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Nebular emission lines in kilonovae spectra: Insights from atomic calculations

Leo Patrick Mulholland

HEAVYMETAL VI @ MacDonald Forest Hills

Queen's University Belfast BT71NN
Luke Shingles, Zewei Xiong, Niamh Ferguson, Michael McCann, Albert Sneppen
Niall McElroy, David Dougan, Fiona McNeill, Steve Bromley, Stuart Loch, Oli Just,
Andreas Bauswein, Beth Campbell
Catherine Ramsbottom, Connor Ballance and Stuart Sim

And the HEAVYMETAL consortium

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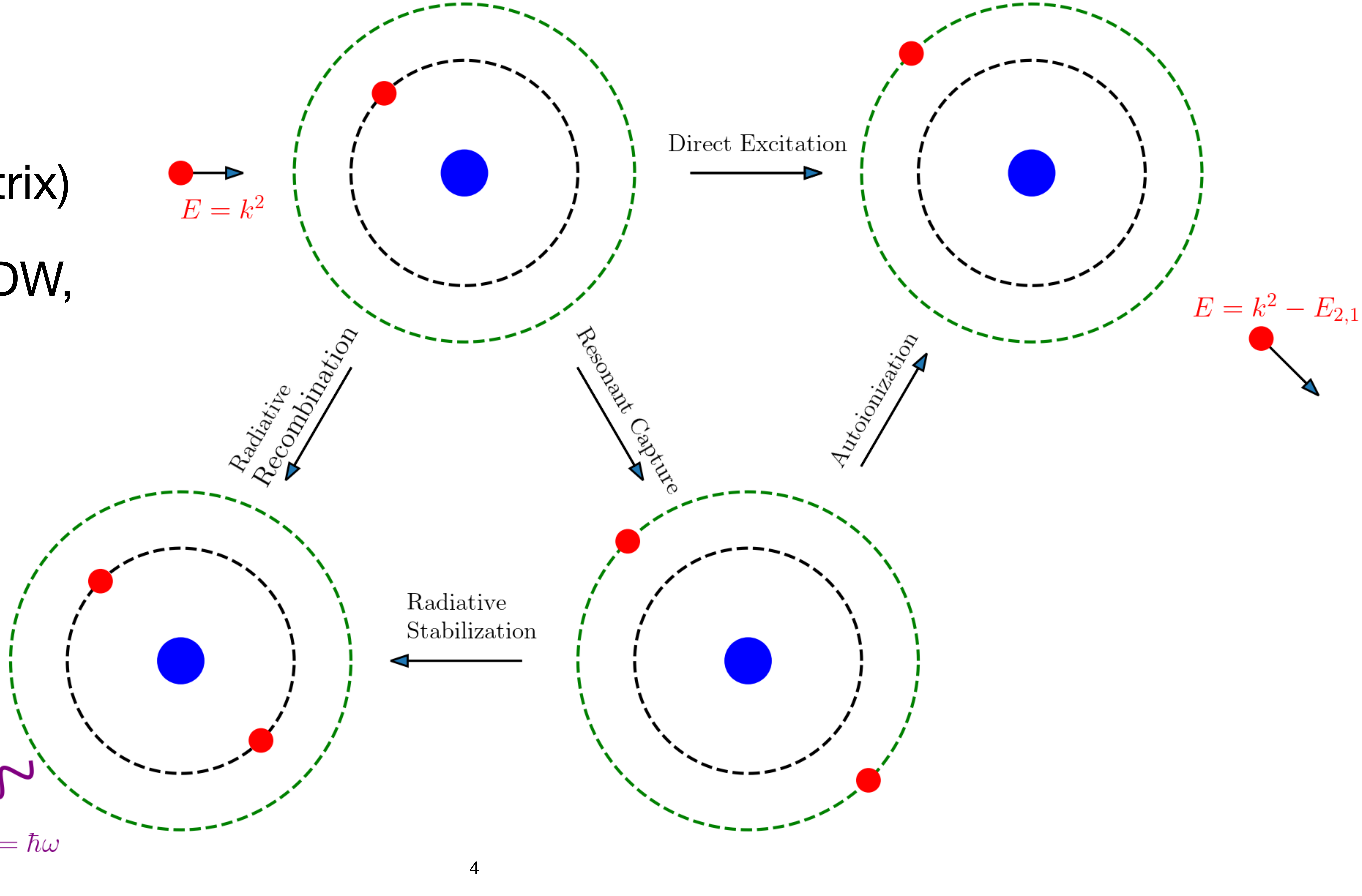
Outline

1. Atomic data
2. Te
3. Ce
4. First peak

1. Atomic data

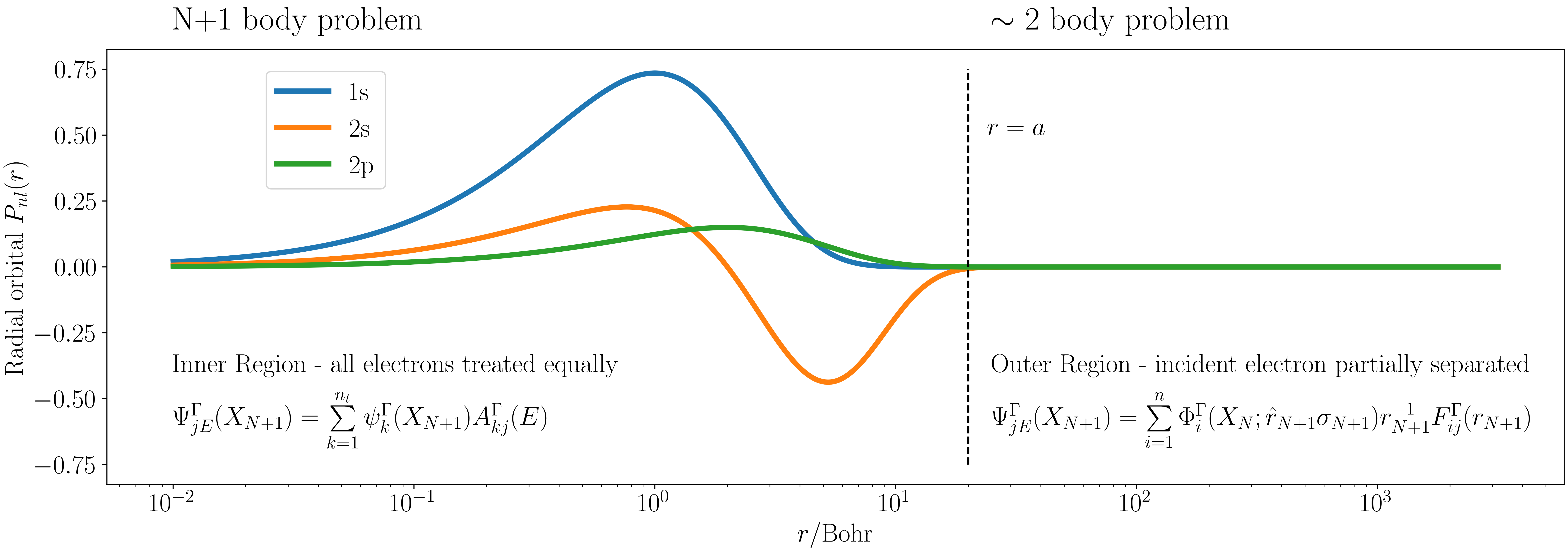
Atomic Processes of Interest

- Excitation (R-matrix)
- Recombination (DW, autostructure)



R-matrix method

For collisional excitation



A note on analytic formulae

For collisional excitation

On the use of the Axelrod formula for thermal electron collisions in astrophysical modelling

Leo P. Mulholland [a],*, Steven J. Bromley [b], Connor P. Ballance [a], Stuart A. Sim [a], Catherine A. Ramsbottom [a]

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- Allowed transitions: formula of van Regemorter: $\Upsilon_{ij} = 2.39 \times 10^6 \lambda^3 A_{ji} g_j G(E/kT)$
- Forbidden, $\Upsilon_{ij} = \alpha g_i g_j$, $\alpha = 0.004$ from Axelrod's thesis
- Forbidden lines generally the bottleneck
- Can be (almost) remedied by rescaling

