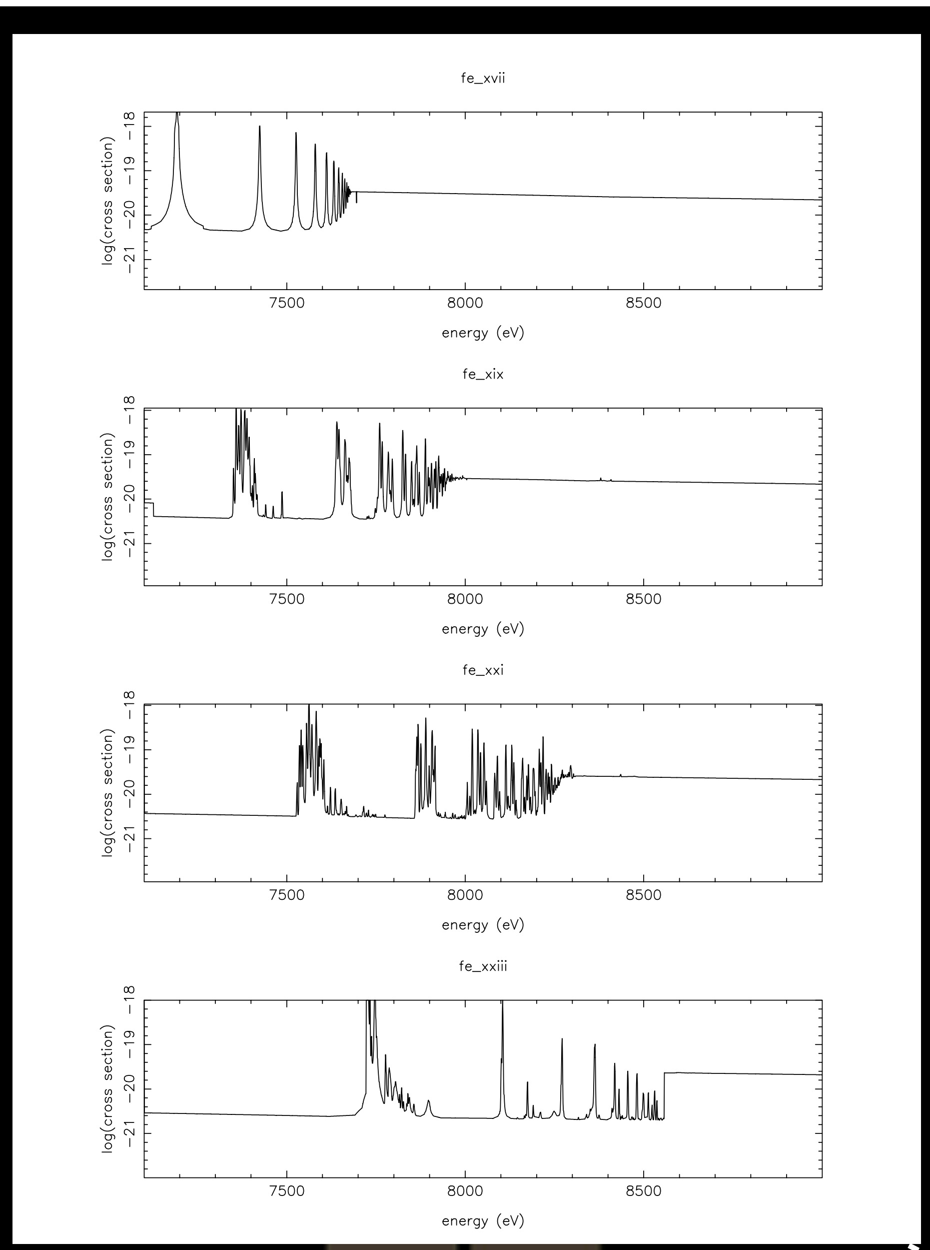

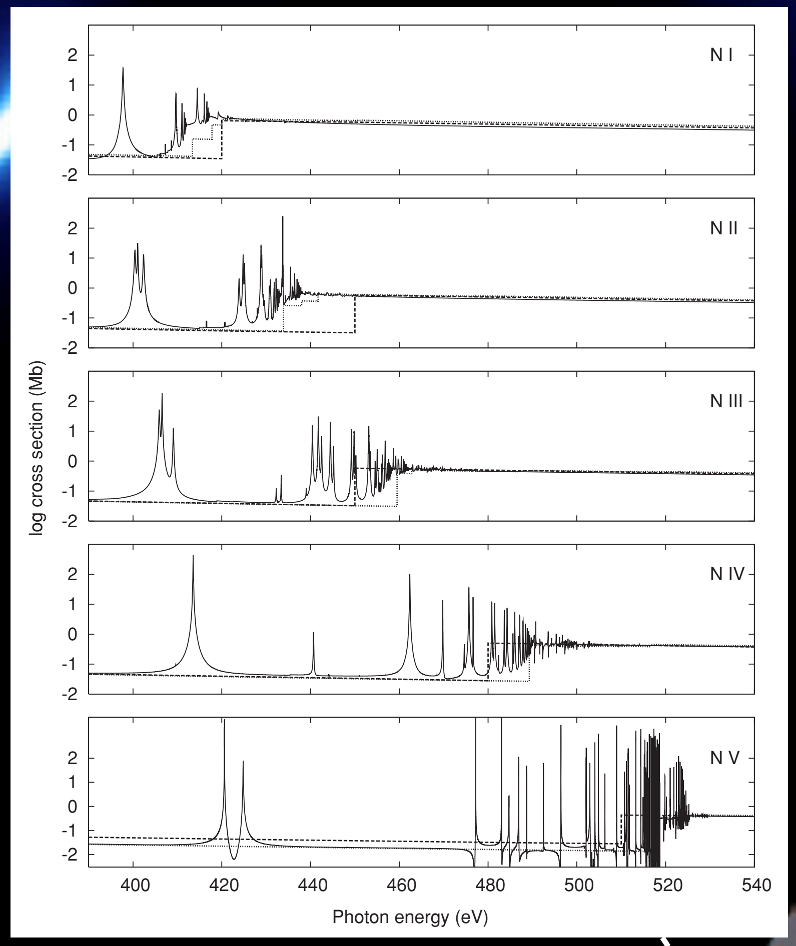

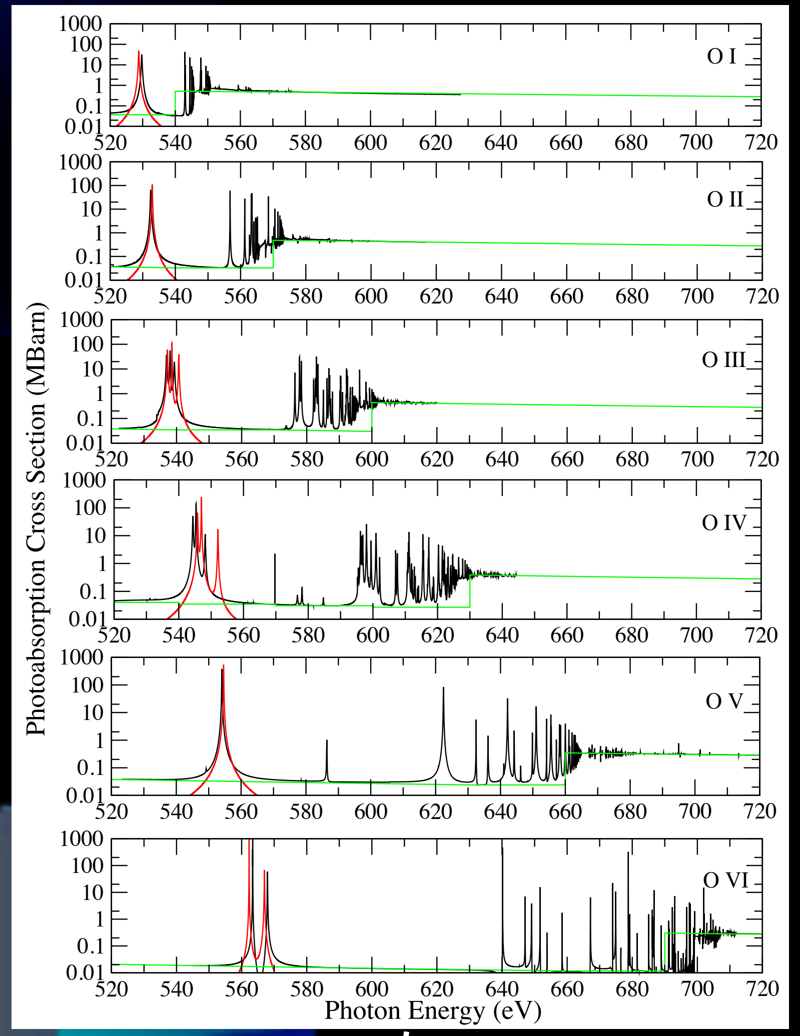

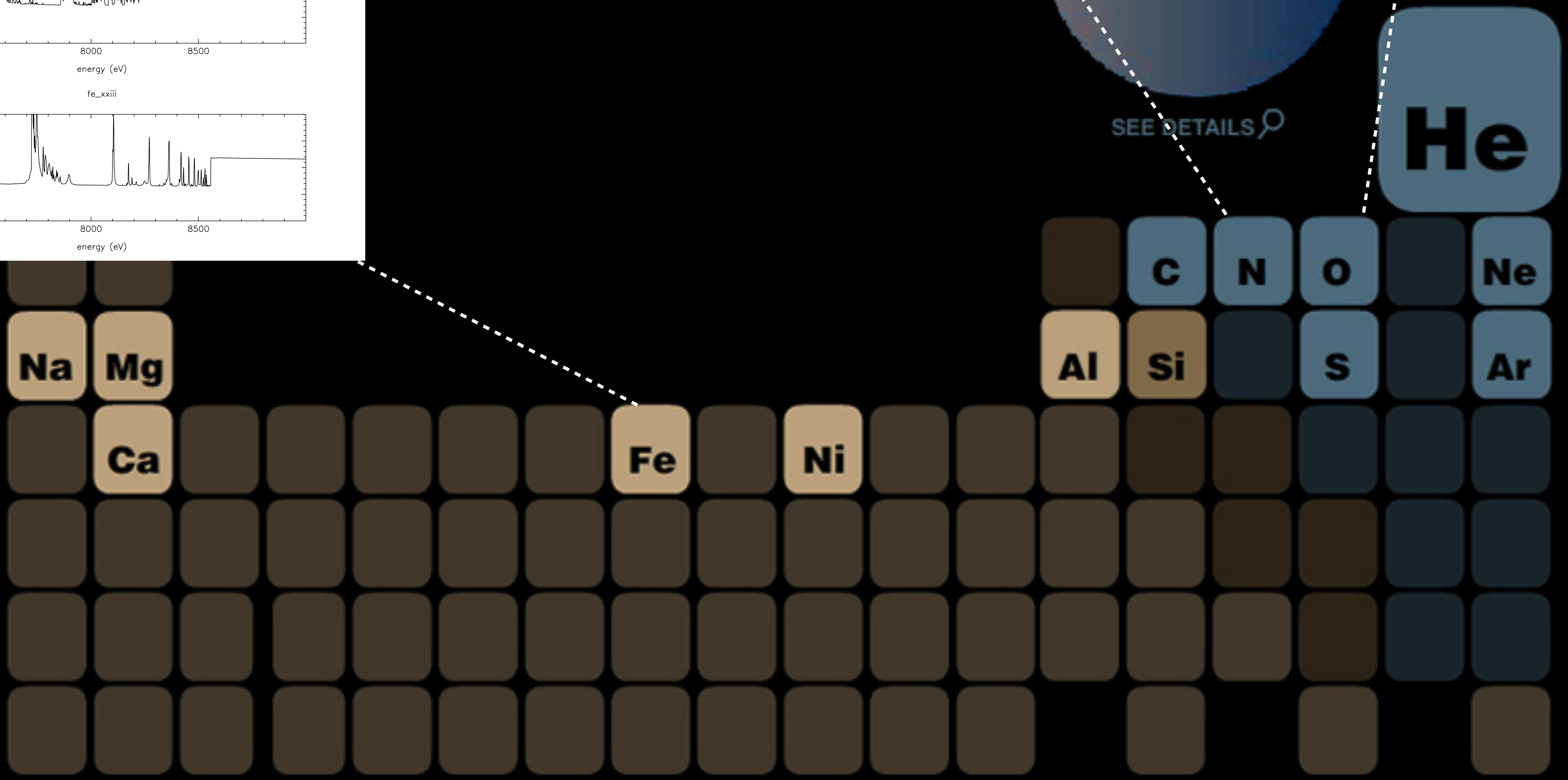

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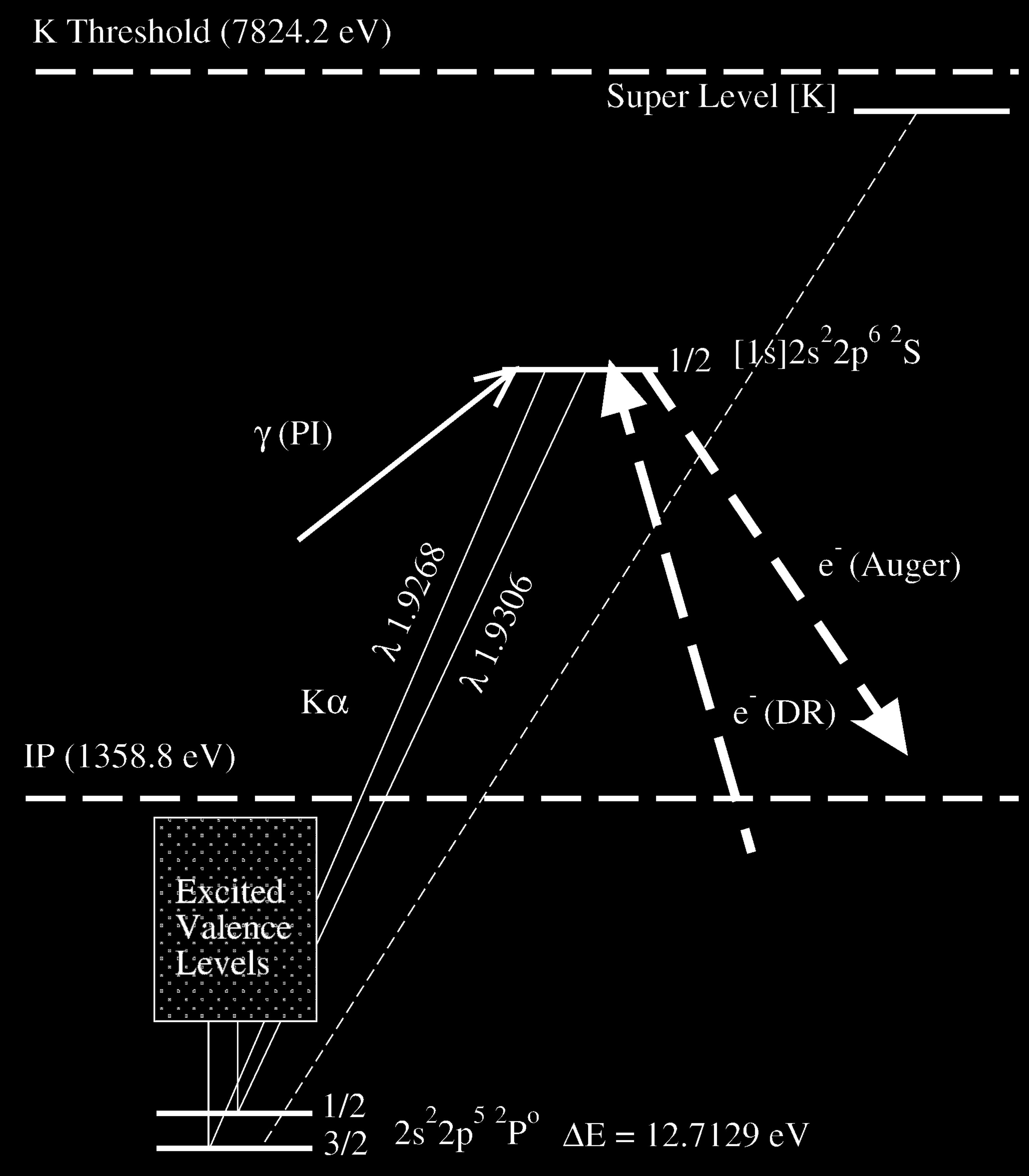

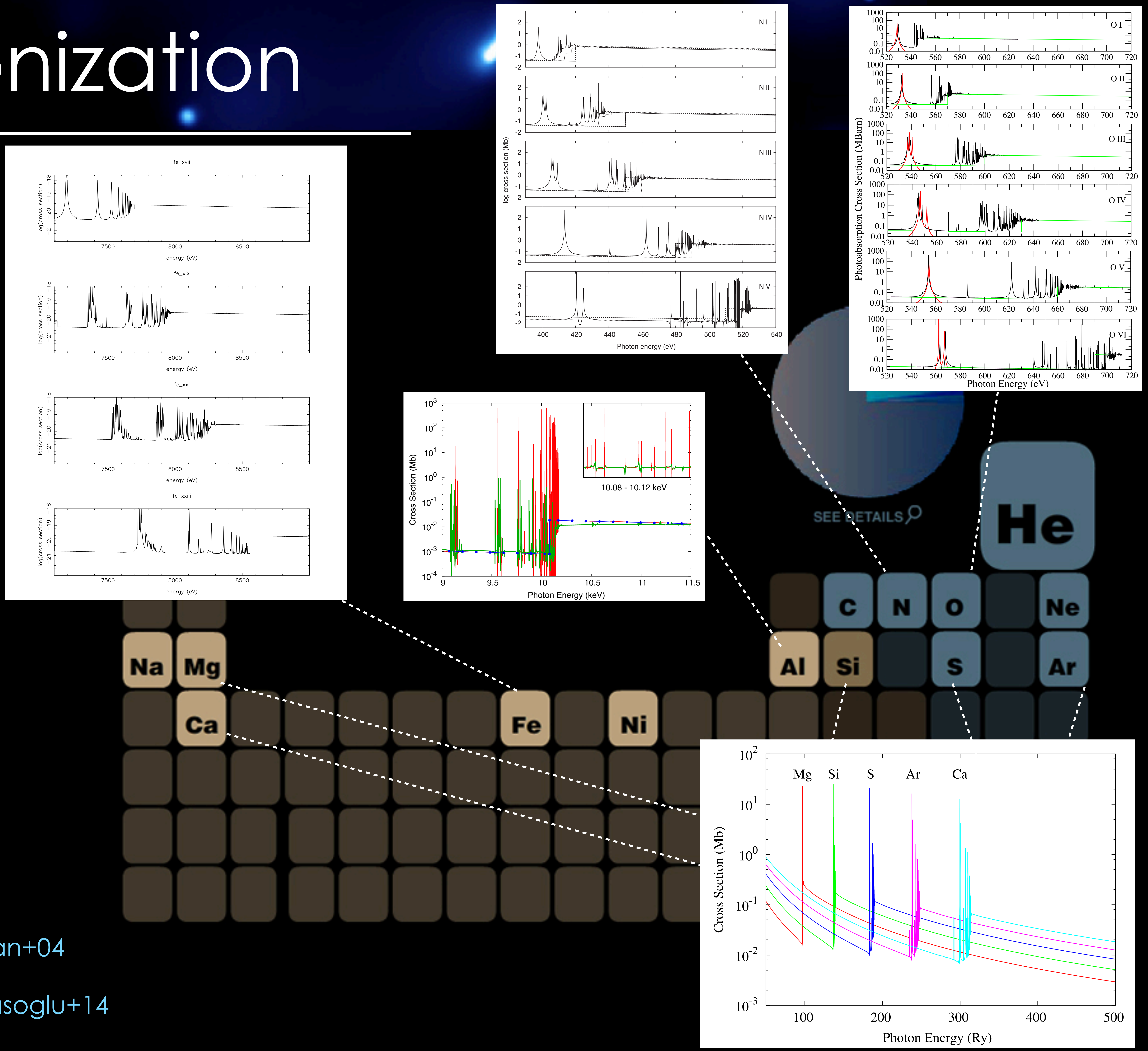

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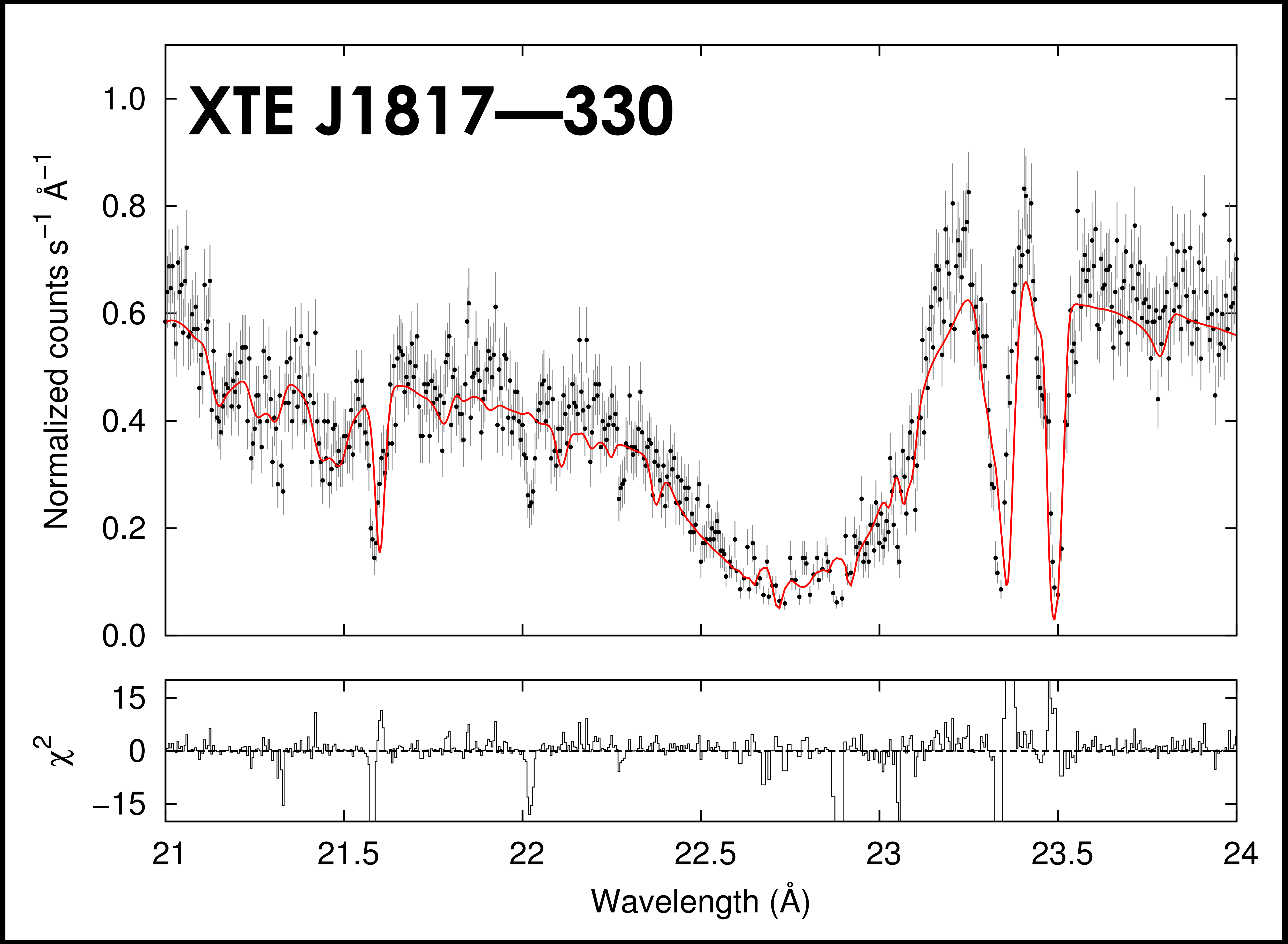
García+05; Gorczyca+13; García+09; Witthoeft+11a,b; Hasoglu+14

Case of Study I: The Oxygen Controversy

Chandra HETG spectrum of the low-mass X-ray binary XTE J1817—330. The oxygen K-band shows several features identified with ionized species.



Gatuzz, JG+13

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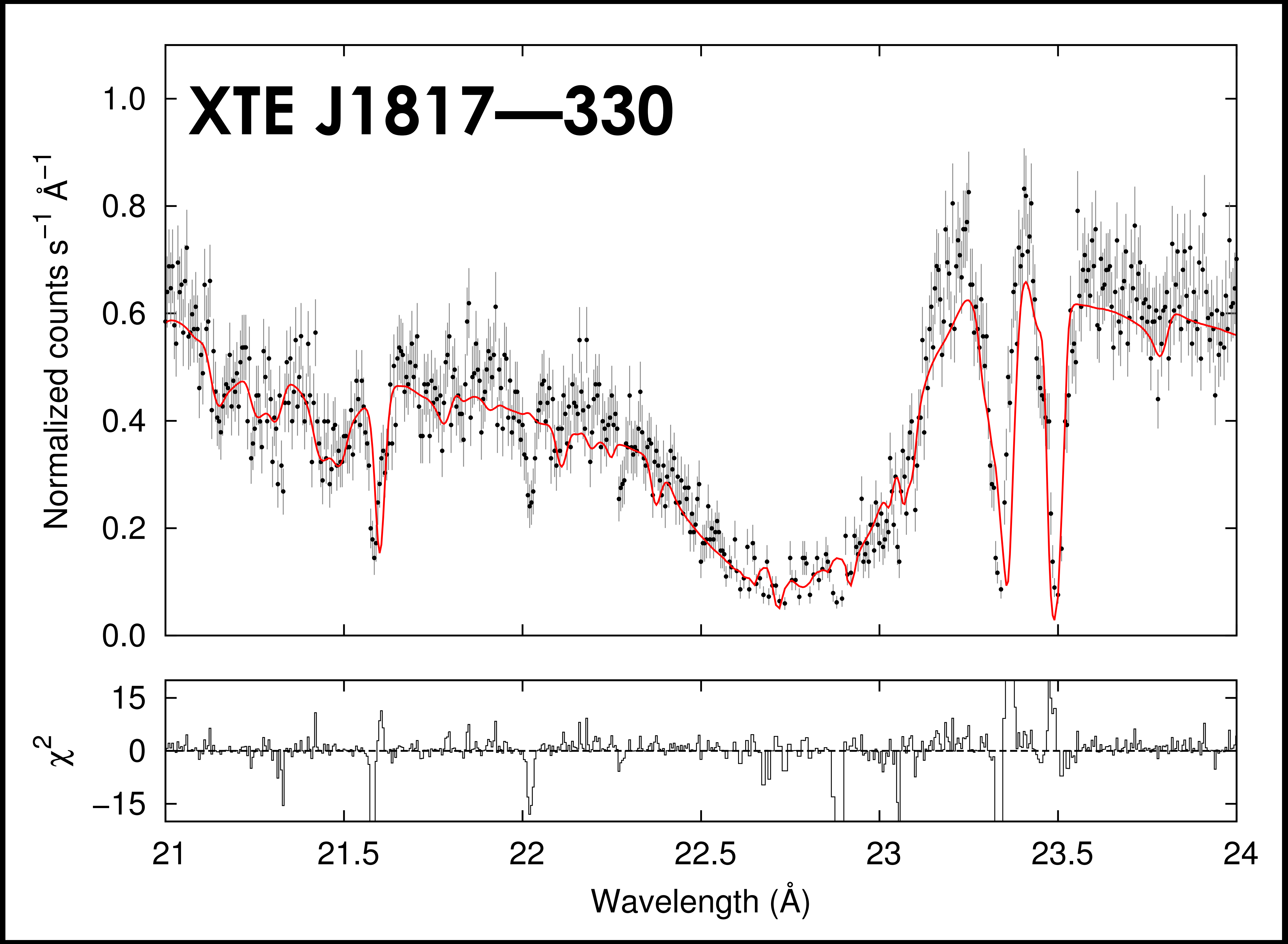

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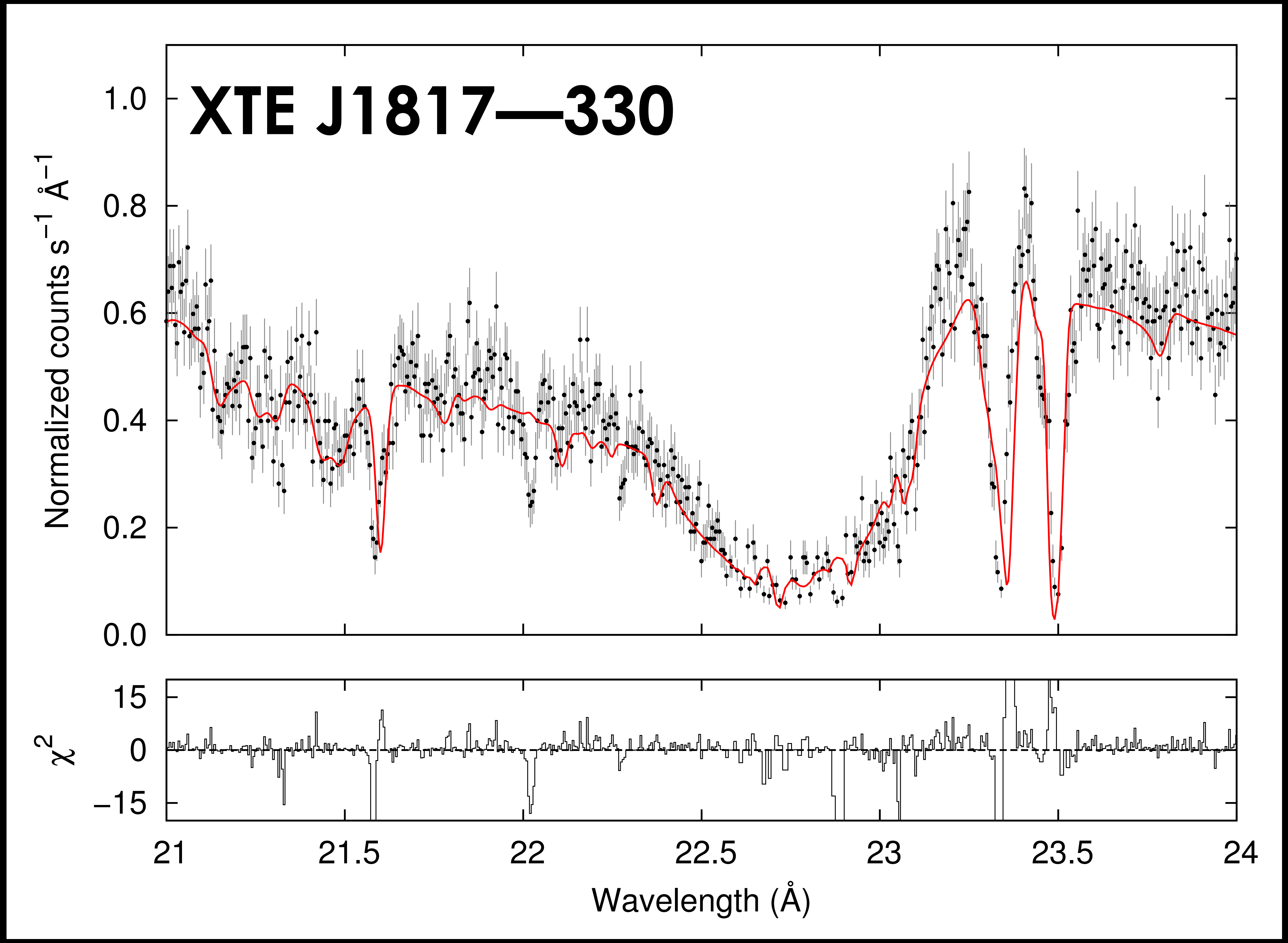