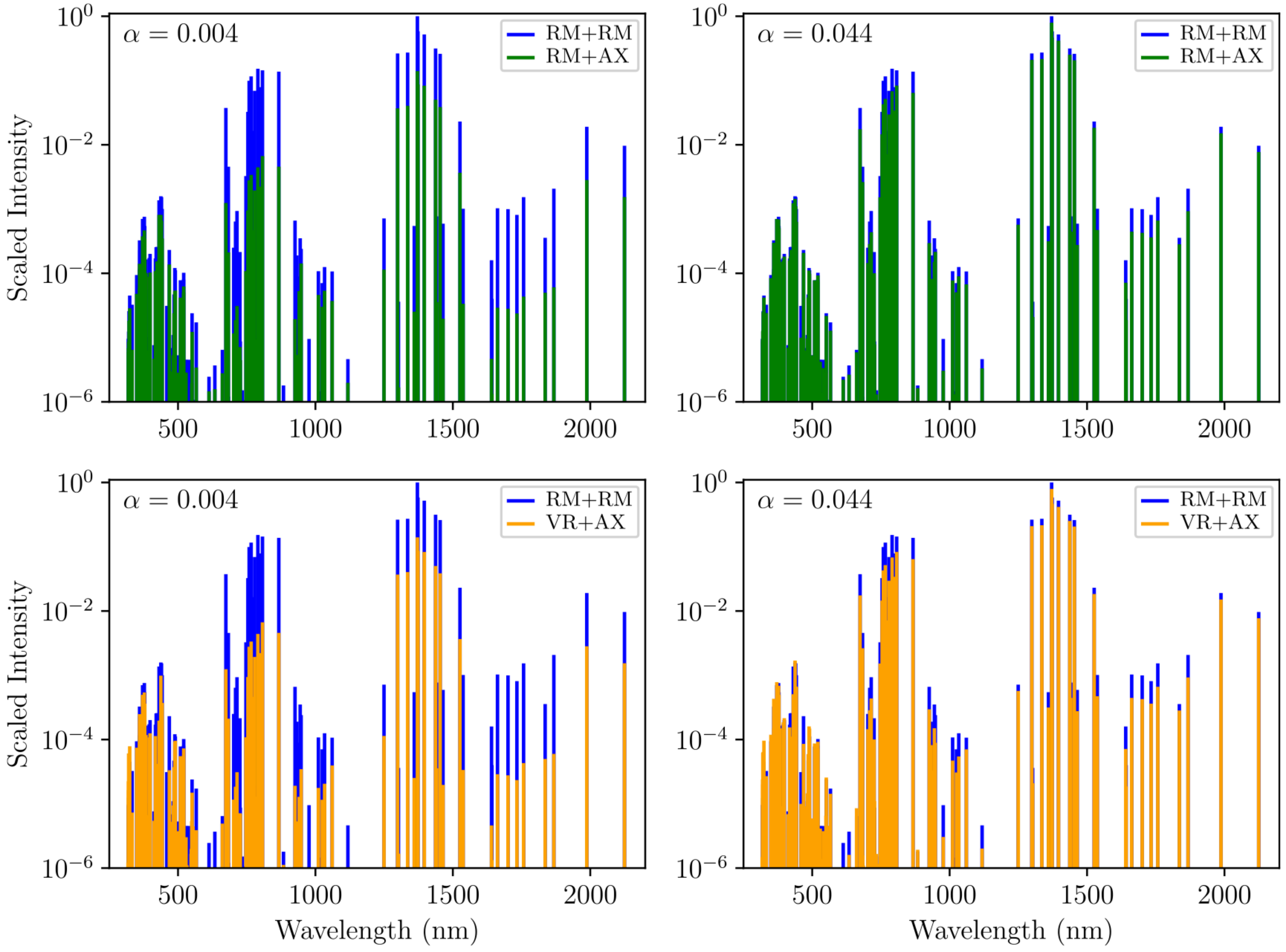
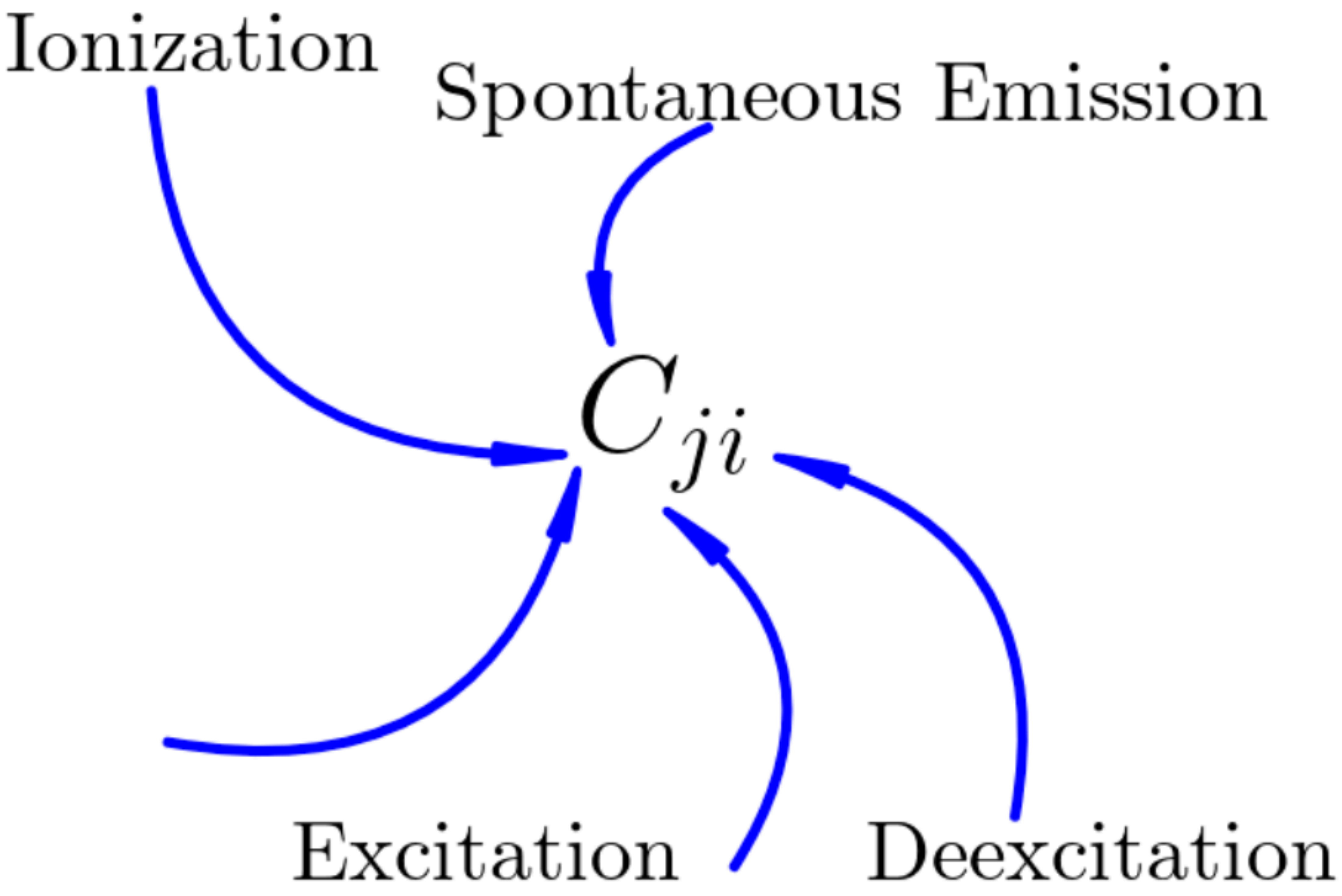


Fig. 1. Optically thin emission spectra of Y II at an electron temperature of 2900 K and electron density 10^6 cm^{-3}.