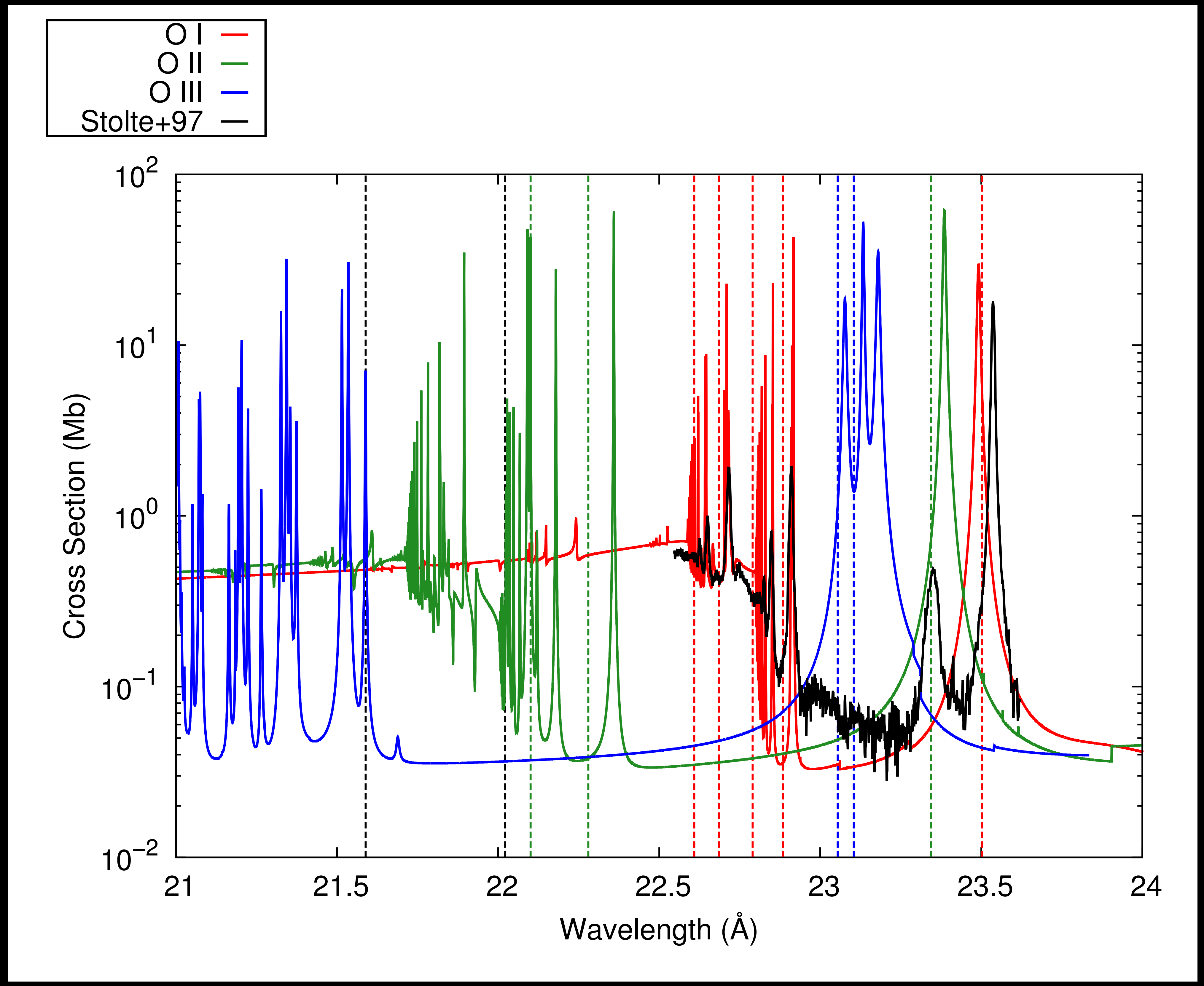

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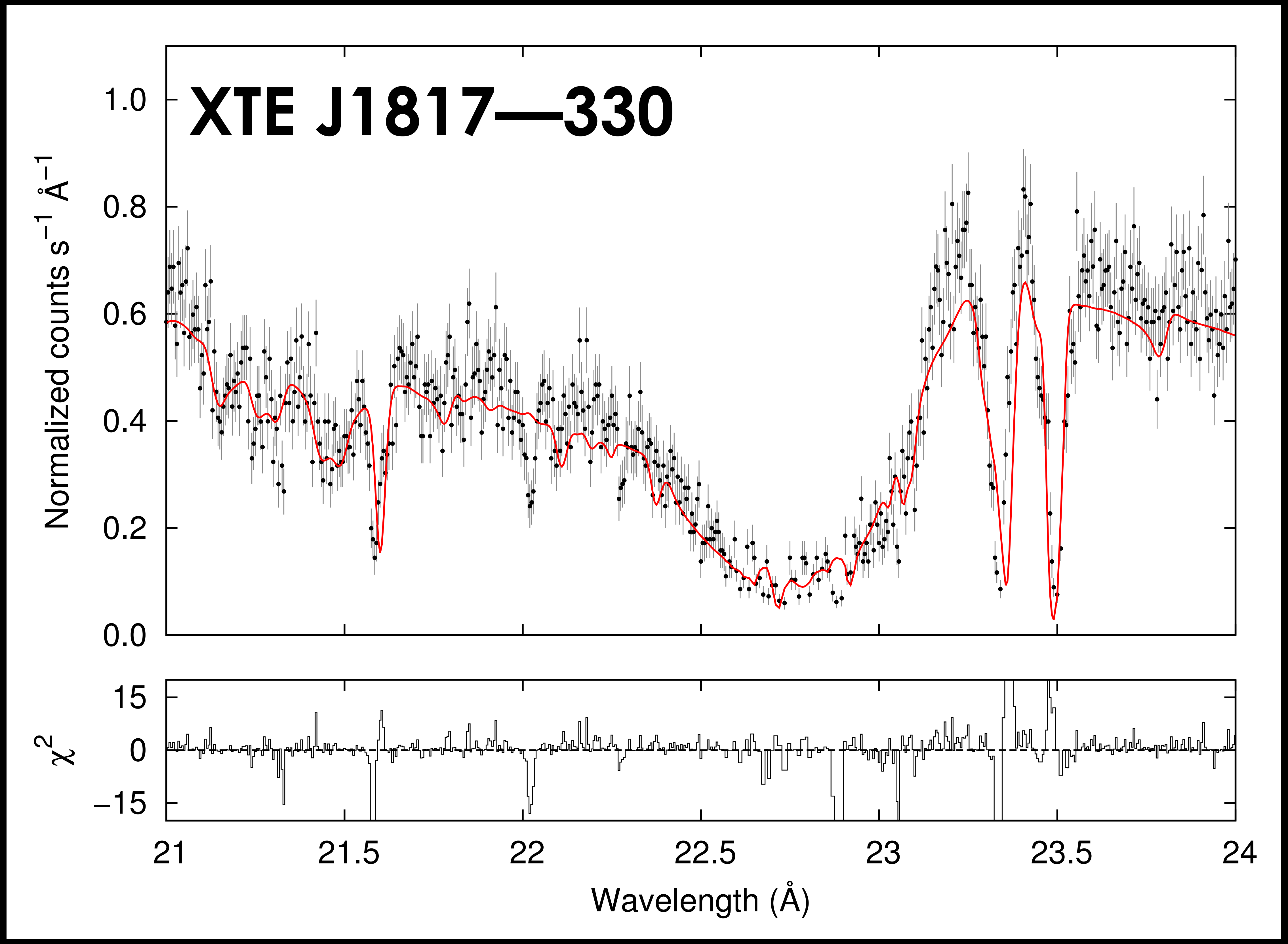

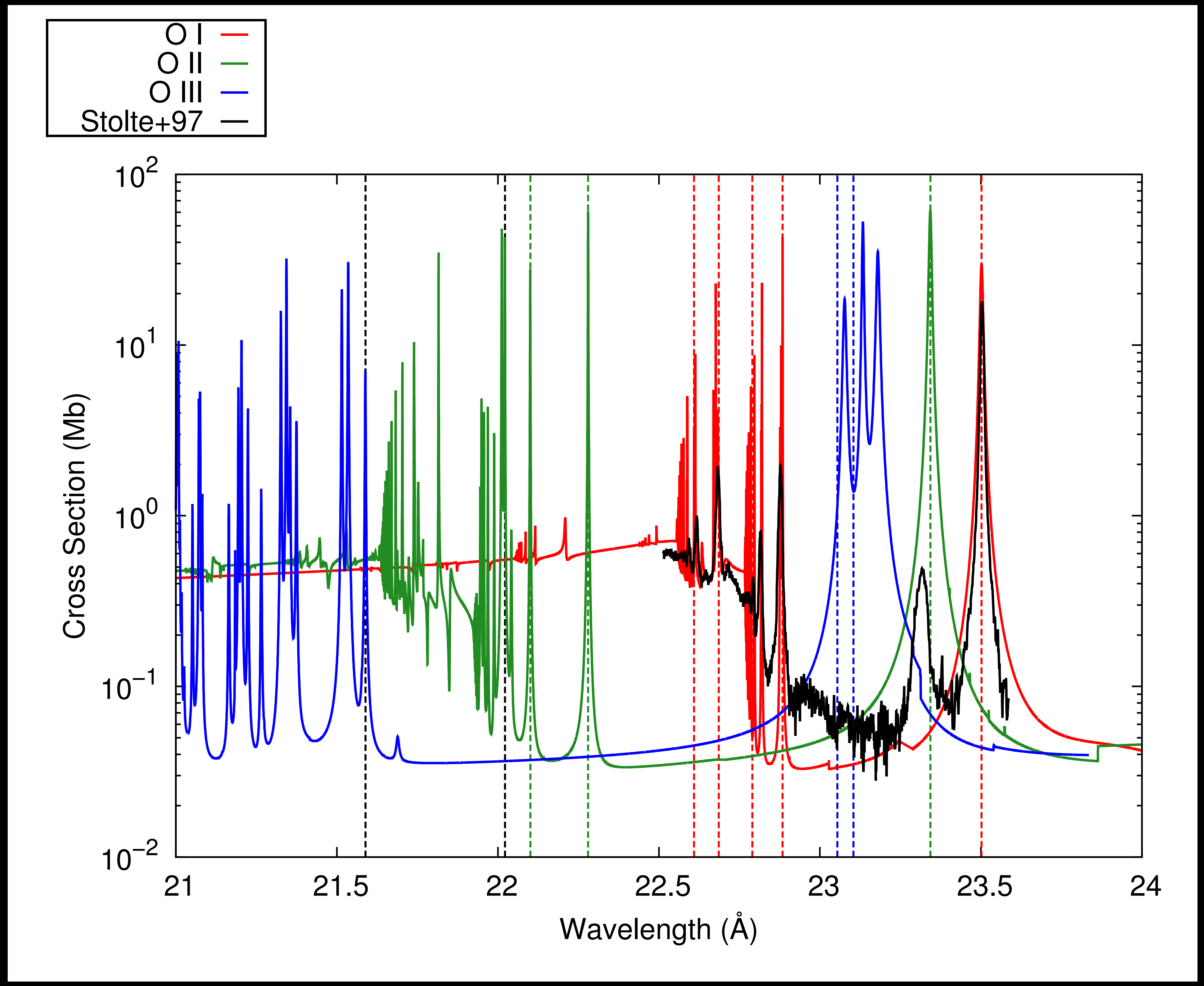

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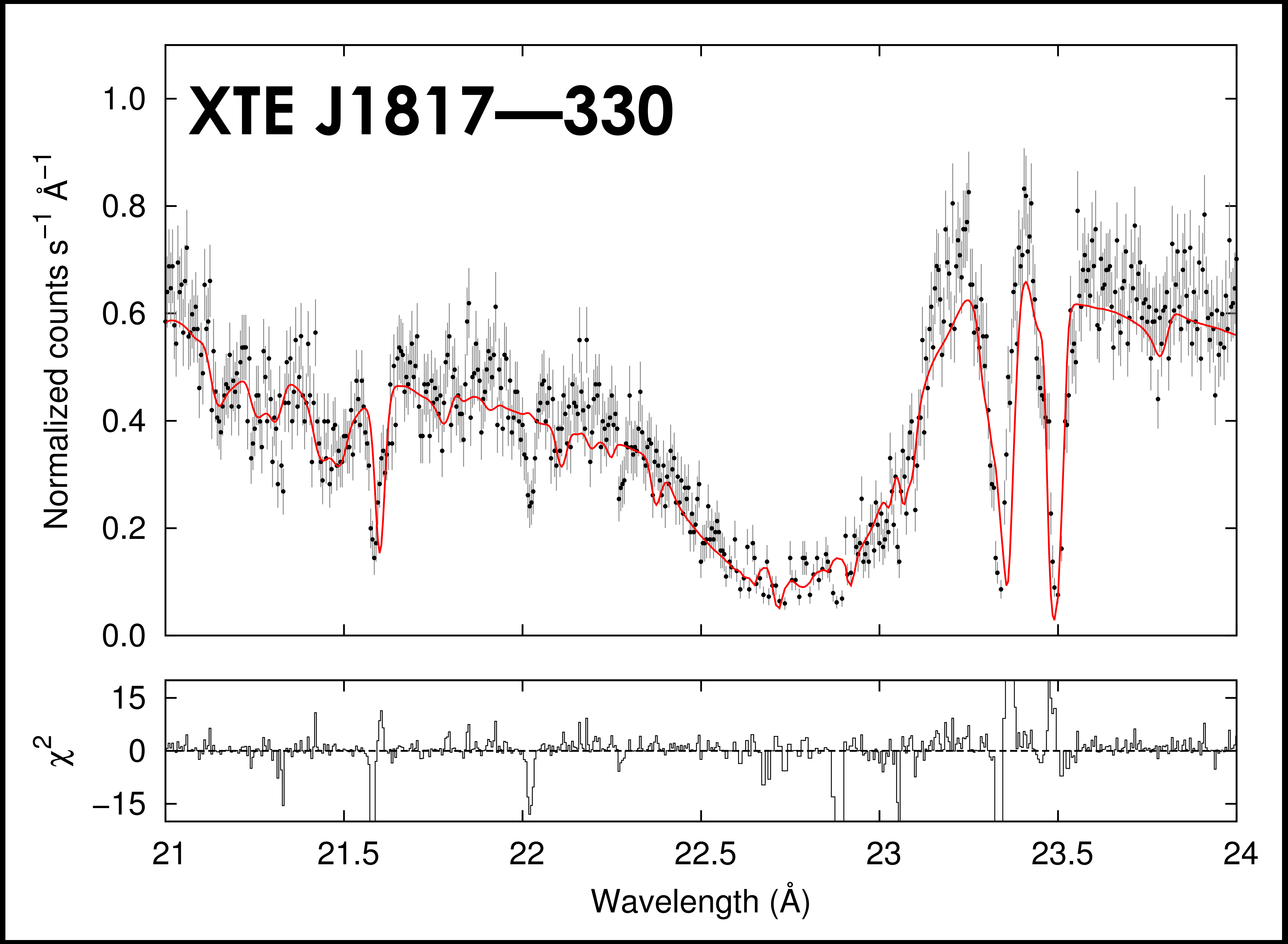

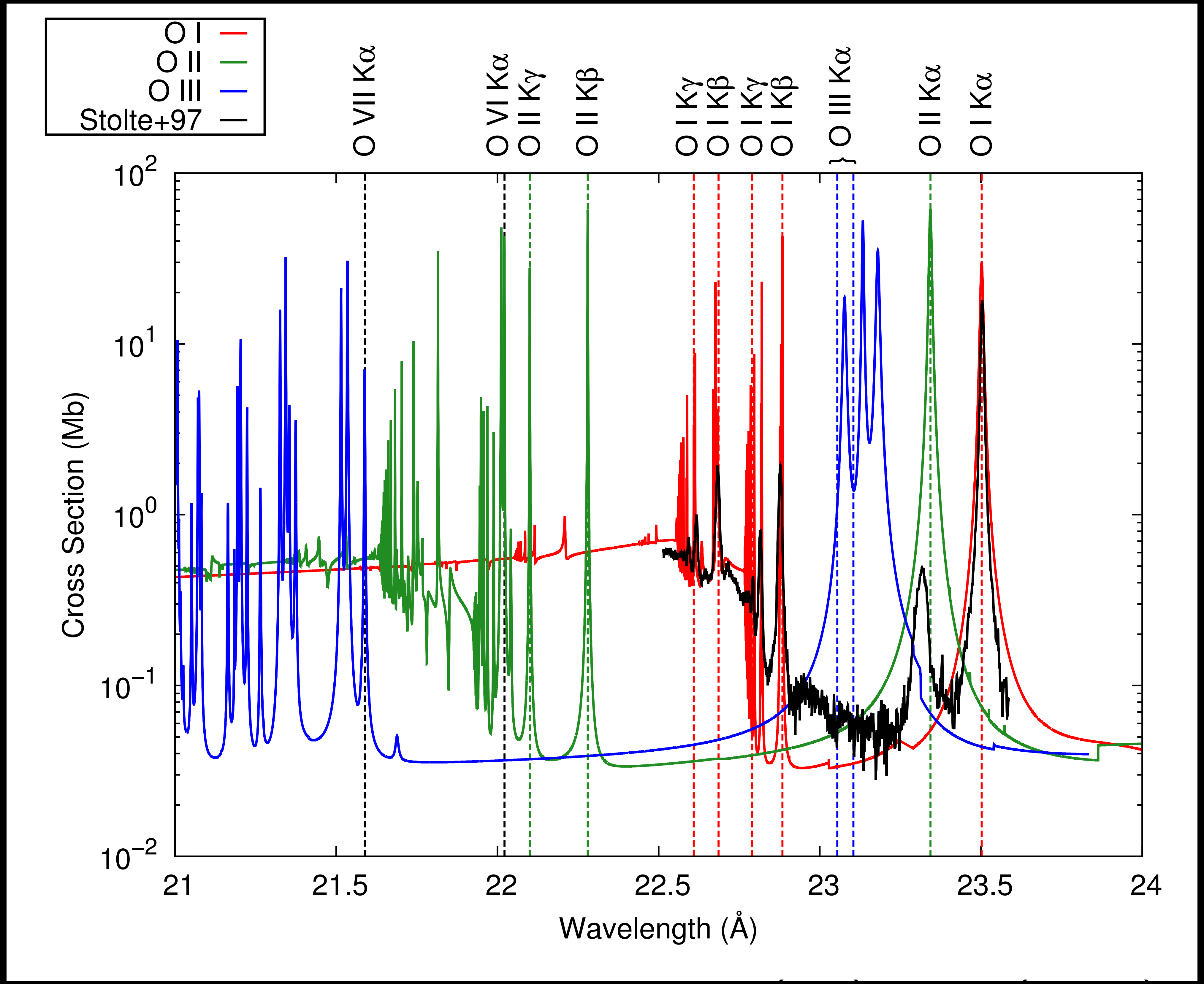

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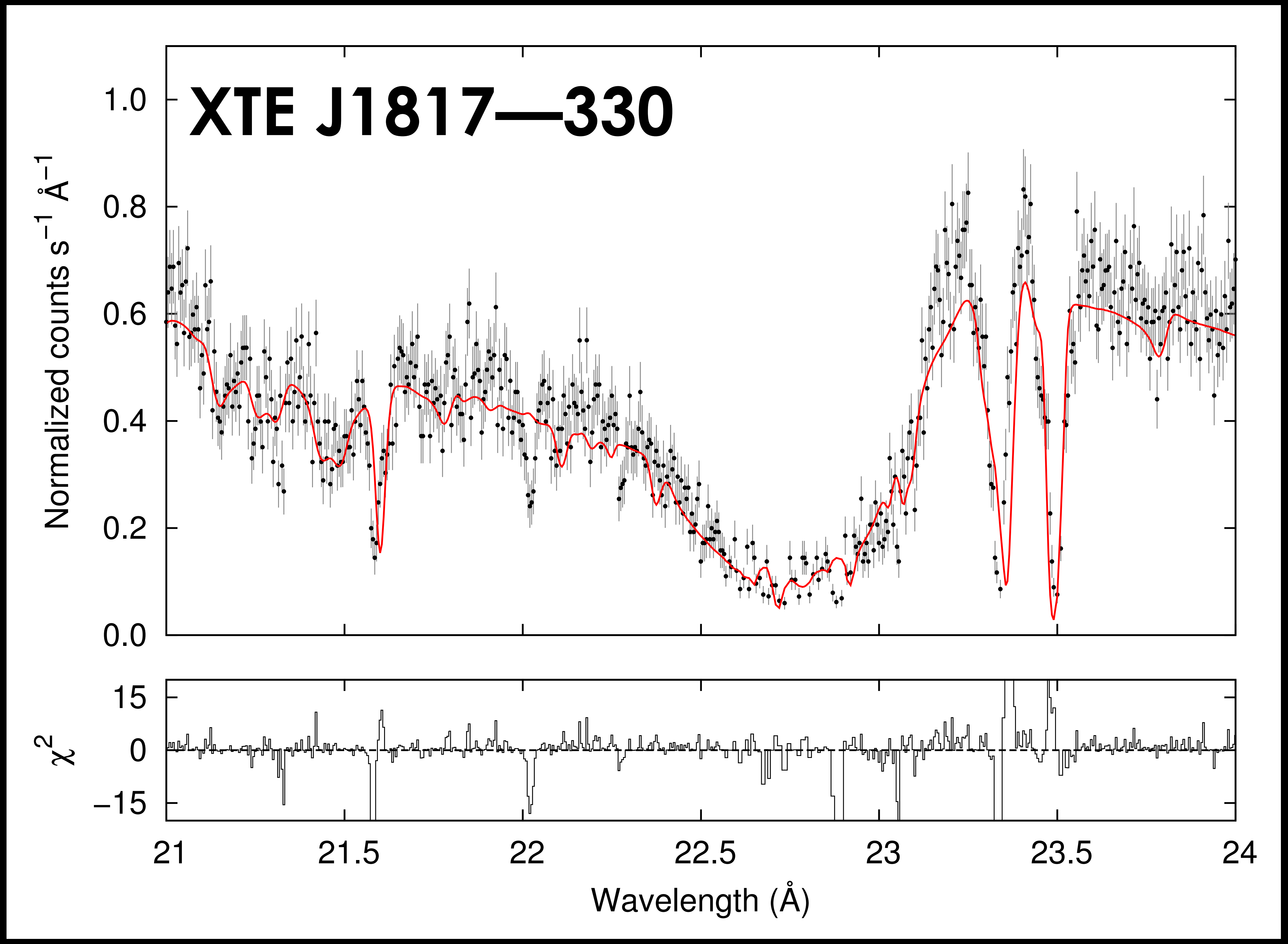