Mulholland+25 (see also Andreas Flörs' PhD thesis)

Collisional Radiative Modelling

101 Definitions of NLTE



$$\frac{dN_i}{dt} = \sum_{j \neq i} N_j R_{j \to i} - N_i \sum_{j \neq i} R_{i \to j}$$

Self Opacity:

$$\tau_{i \to j} \propto A_{i \to j} \lambda^3 N_i$$

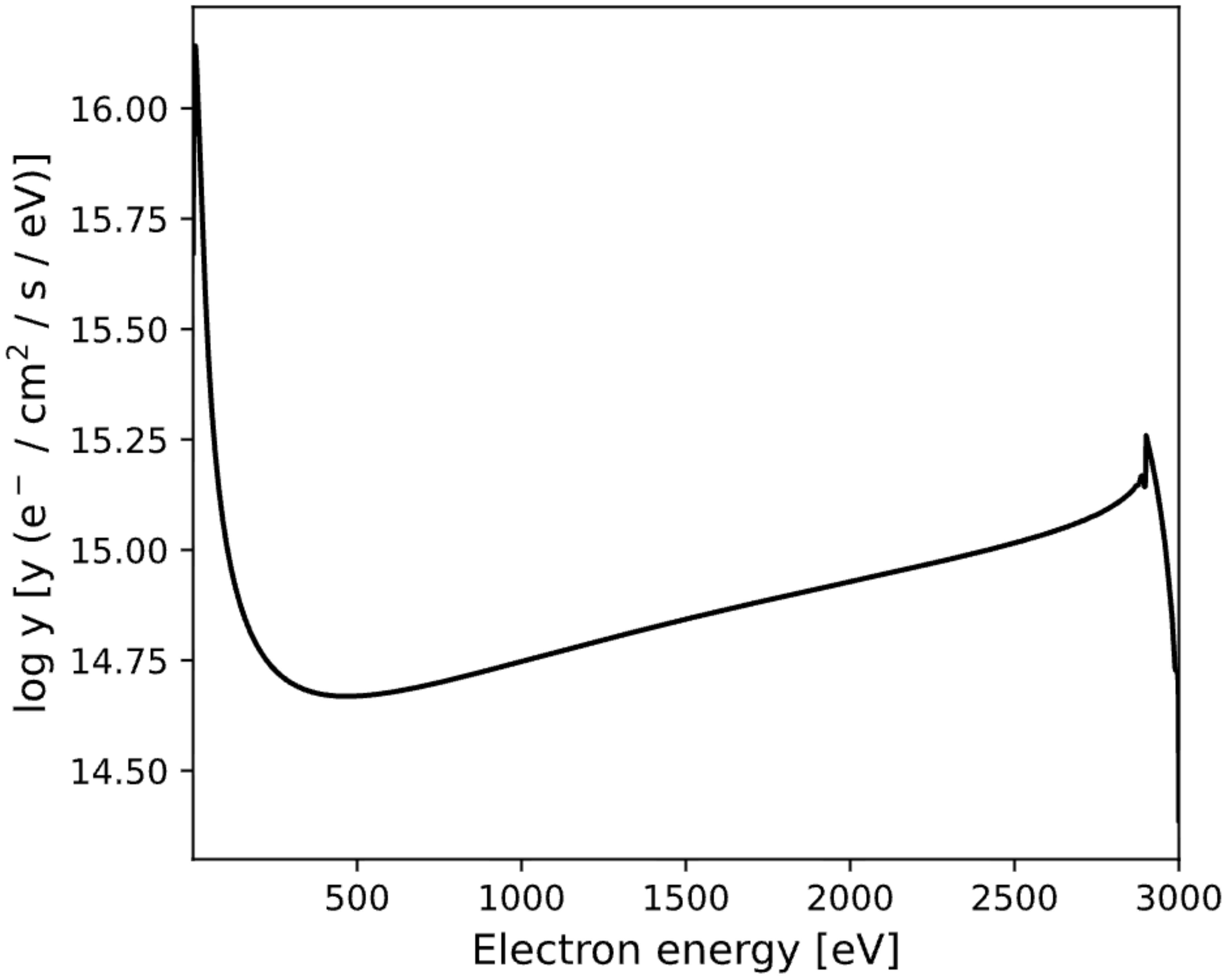
Emission lines:

$$L_{line} \propto N_j \beta^{esc}_{j \to i} A_{j \to i}$$

Collisional Radiative Modelling

101 Definitions of NLTE

- Ionization balance:
  $N^{z+1} R^{eff}_{z+1 \rightarrow z} = N^{z} S^{eff}_{z \rightarrow z+1}$
- Recombination rates from AS
- Ionization rates from pynonthermal (Shingles, Axelrod, Lotz)
- R-matrix ionization coming... (see Dougan+26)



Shingles+26, Kozma+92

2. Tellurium

Tellurium

Electron impact excitation of Te IV and V and level resolved R-matrix photoionization of Te I–IV with application to modelling of AT2017gfo

Leo P. Mulholland [1★], Catherine A. Ramsbottom [1], Connor P. Ballance [1], Albert Sneppen [2,3] and Stuart A. Sim [1]

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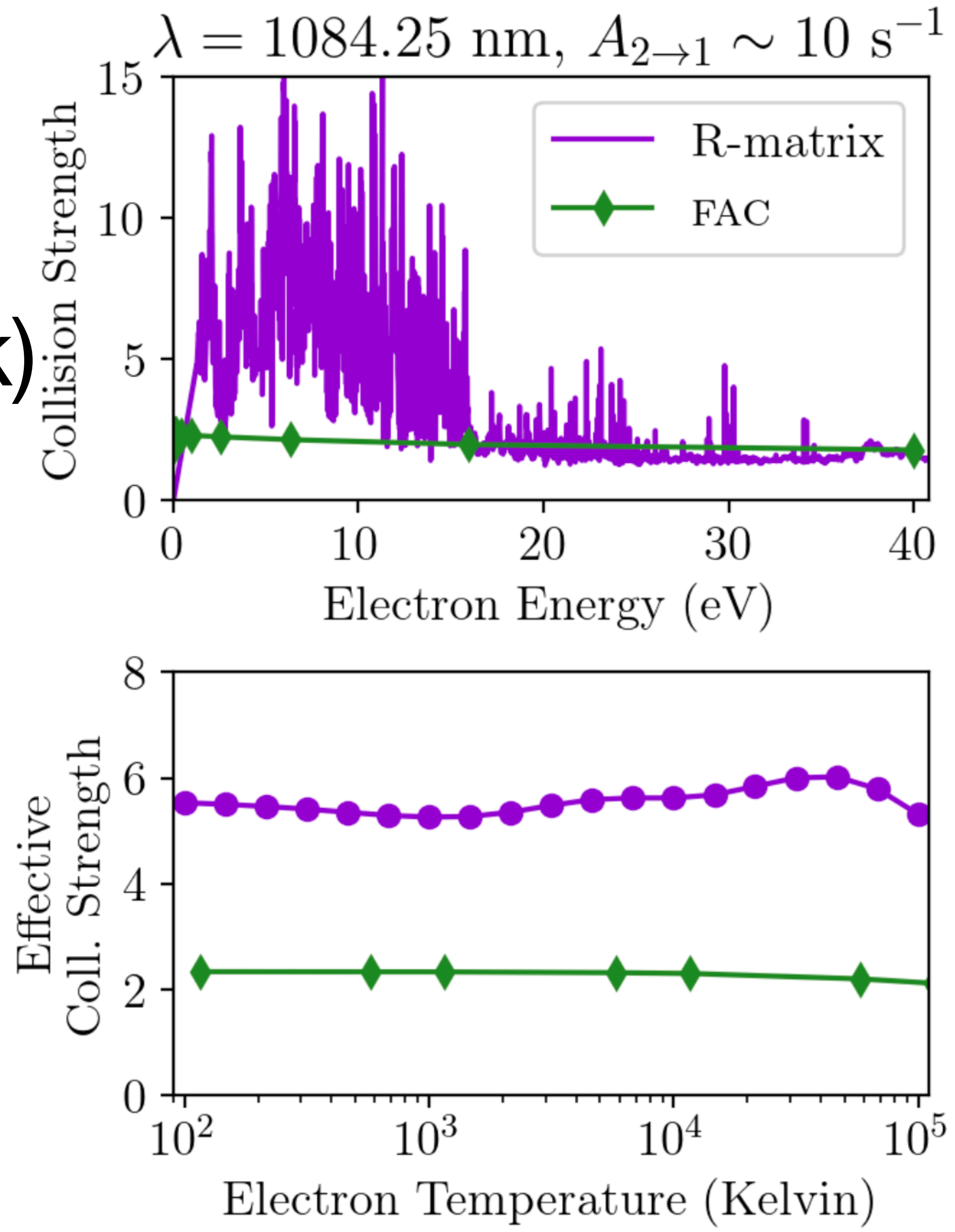
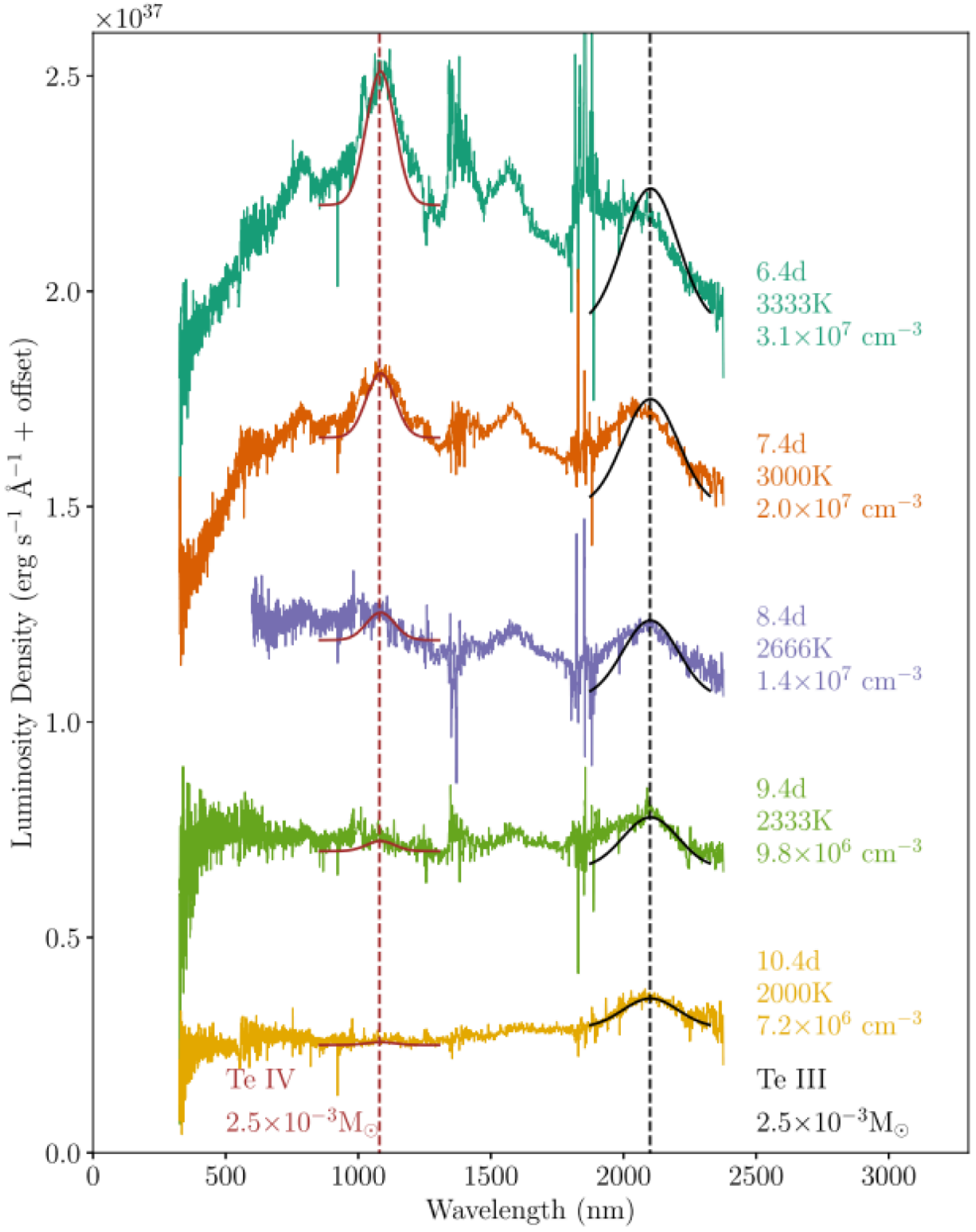
[2] Niels Bohr Institute, University of Copenhagen, Jagtvej 128, 2200 Copenhagen N, Denmark
[3] Cosmic Dawn Center (DAWN), Copenhagen, Denmark

- We (might) hear a lot about Te this week...
- Sr II at 1.08μm... (Aayush' talk)
- Noteworthy that Te IV aligns well with 1.08μm emission in gfo
- Collision strengths, photoionization data public





Mulholland+26a

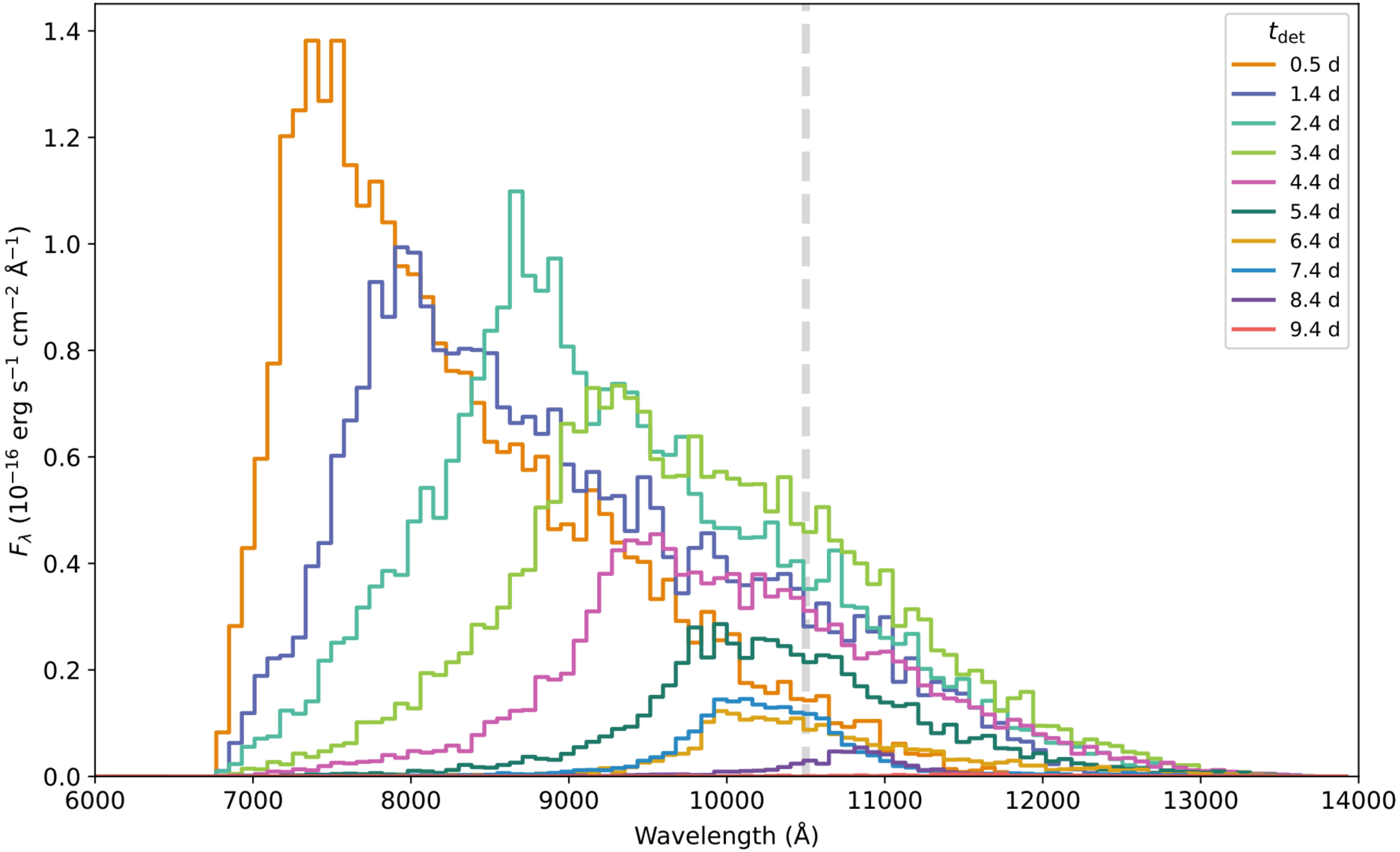
(No ion balance here)

Although...