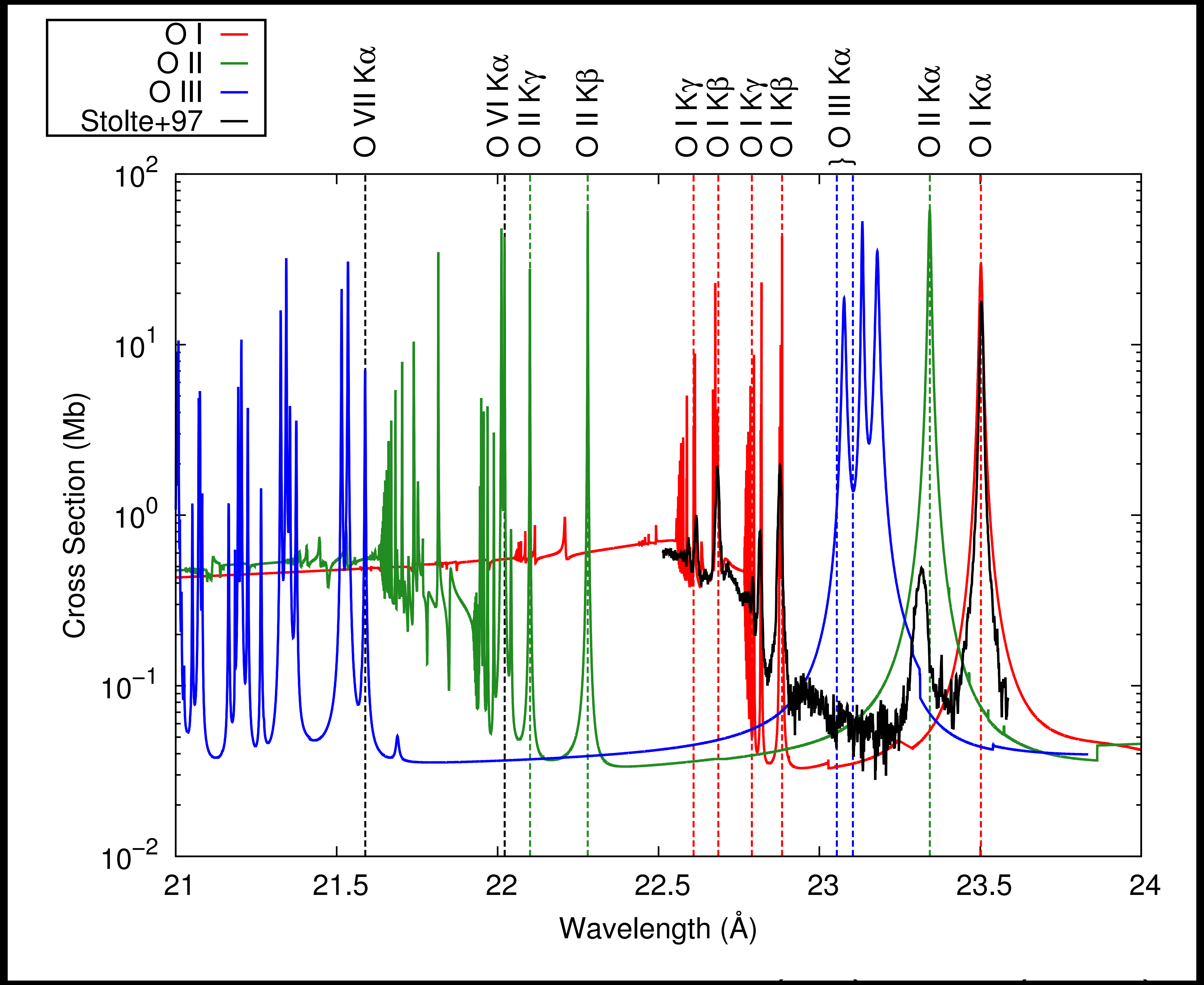

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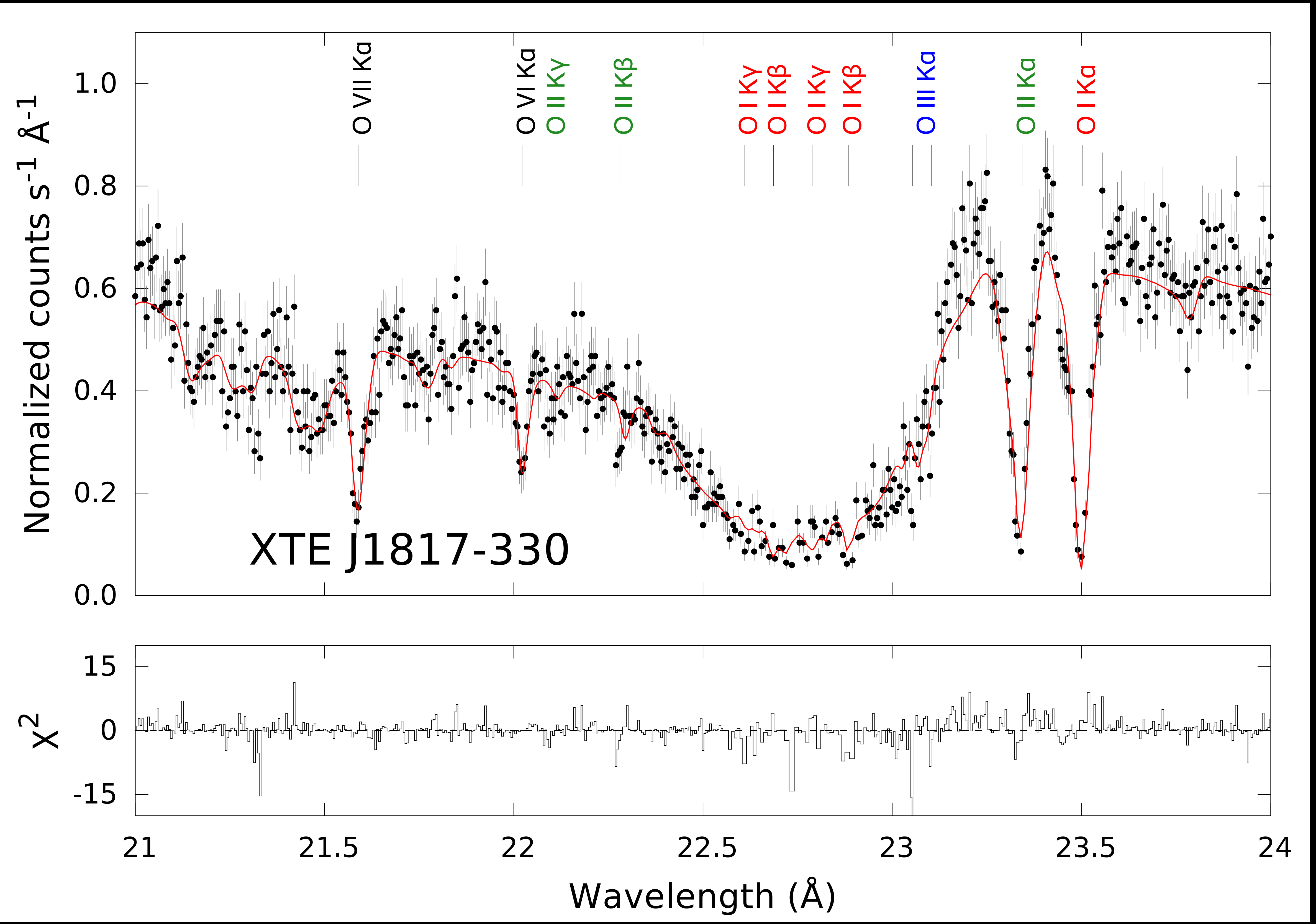
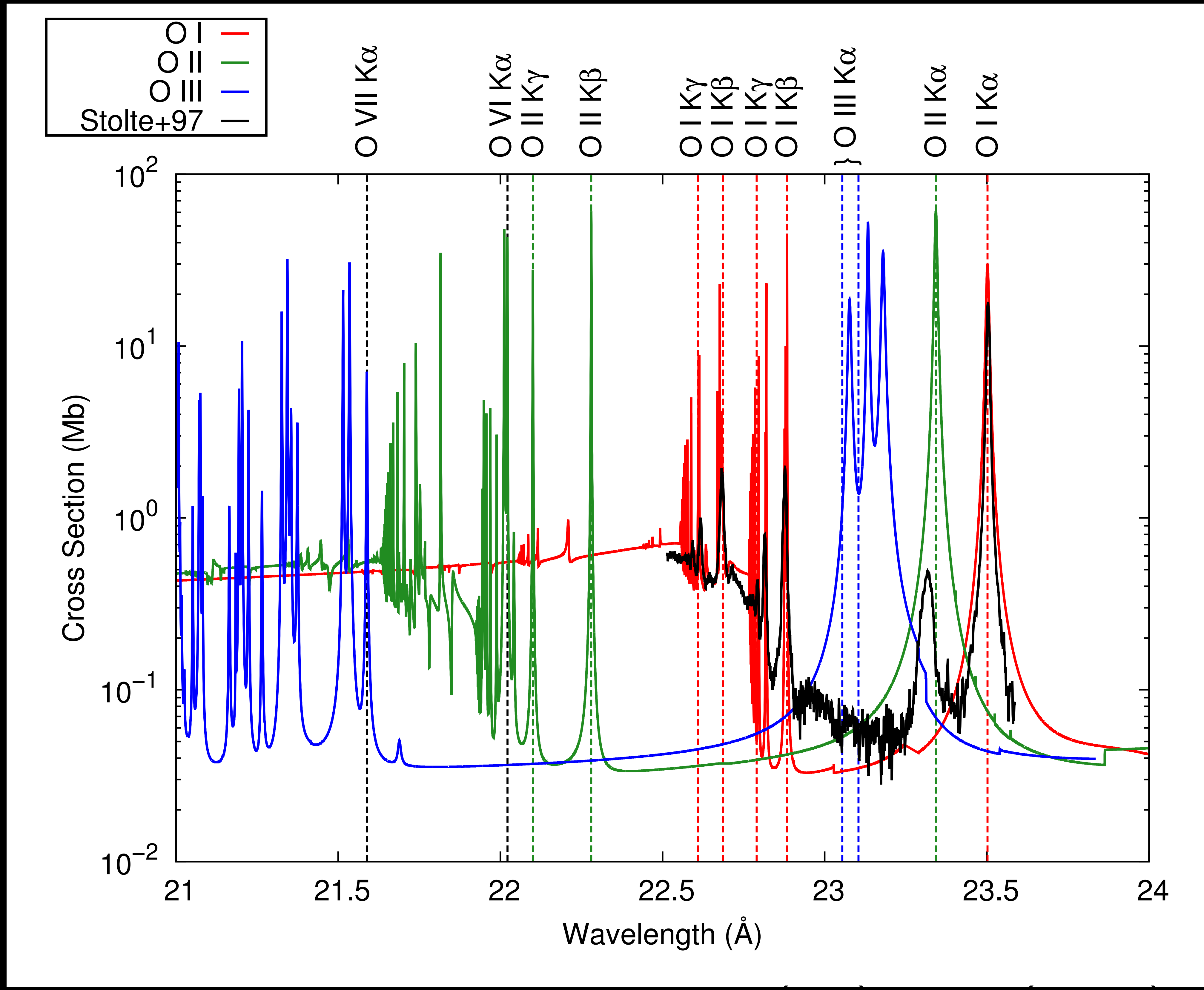
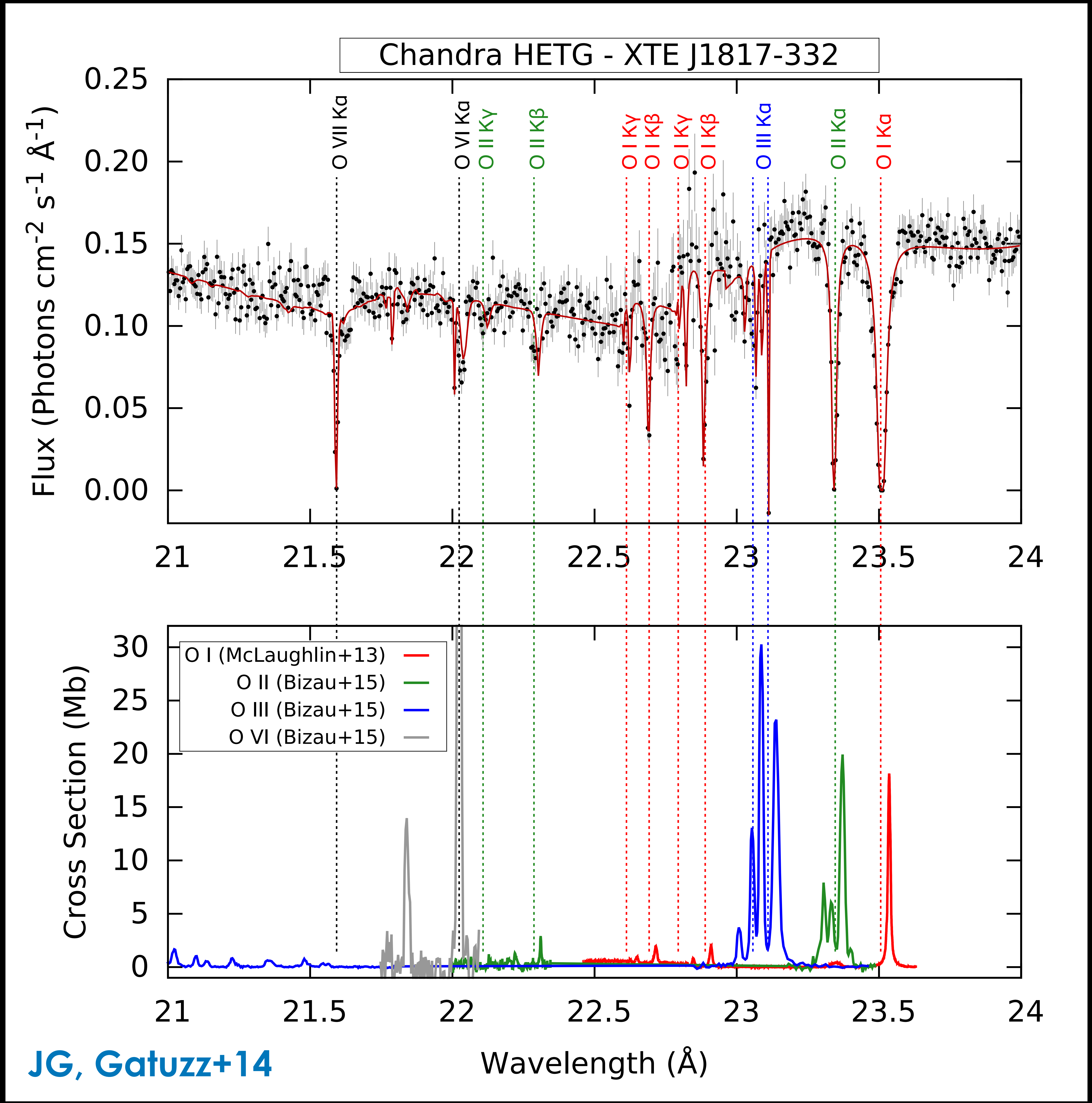




Gatuzz, JG+13

Shifts of ~33 mA for O I and 75 mA O II, Ka different from the high-n resonances

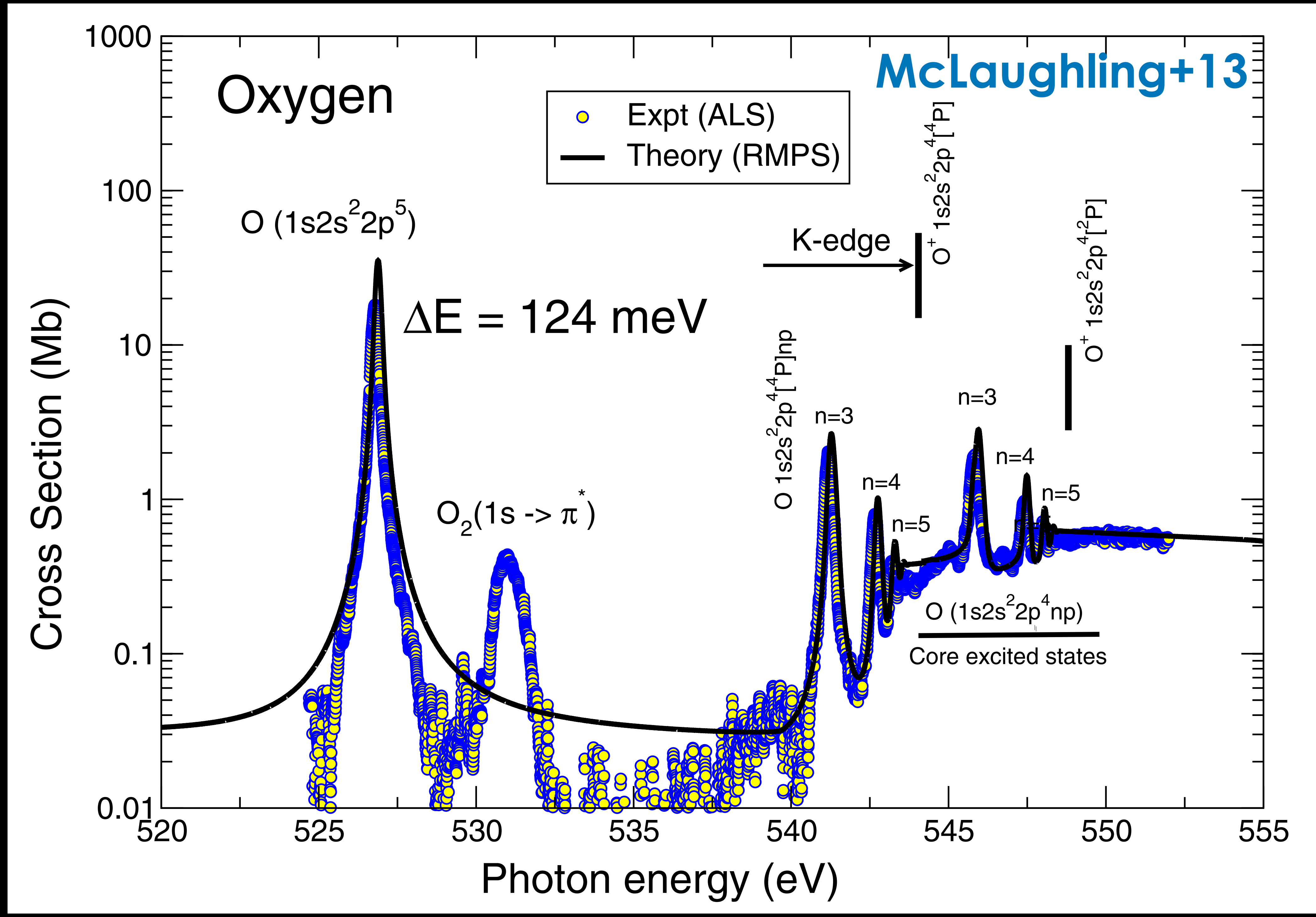
Line Positions: Observations vs Lab Experiment



Resonance positions in disagreement with laboratory experiments

O I shifts of ~580 meV

McLalughlin+13: Gratings on *Chandra* and *XMM* need to be re-calibrated(!?)



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Leutenegger+20: Simutaneous measurement of O VII and O_2 lines provides accurate absolute wavelength calibration

Source	$1s-2p$	$1s-3p\,^4P$
This work	527.26(4)	541.645(12)
Gorczyca *et al.* [16] *XMM*, Mkn 421	527.28(5)	541.93(28)
Gorczyca *et al.* [16] *Chandra*	527.44(9)	541.72(18)
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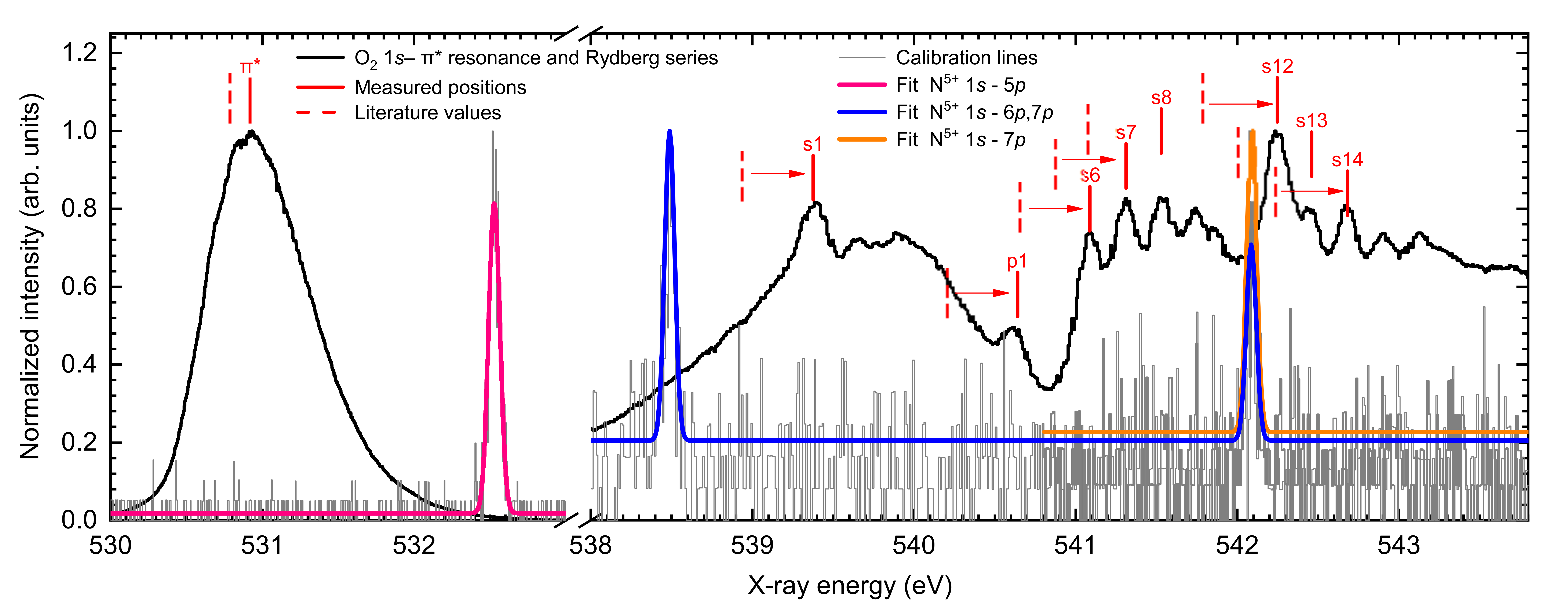

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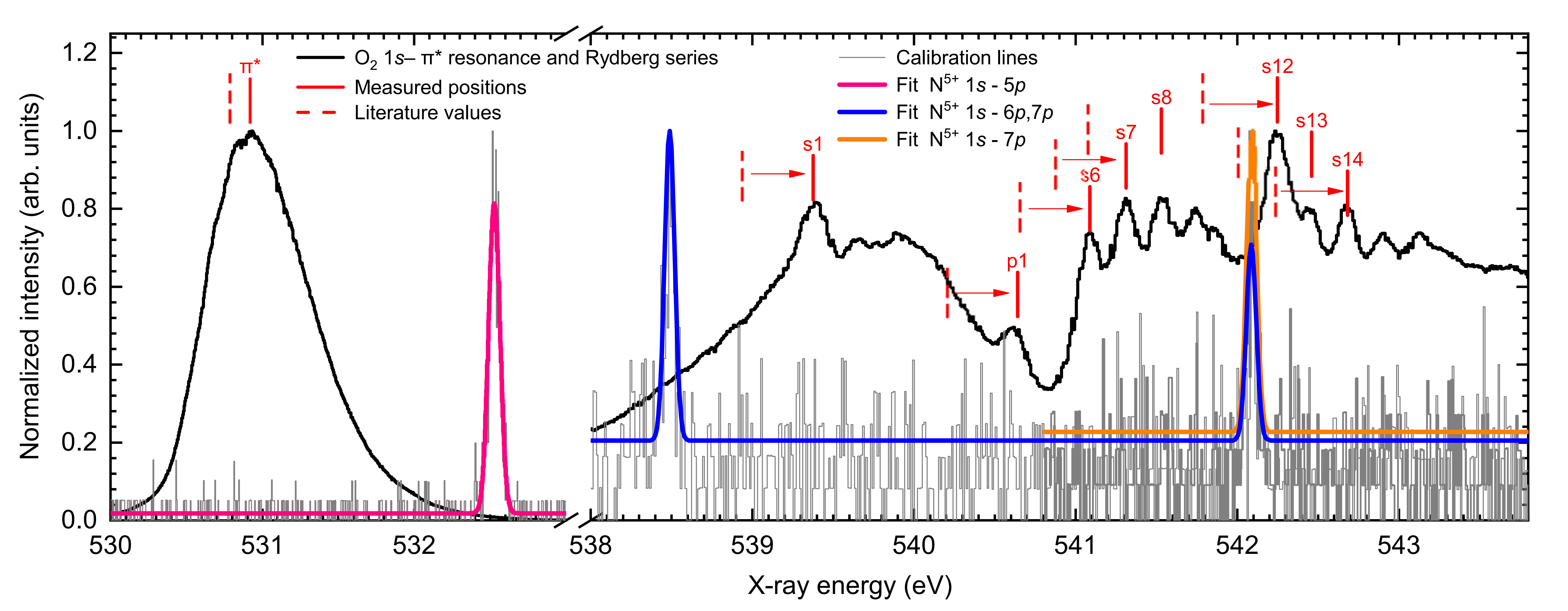

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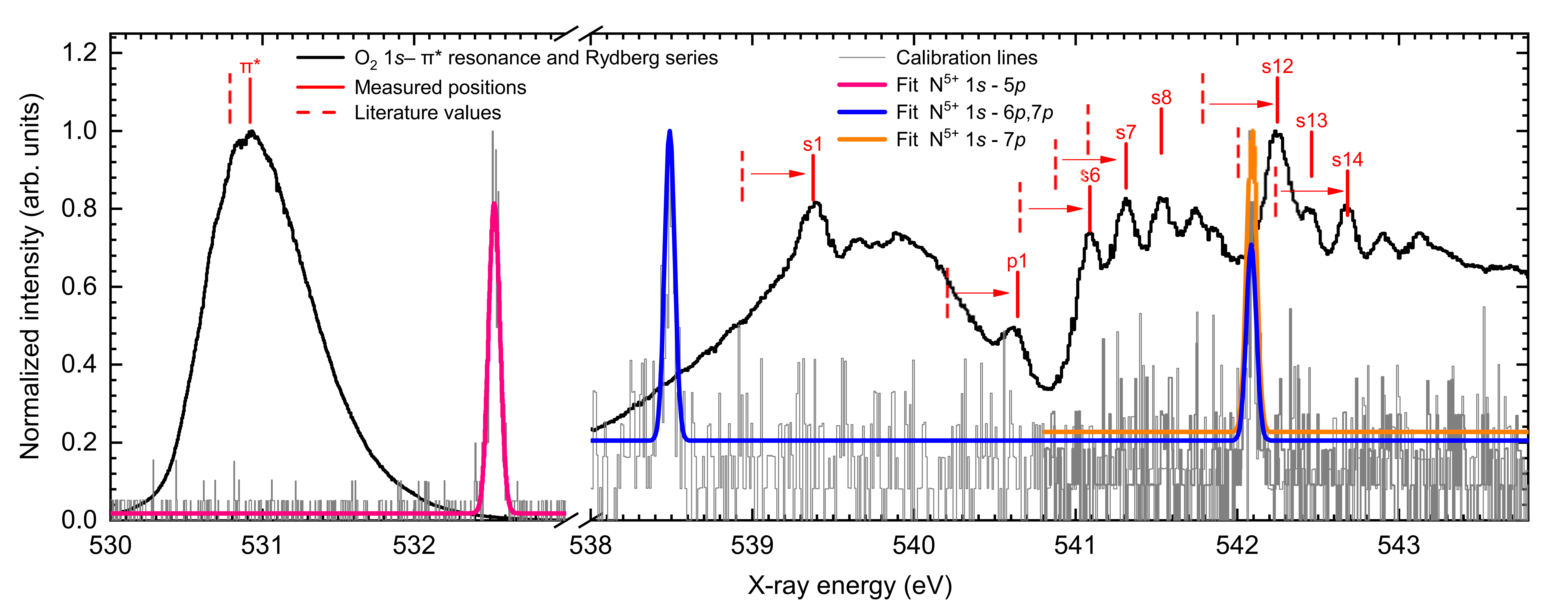

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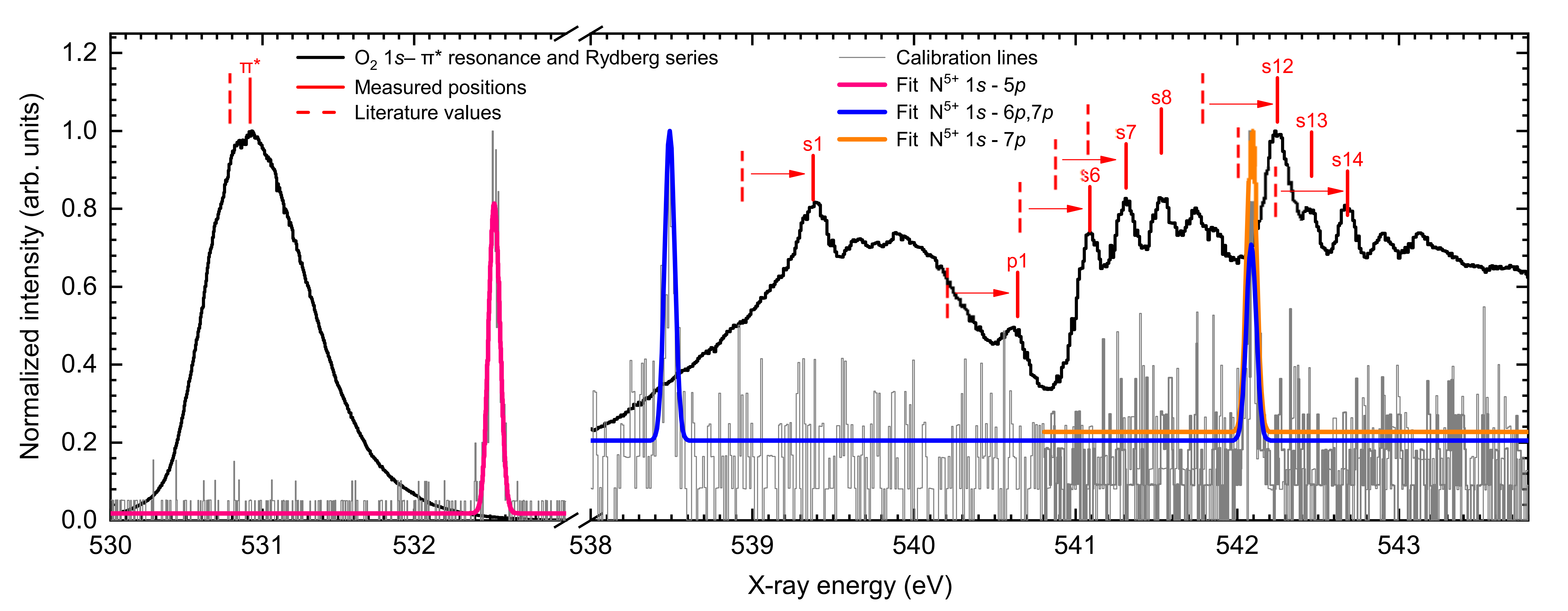