- Reverberation effects of the Sr II lines may also help explain this (McNeill+26)

- Nonetheless - we have the atomic data to model both Sr and Te

- Te IV emission in models could be a sign of too strong ionisation...

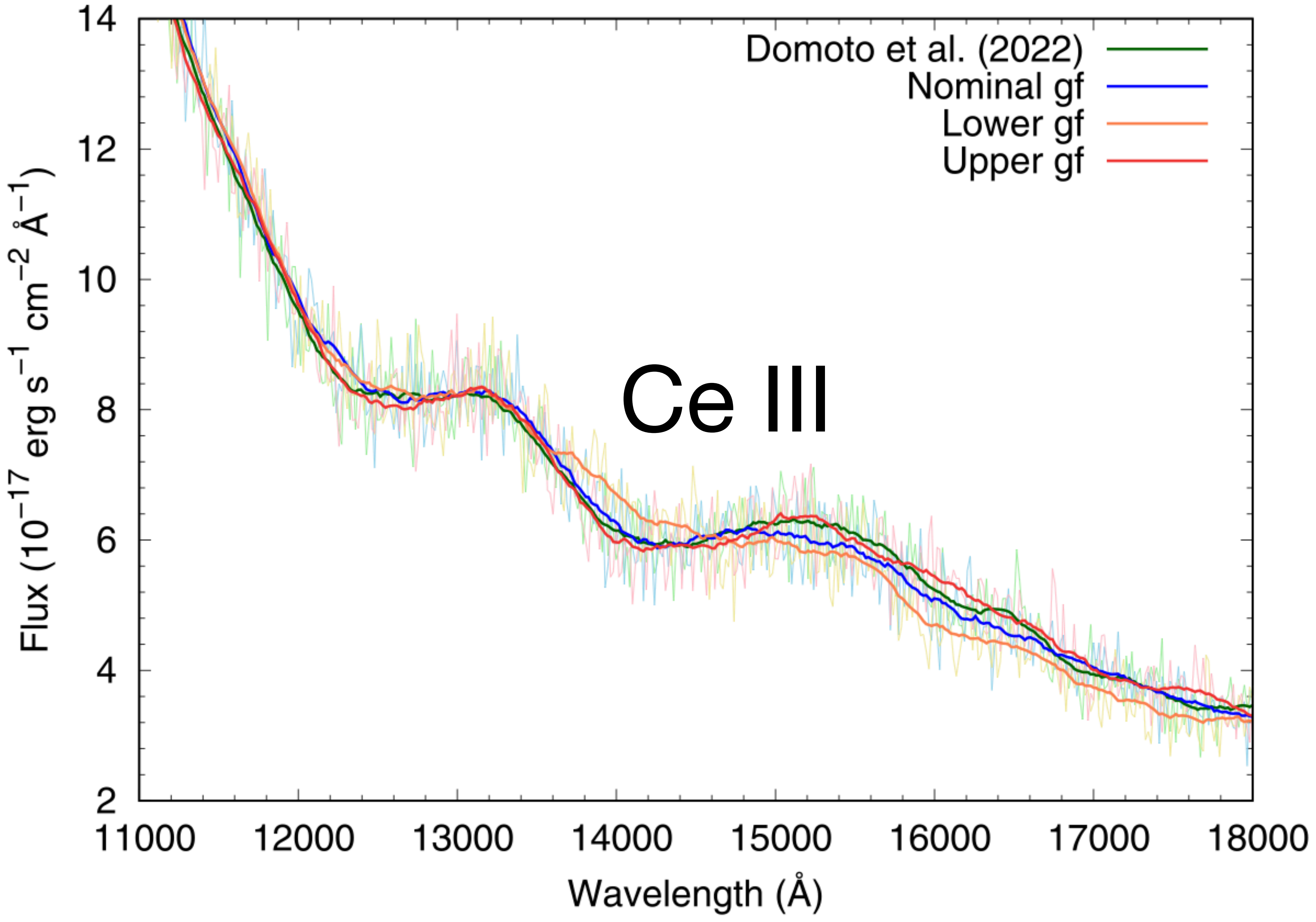


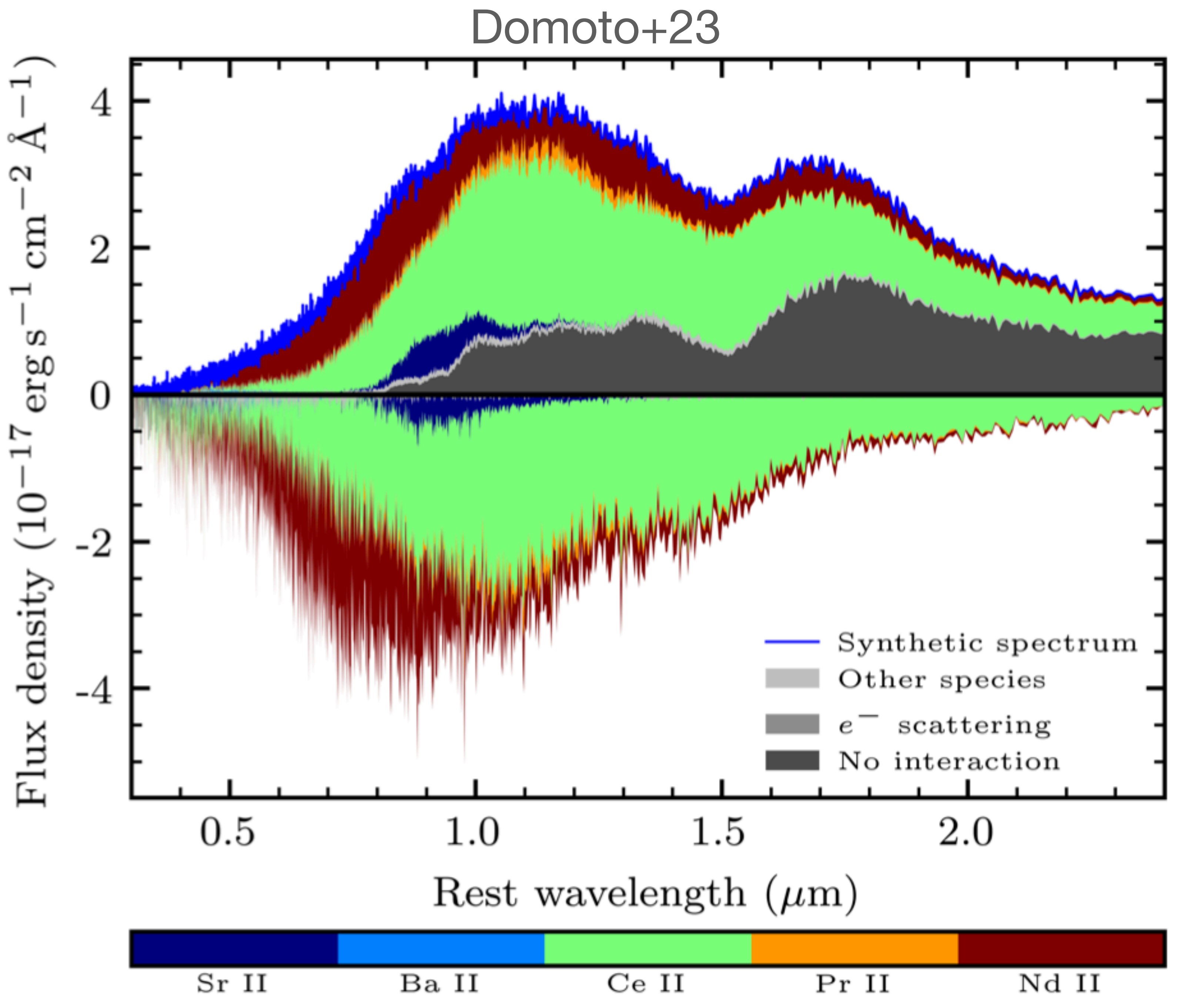
McNeill+26

3. Cerium

Cerium

- Cerium has potential interest across a variety of charge states
- II, III - opacity, cf radiative transfer talks
- III, P-cygni feature, see Domoto+22,23
- IV - potential emission ?
- (cf Tanaka, Flörs yesterday)