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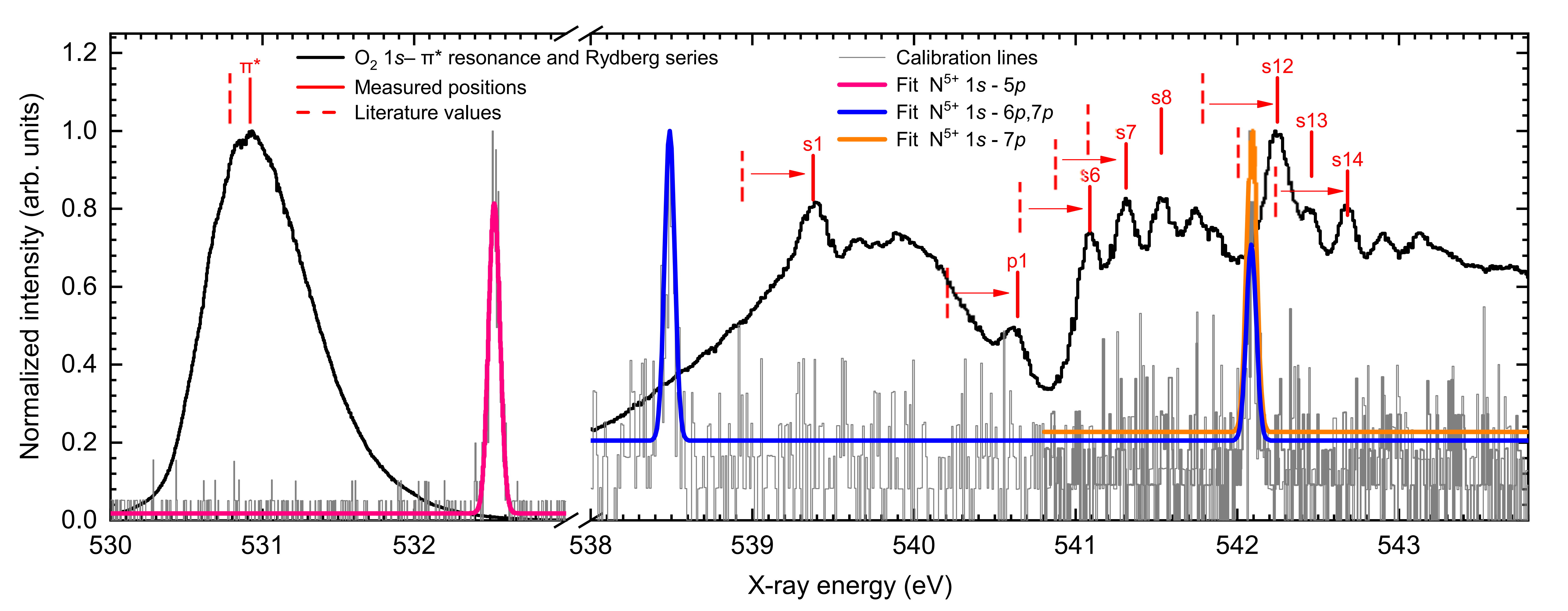
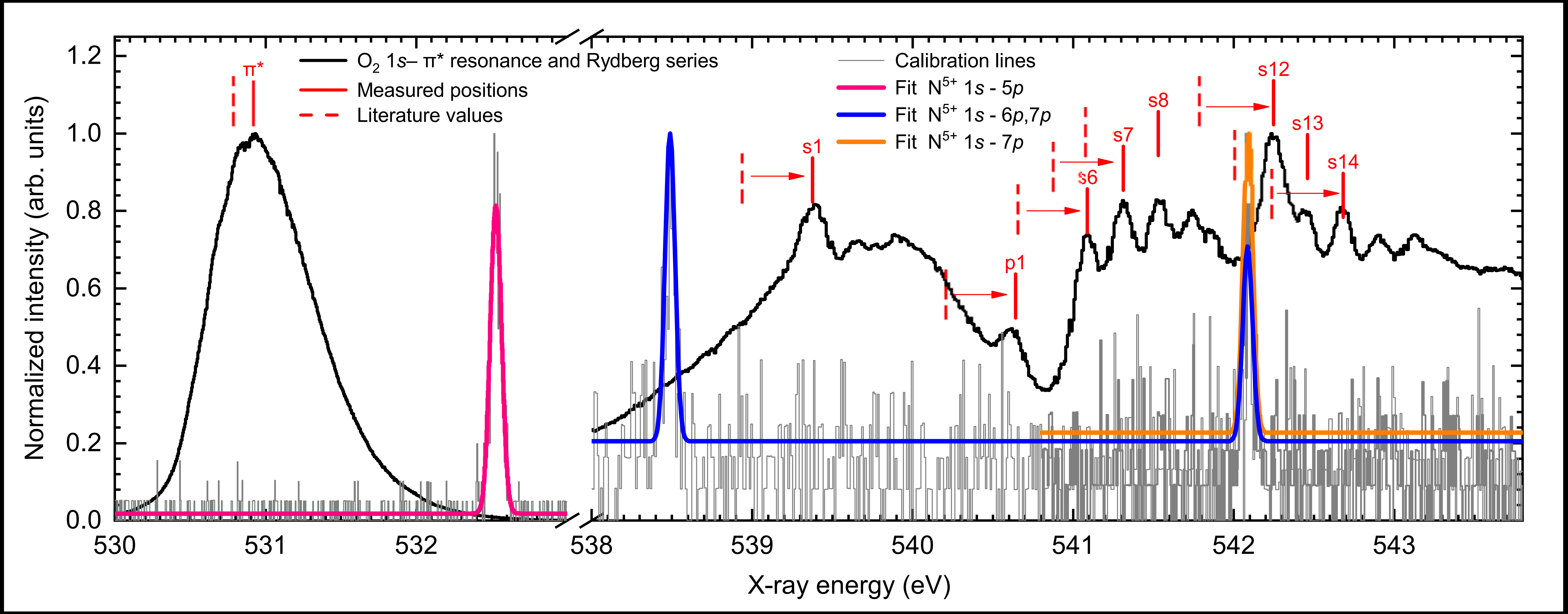


Line Positions: Observations vs Lab Experiment

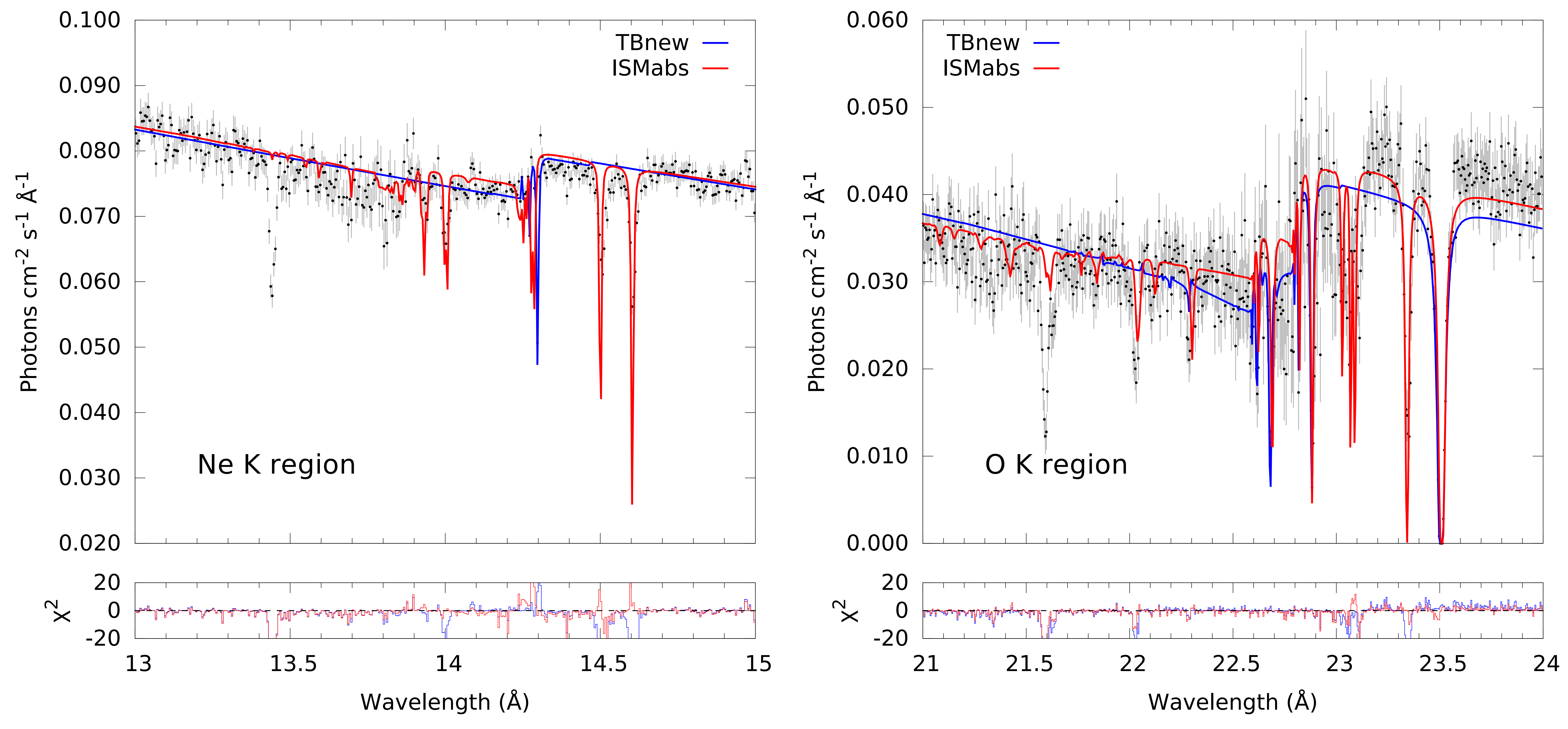
Leutenegger+20: Simutaneous measurement of O VII and O_2 lines provides accurate absolute wavelength calibration

Source	$1s-2p$	$1s-3p\,^4P$
This work	527.26(4)	541.645(12)
Gorczyca *et al.* [16] *XMM*, Mkn 421	527.28(5)	541.93(28)
Gorczyca *et al.* [16] *Chandra*	527.44(9)	541.72(18)
Gorczyca *et al.* [16] *Chandra*, shifted	527.26(9)	
Liao *et al.* [38] *Chandra*, average	527.39(2)	
McLaughlin *et al.* [18] ALS	526.79(4)	541.19(4)



ISMabs: Ionized (Atomic) Absorption Model

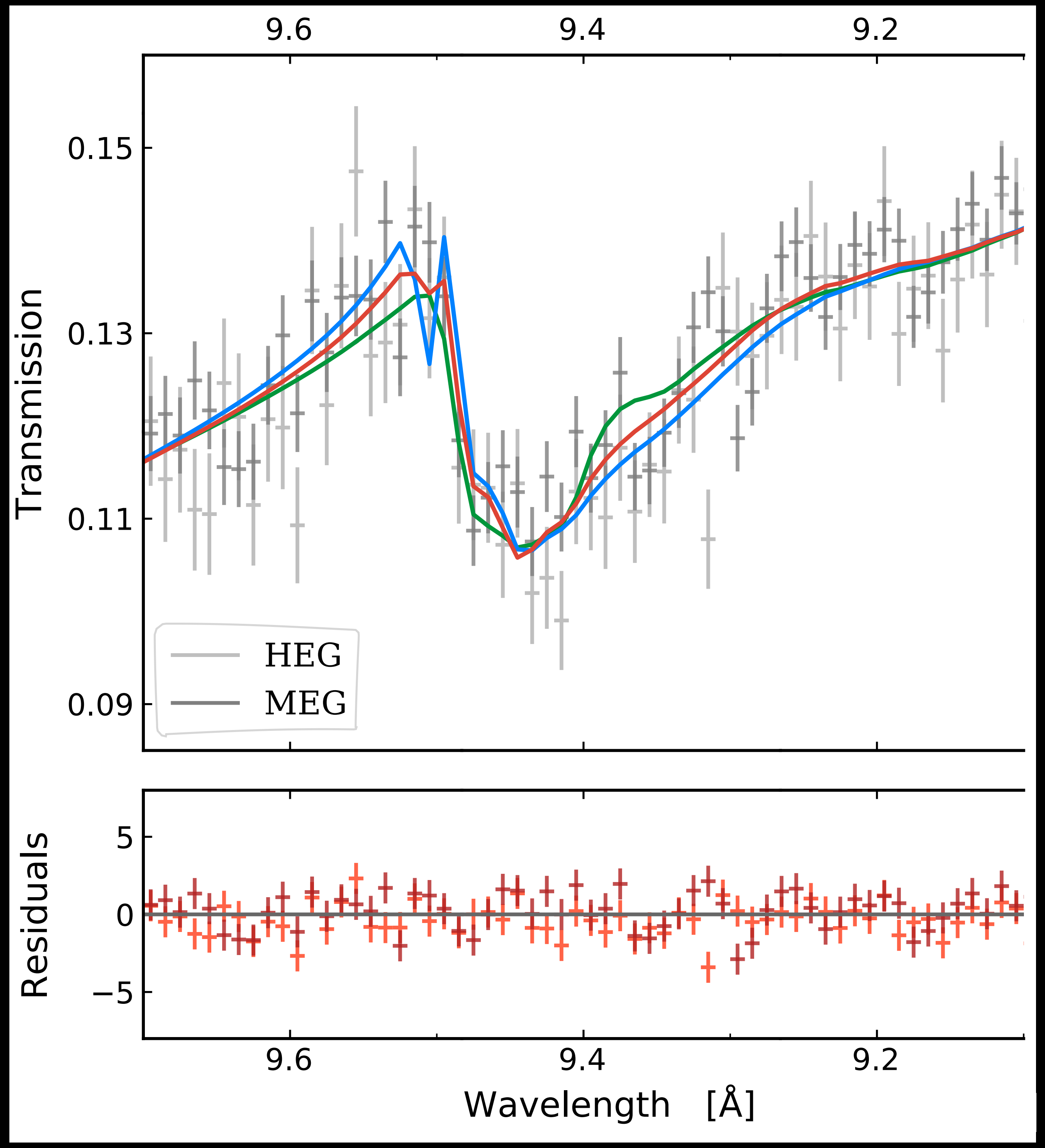
* Includes H, He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe
* Only neutrals, single and double ionized species (e.g., O I, O II, O III)
* Fit for column densities of each ion (no ionization equilibrium)