Gillanders, Flörs & da Silva (2026)

Cerium

Bound-bound data

- Einstein A-values, R-matrix collision strengths
- Calculated for Ce II - IV

(Mulholland+26b, in prep)

Cerium

Bound-bound data

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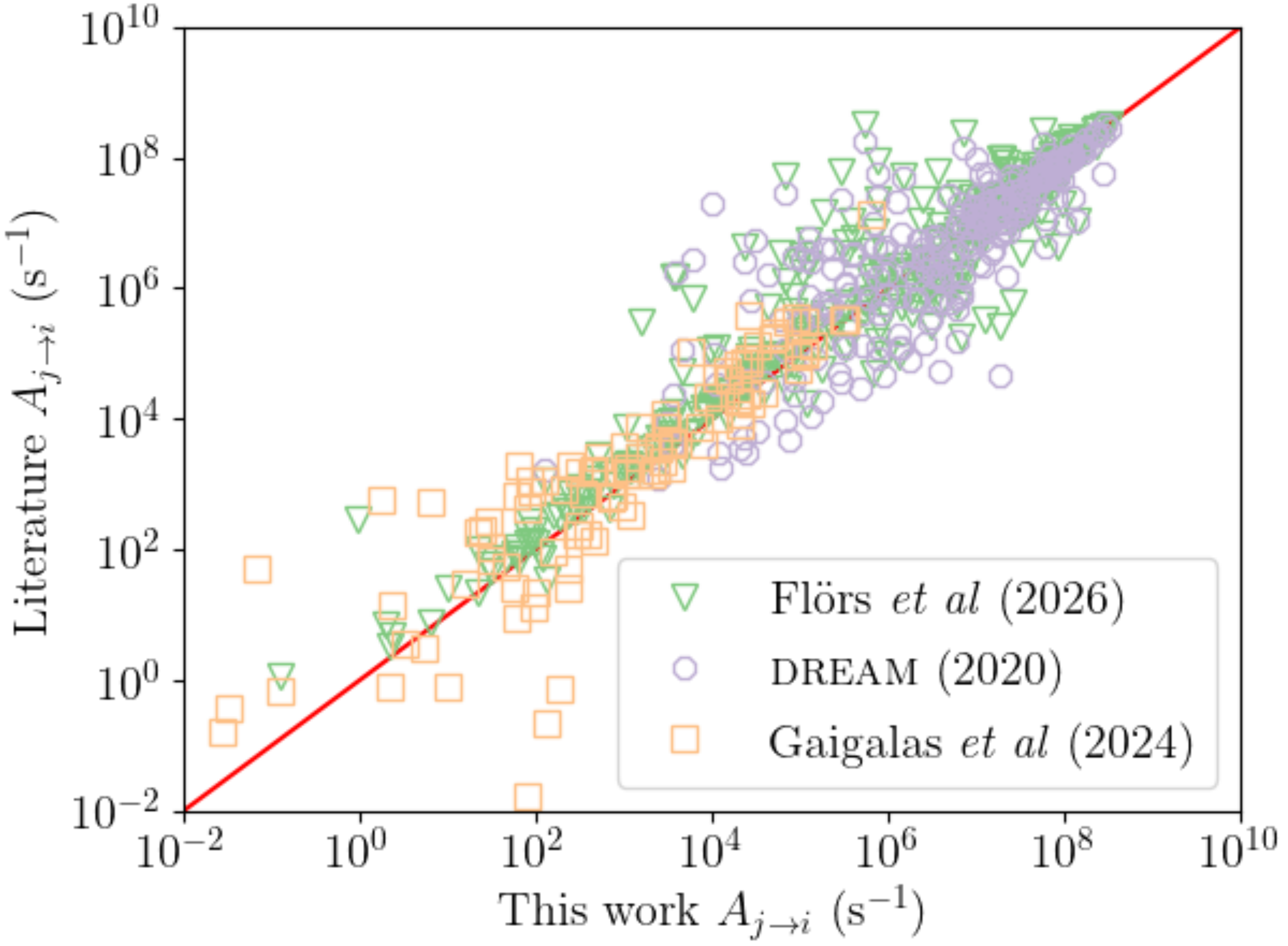
Ce III A-values



(Mulholland+26b, in prep)

Cerium

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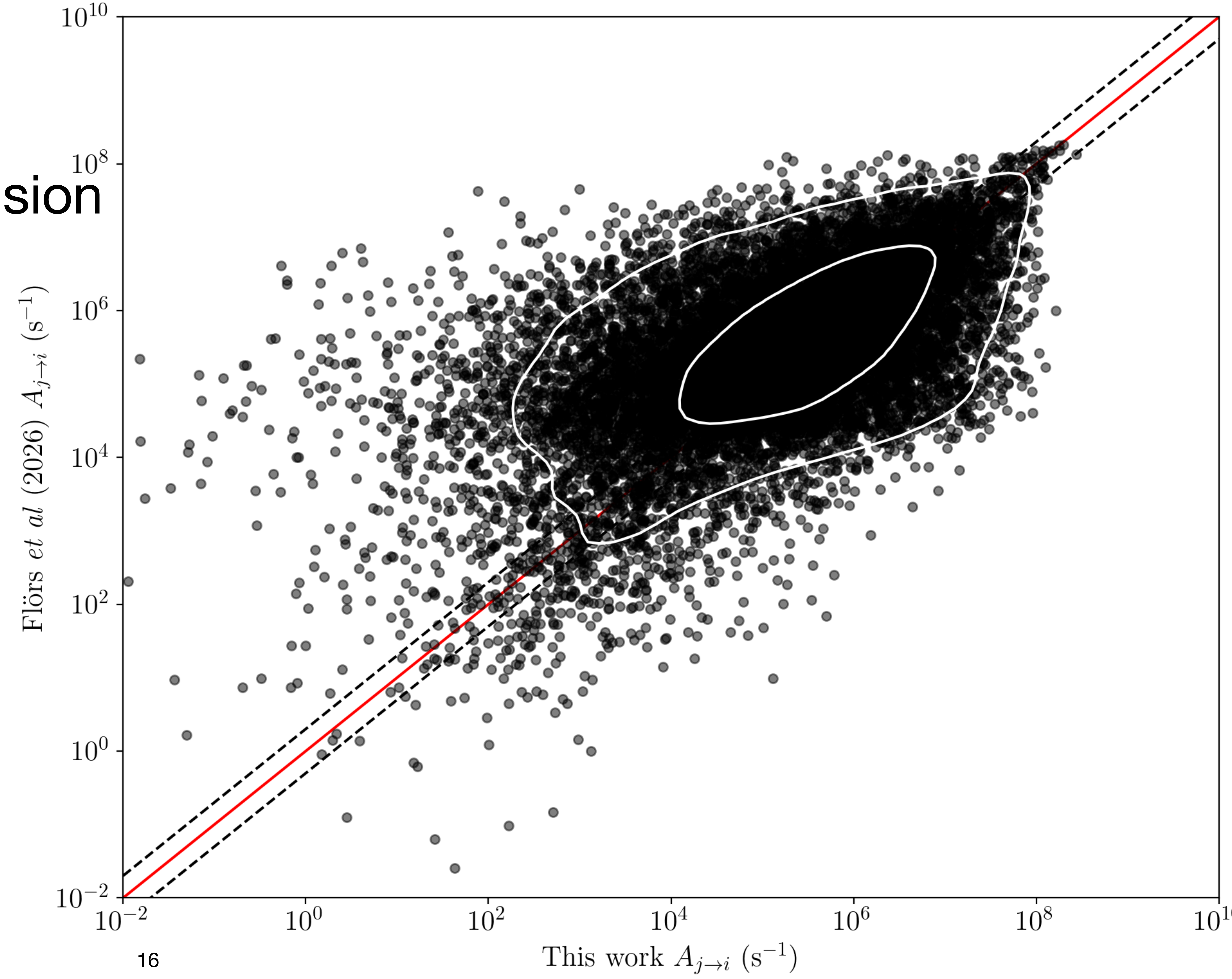
(Mulholland+26b, in prep)