Gatuzz, JG+15

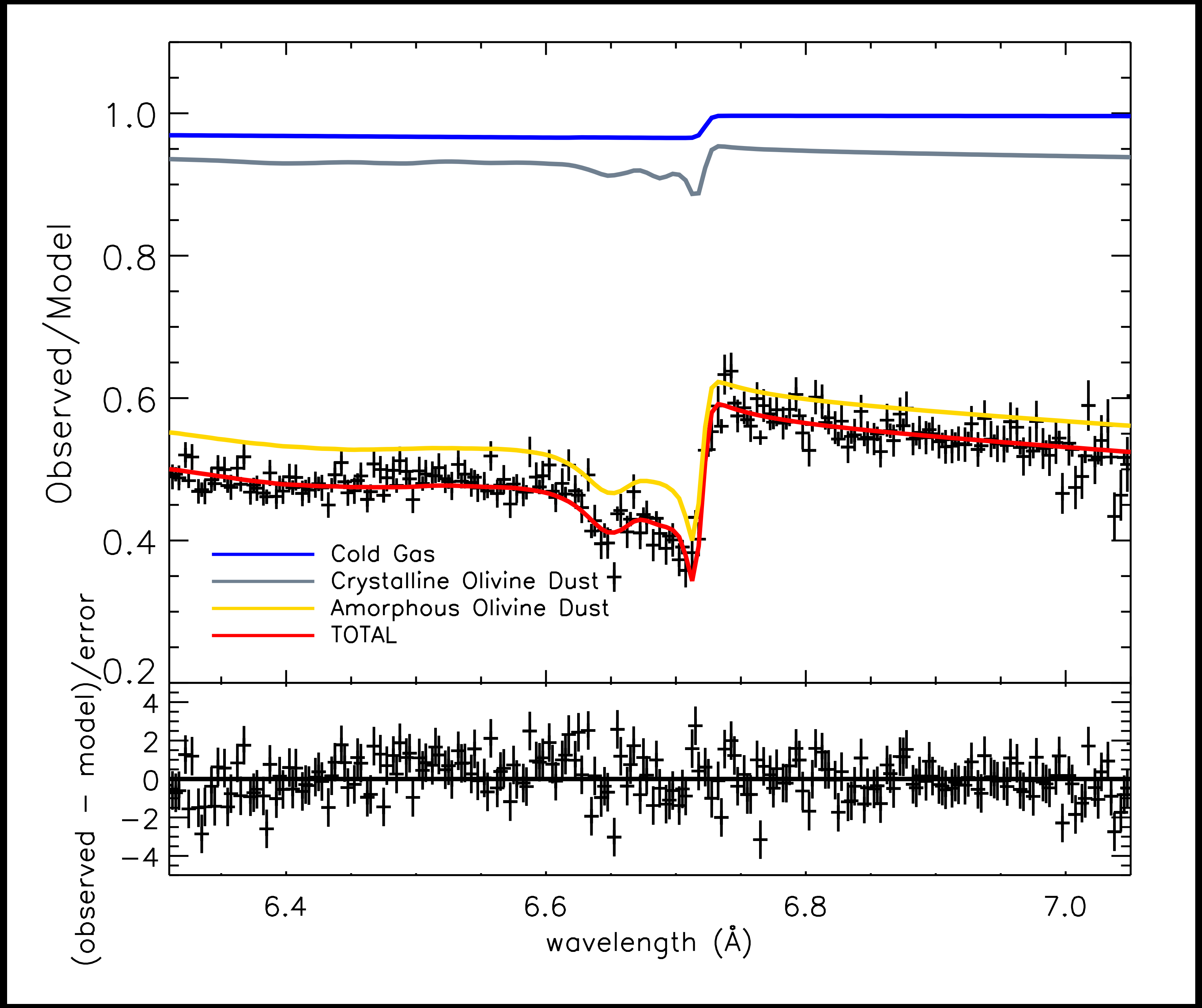
Other Compounds

Mg K-edge



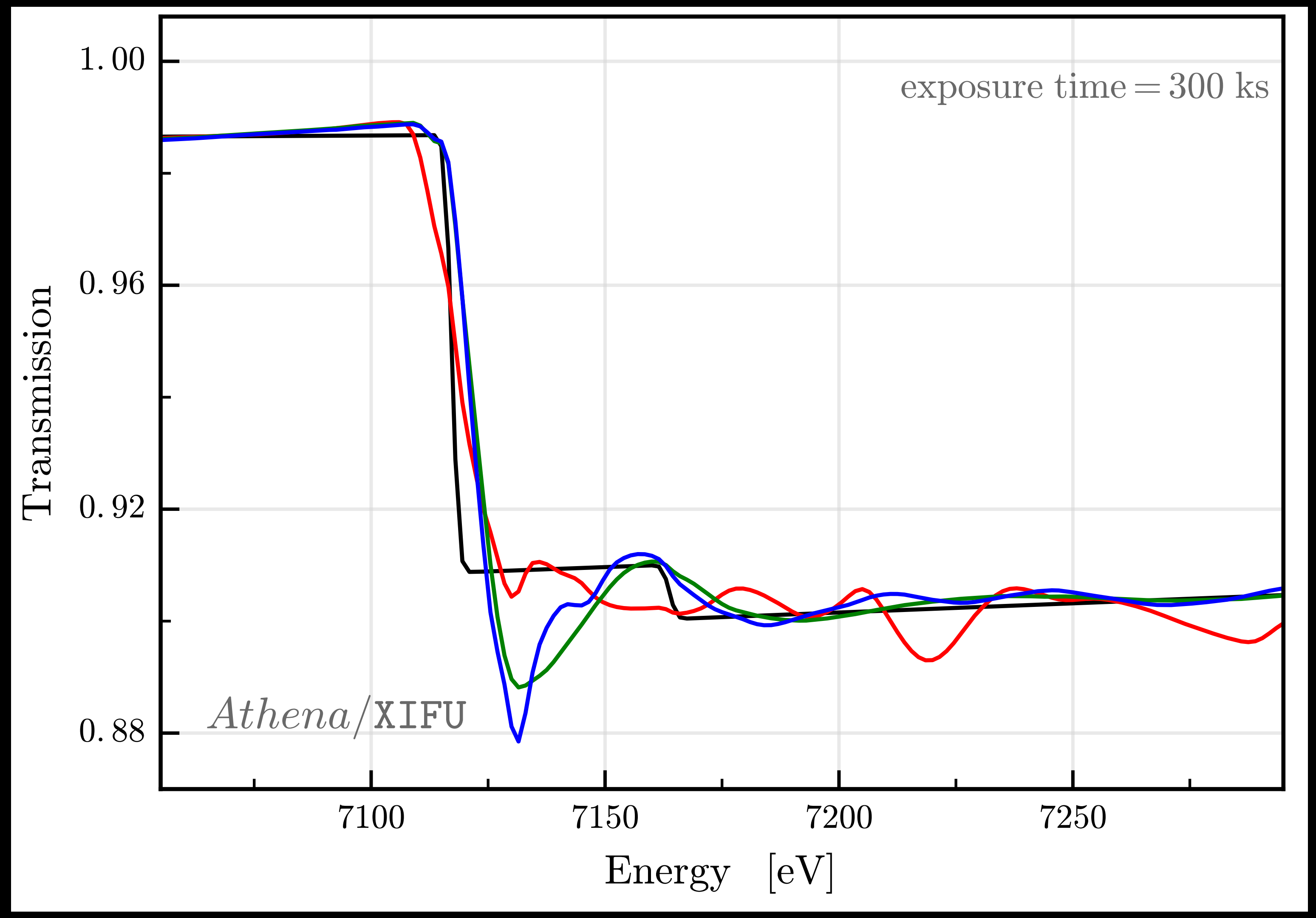
Rogantini+19

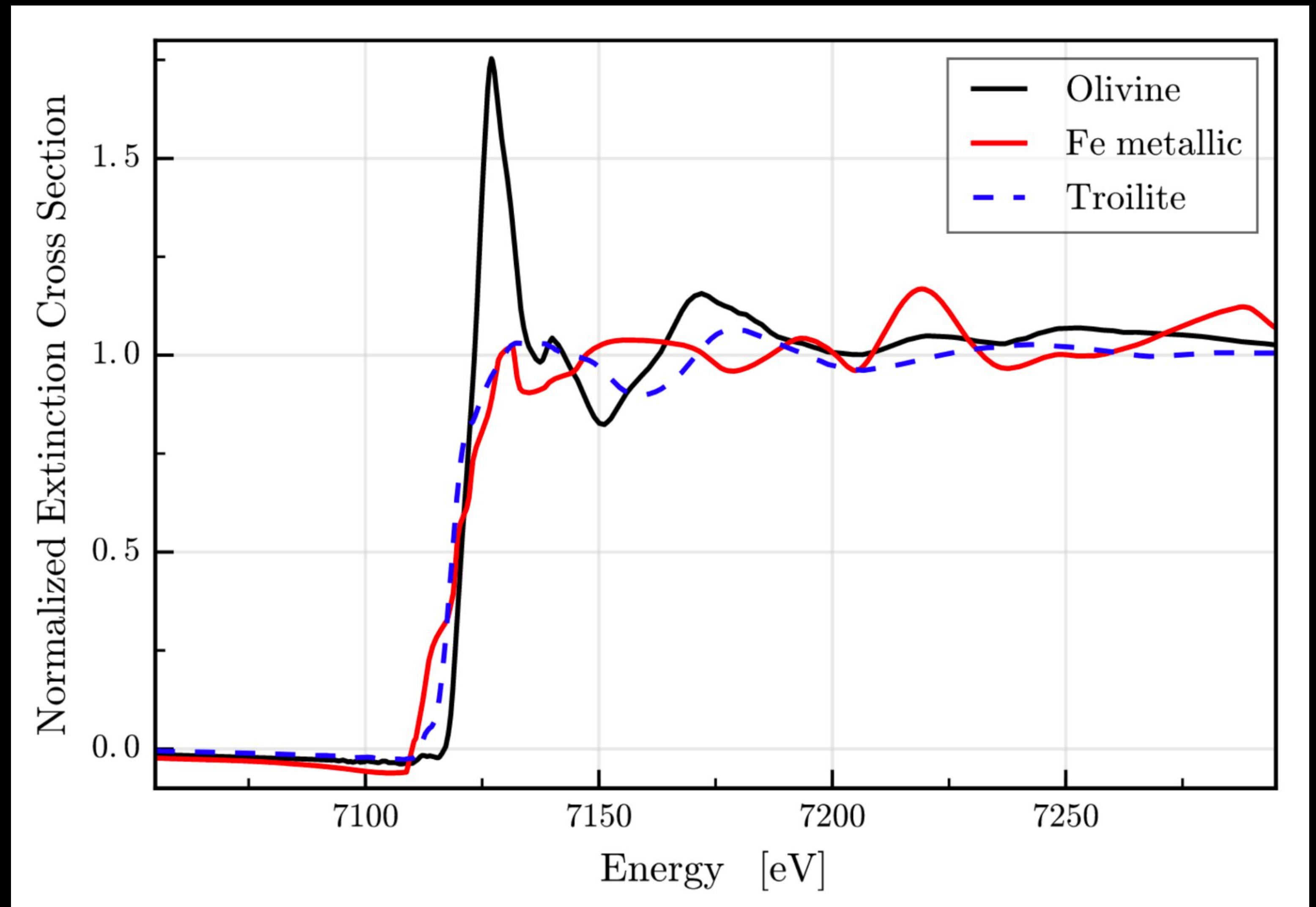
Si K-edge



Zeegers+15,+19

Fe K-edge

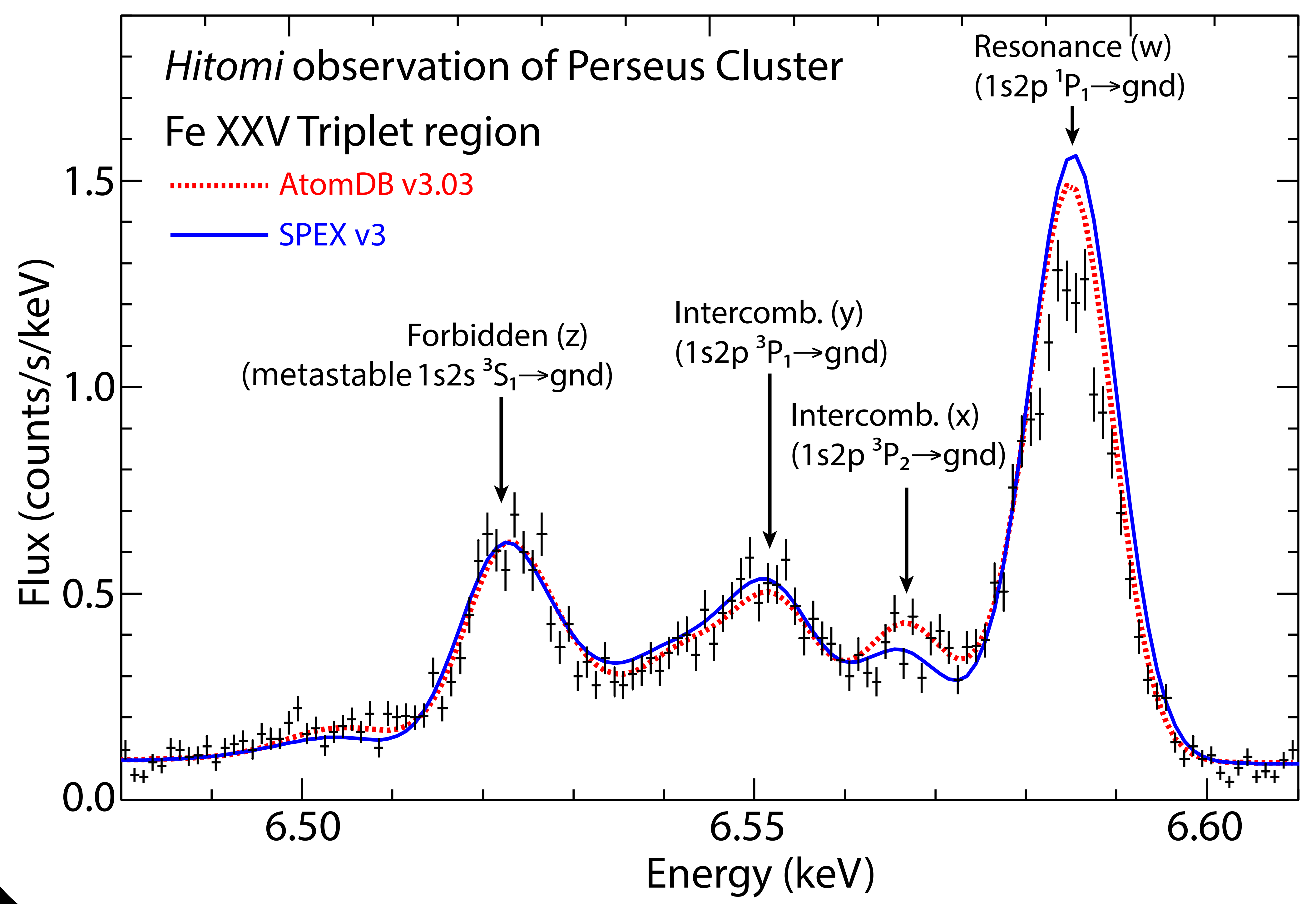




Rogantini+18

Case II: The Perseus Cluster with Hitomi

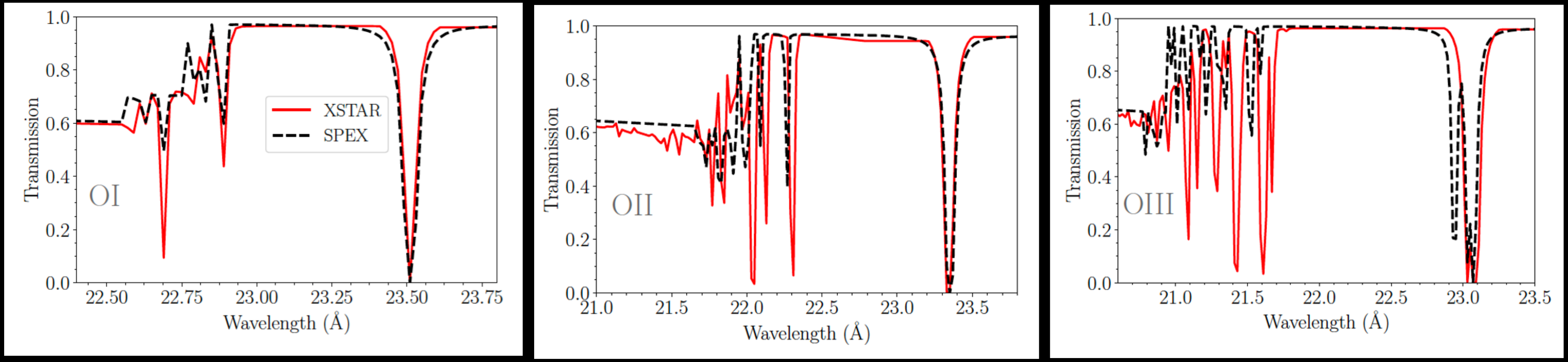
- Analysis with different plasma codes gives statistically acceptable fits
- 16% difference in Fe abundance between SPEX and APEC
- Reason: Different collisional excitation and dielectronic recombination rates



Hitomi Collaboration+18

Atomic Data Uncertainties

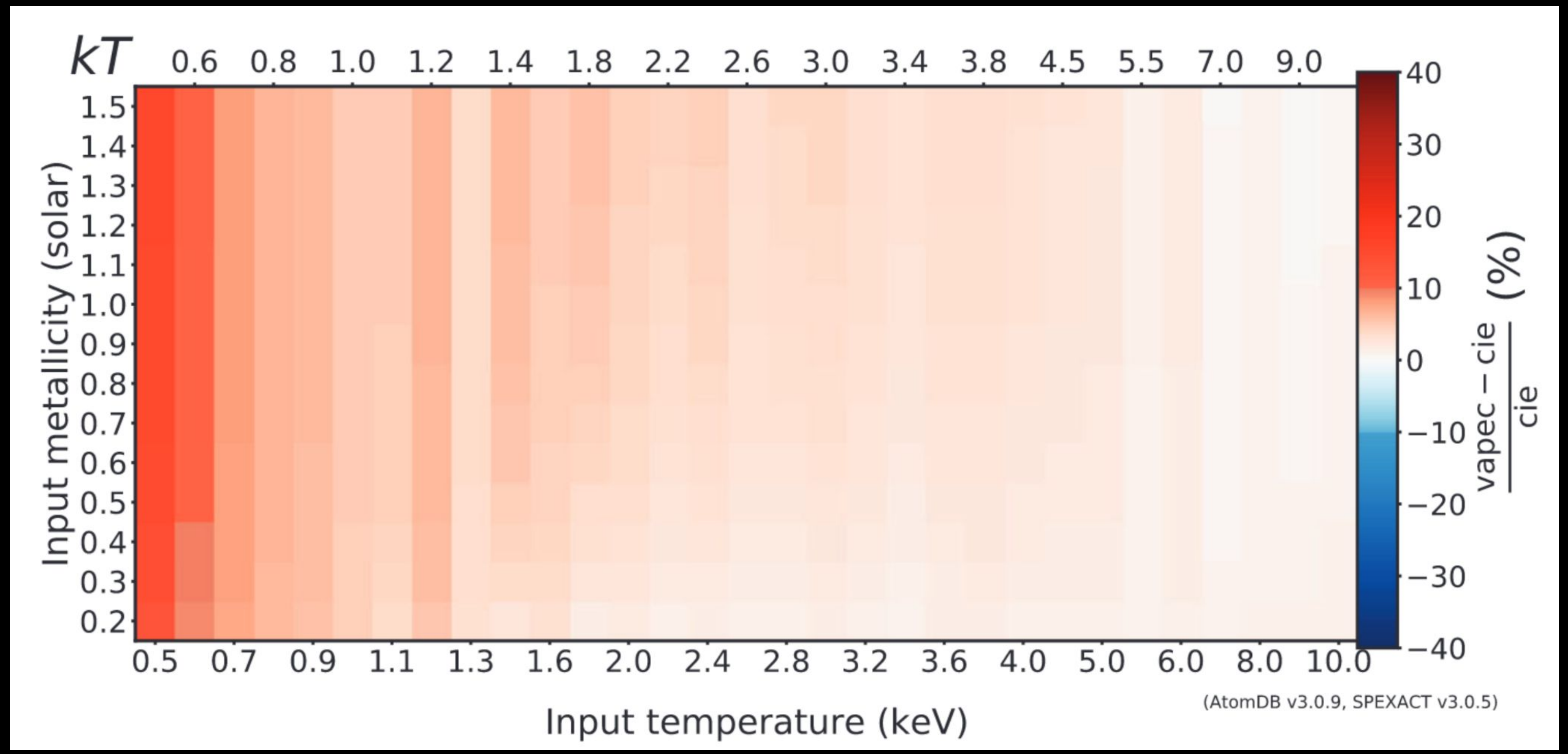
Database Comparison Approach



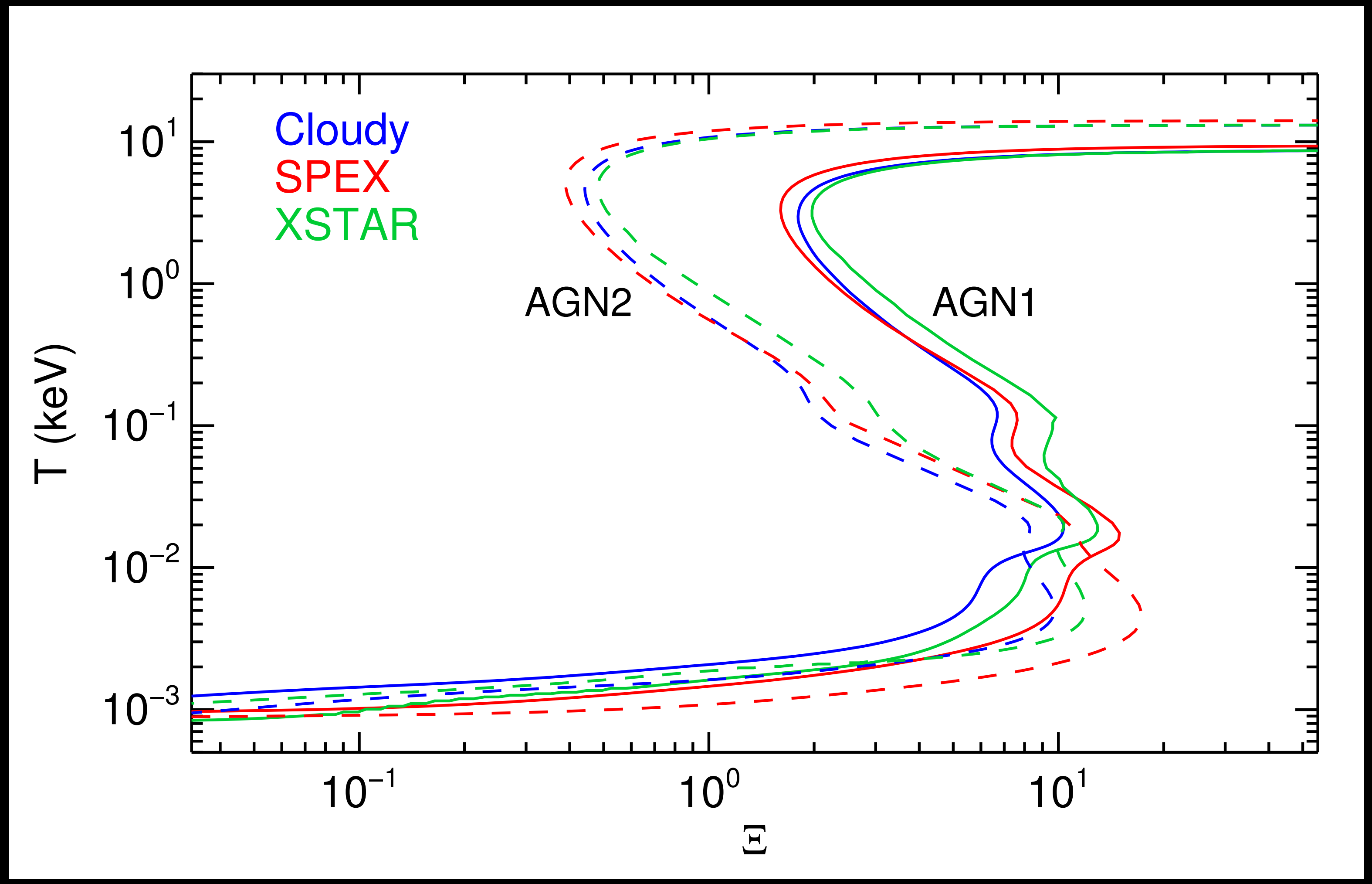
Sources of atomic data:
XSTAR—-García+05
SPEX—-Kaastra+18

Psaradaki+20

Model Comparison Approach



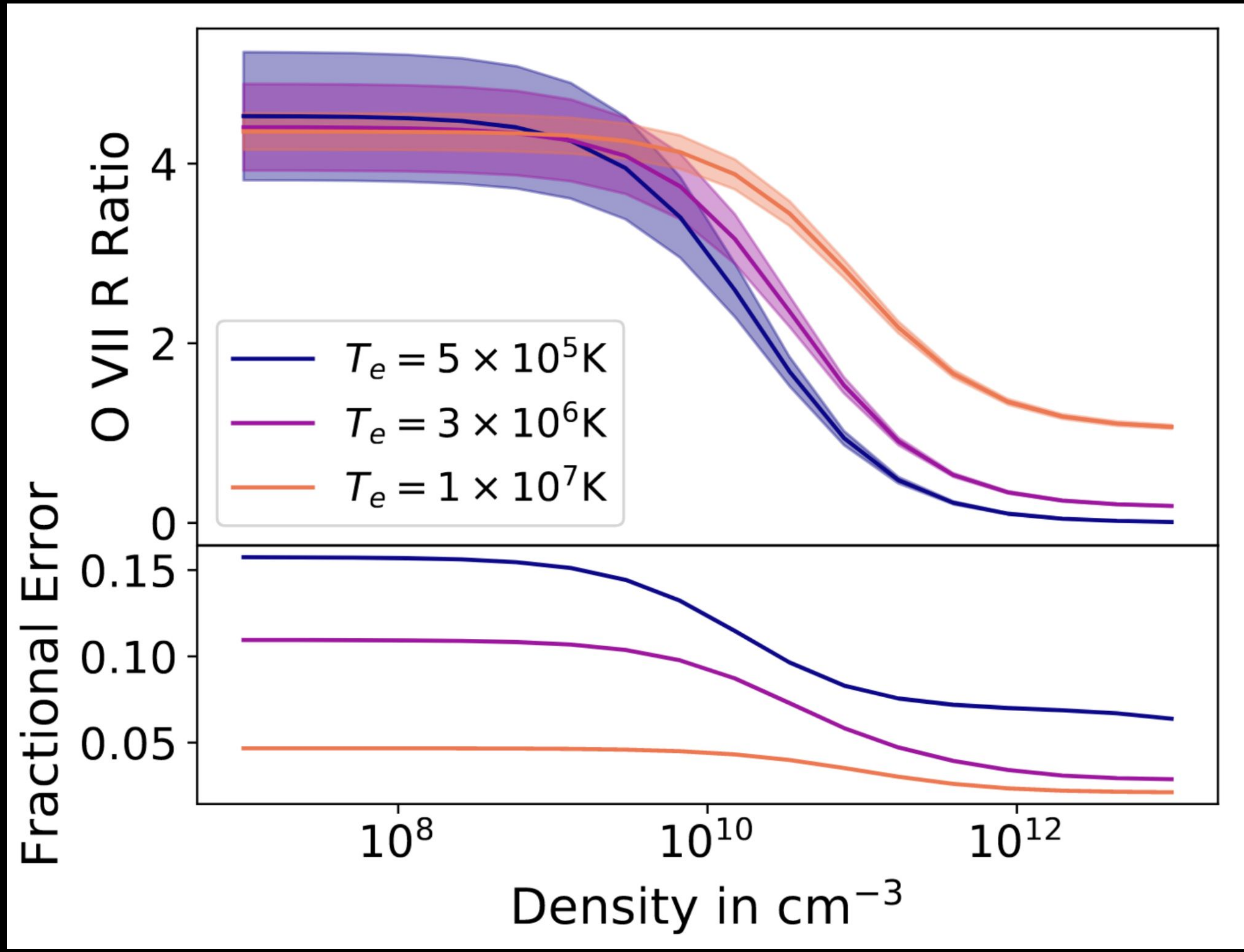
Mernier+20



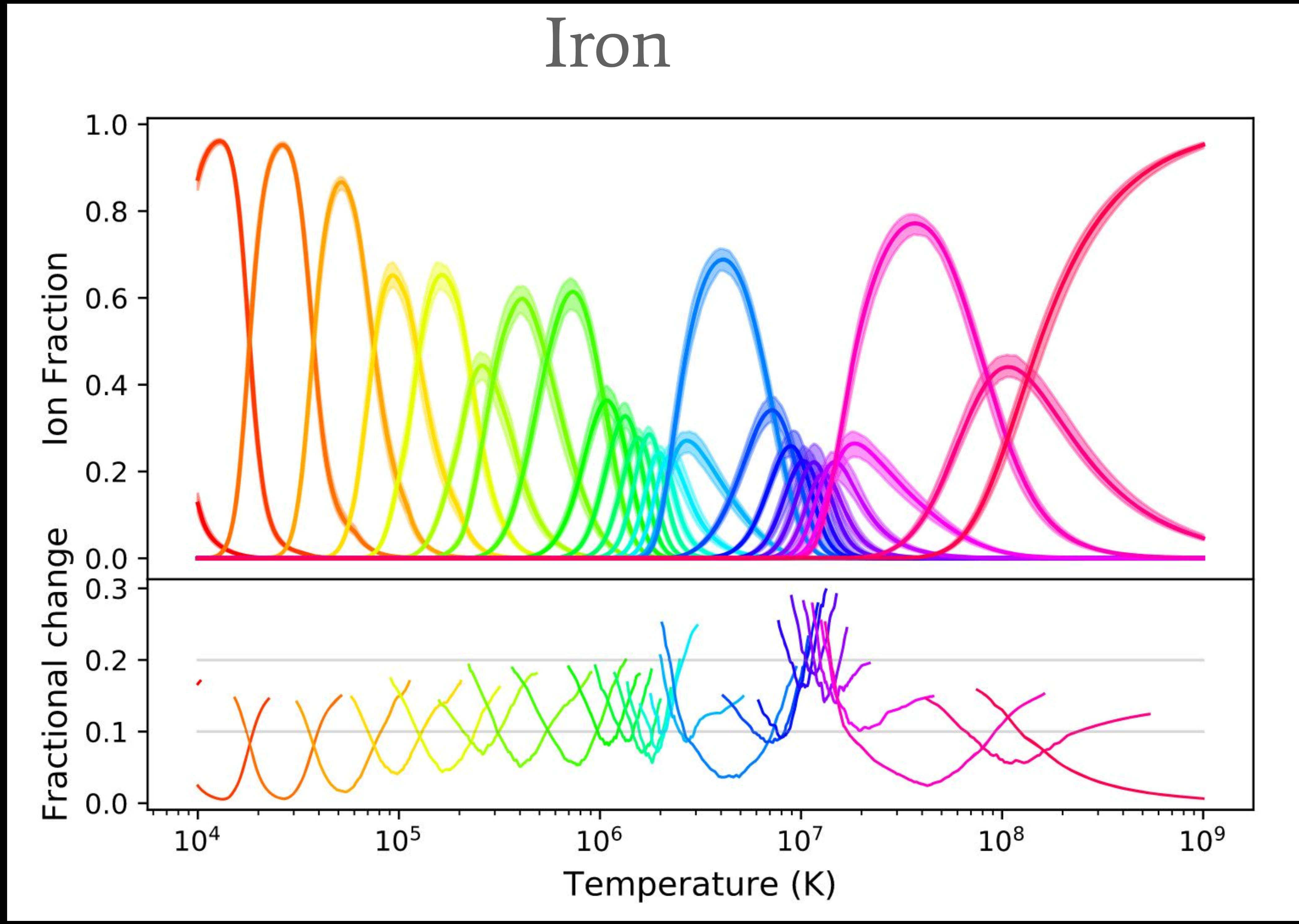
Mehdipour+Kaastra+Kallman16

Atomic Data Uncertainties

Monte Carlo Approach



Foster+Heuer20

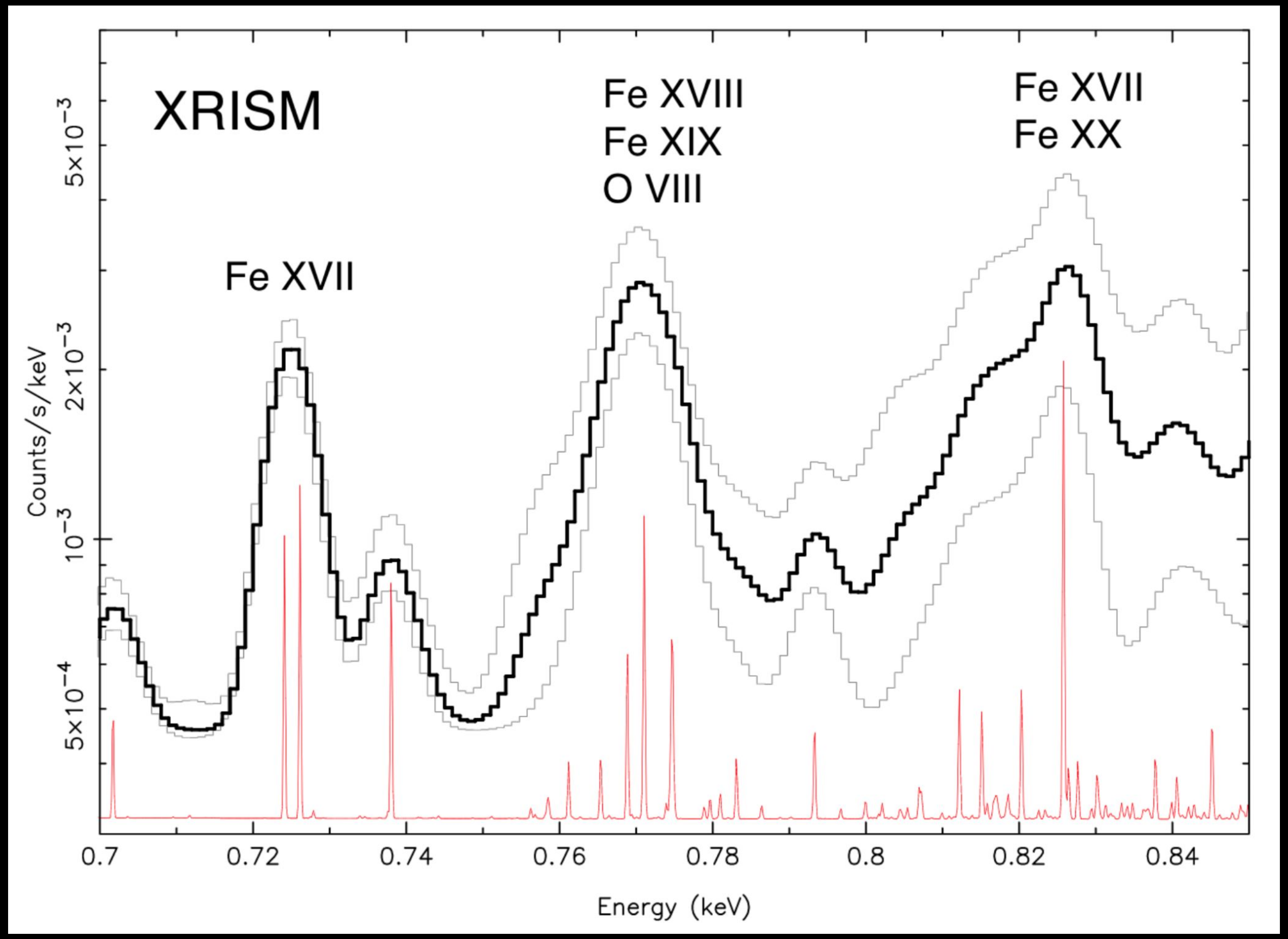


Heuer, Foster+Smith21

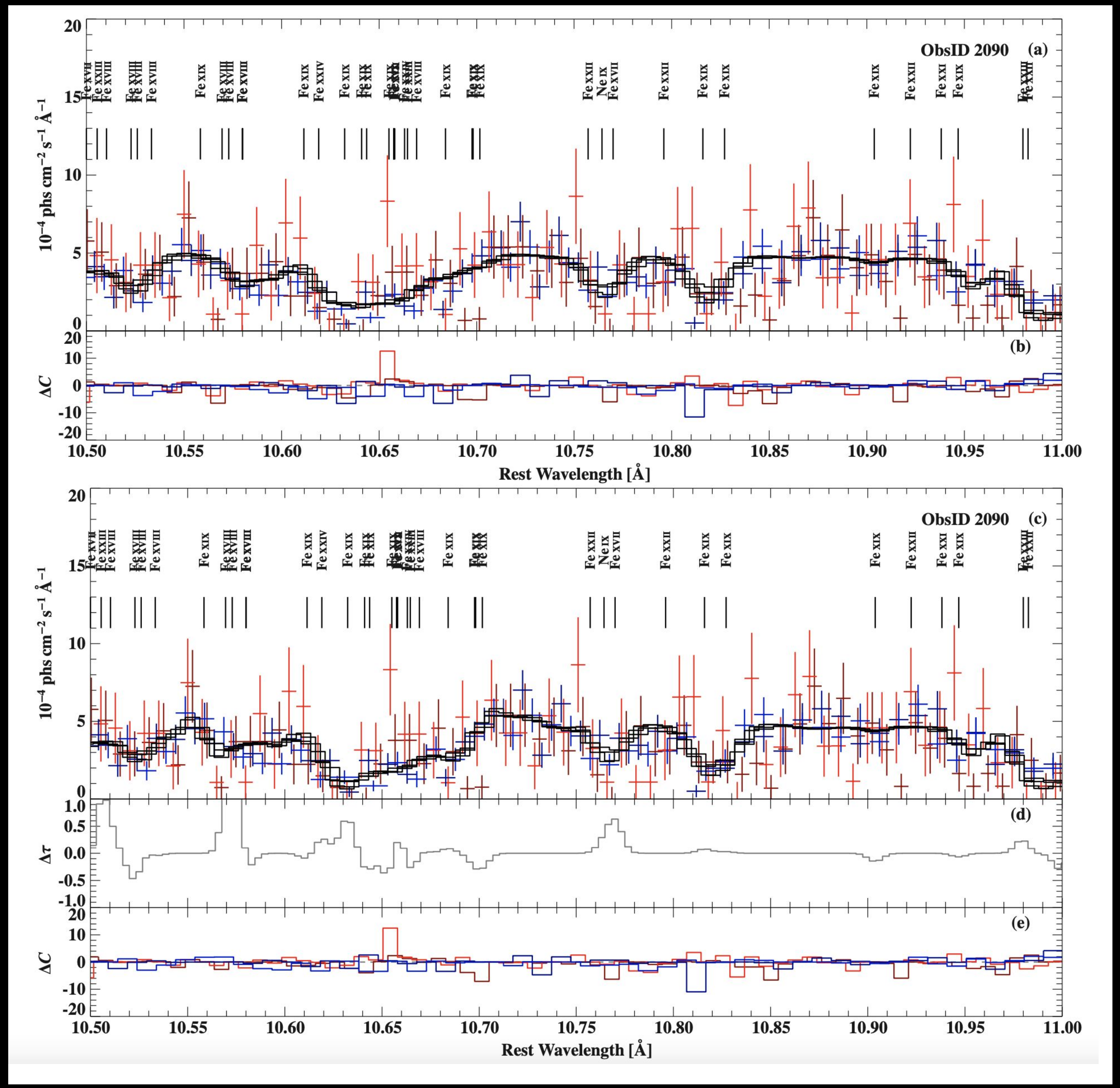
O VII R ratio with a ±15% uncertainty on the DE rates and A-values of the forbidden, resonance, and inter- combination lines

Atomic Data Uncertainties

Data Driven Approach



Gu+22



Ballhausen+23

Good: Atomic data uncertainties can account for some of the fit deficiencies, but not entirely!

Bad: the statistical treatment is not trivial

Simulated spectra for a CIE plasma

Derived systematic uncertainties in temperature, abundances, and line emission

Final Remarks

Laboratory astrophysics plays a fundamental role in the study of astrophysical sources and thus needs to be considered with care

- The higher the resolution and/or signal, the larger is the pain! Atomic data uncertainties can be important (10's %), and still not fully understood

- Be mindful of your limitations regarding model and data: with great data comes great responsibility. Spectral models are highly complex and need to be used in the way they are intended

- The ultimate goal is to understand the physics, ***not just to have a good fit!***

=> Talk to your Lab Astro or Atomic Physicist of trust, they will help you!

Other Resources

* Ralf Ballhausen’s talk from the 1st XRISM Workshop (2023)
* Randall Smith’s online slides on spectral codes
* NIST website
* AtomDB
* UADB