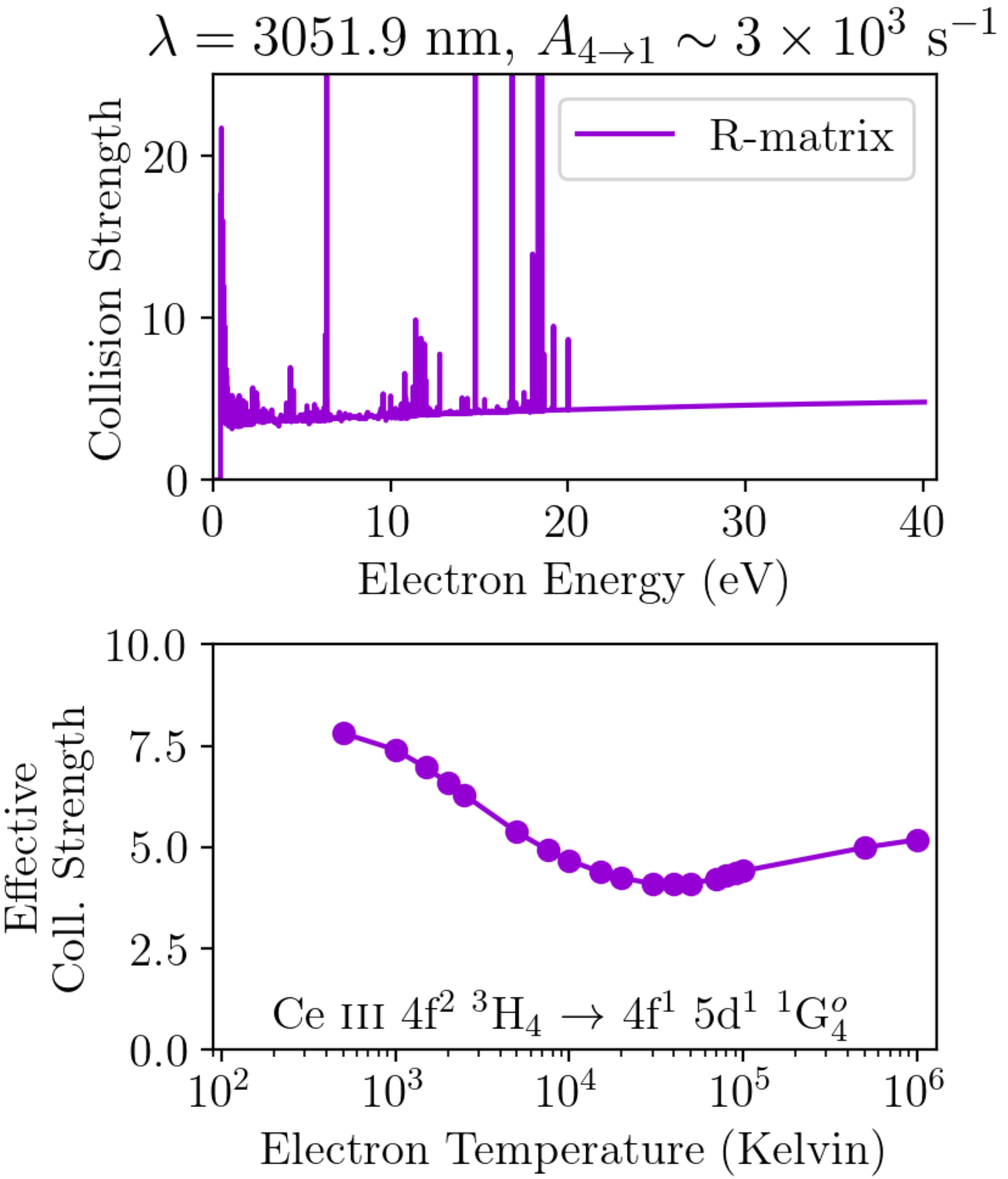
Ce II A-values



Cerium

Bound-bound data

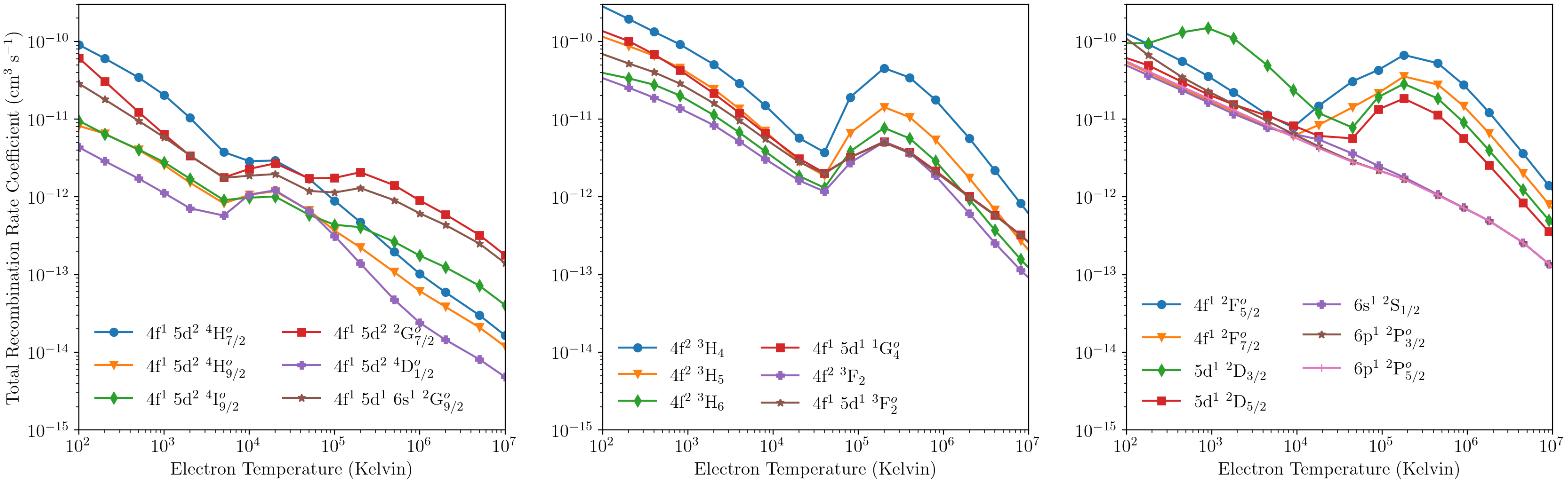
- Einstein A-values, R-matrix collision strengths
- Calculated for Ce II - IV
- Forbidden: $\Upsilon_{ij} = \alpha g_i g_j$
- $\alpha \sim 10^{-3} - 10^{-2}$
- (cf Fe III 4×10^{-3}, Axelrod 1980)



(Mulholland+26b, in prep)

Cerium

Recombination rate coefficients



- RR and DR using autostructure
- Quantum chaos? See John Sheil

(Mulholland+26b, in prep)

Cerium
Charge state balance

- Solar X[Ce] = $\sim 1.6 \times 10^{-3}$ (Prantzos+20, r-residual)
- Dynamical ejecta of gfo, vfi $\sim 5 \times 10^{-2} M_{\odot}$
- Solar expectation $\sim 10^{-4} M_{\odot}$
- Domoto+22 ~ MF $\sim 10^{-5} - 10^{-3}$
  - $\lesssim 5 \times 10^{-5}M_{\odot}$

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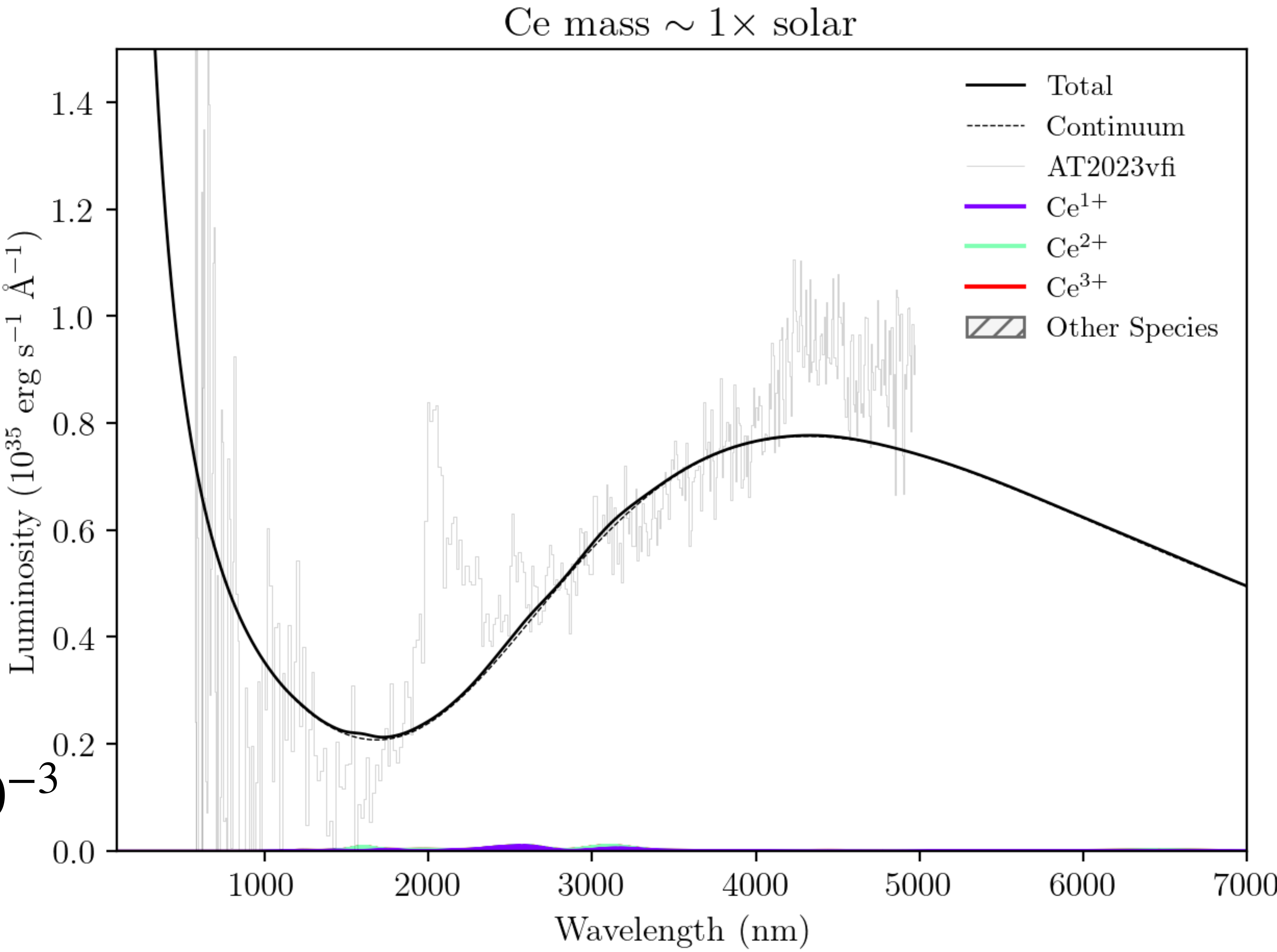
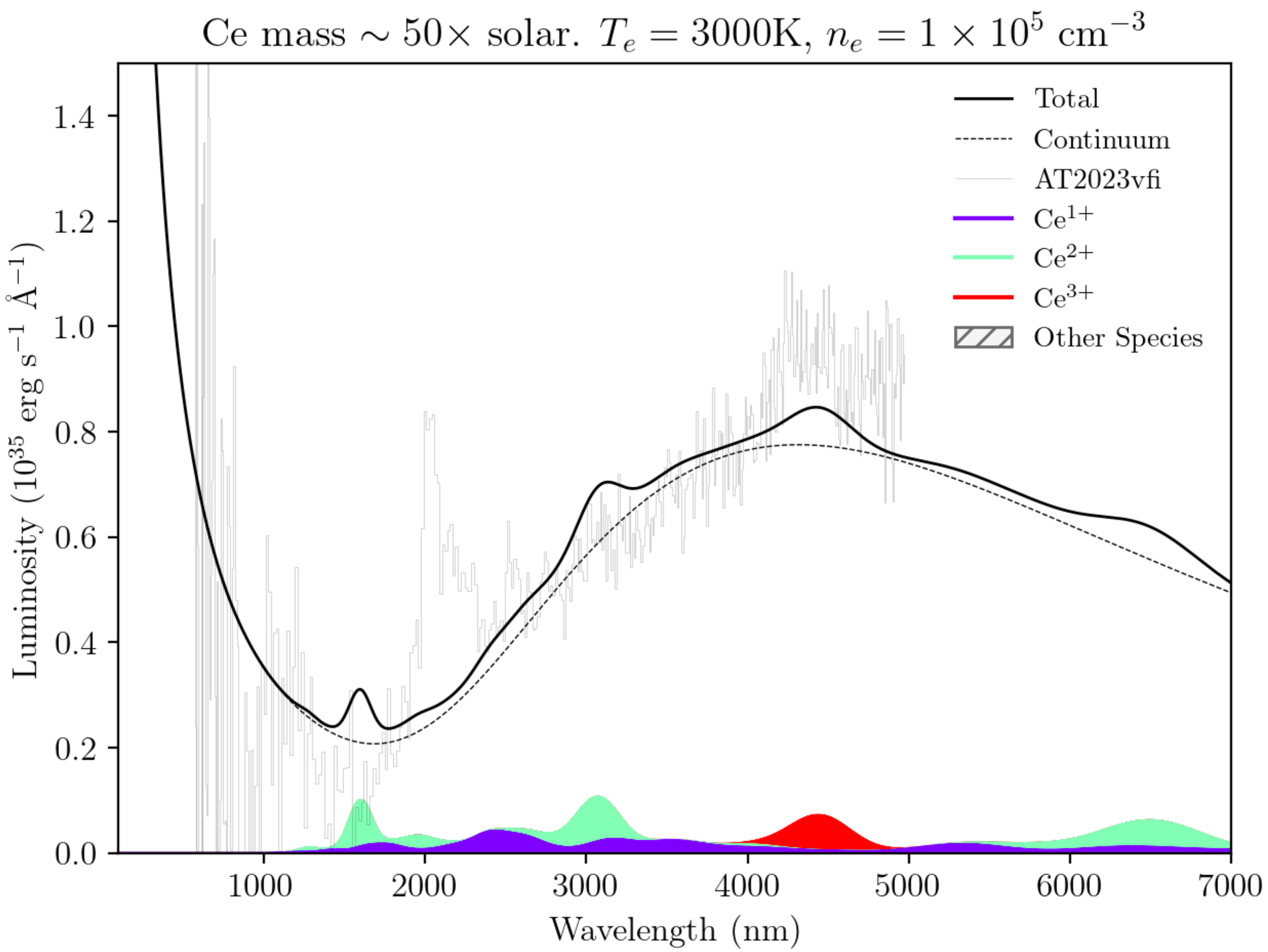
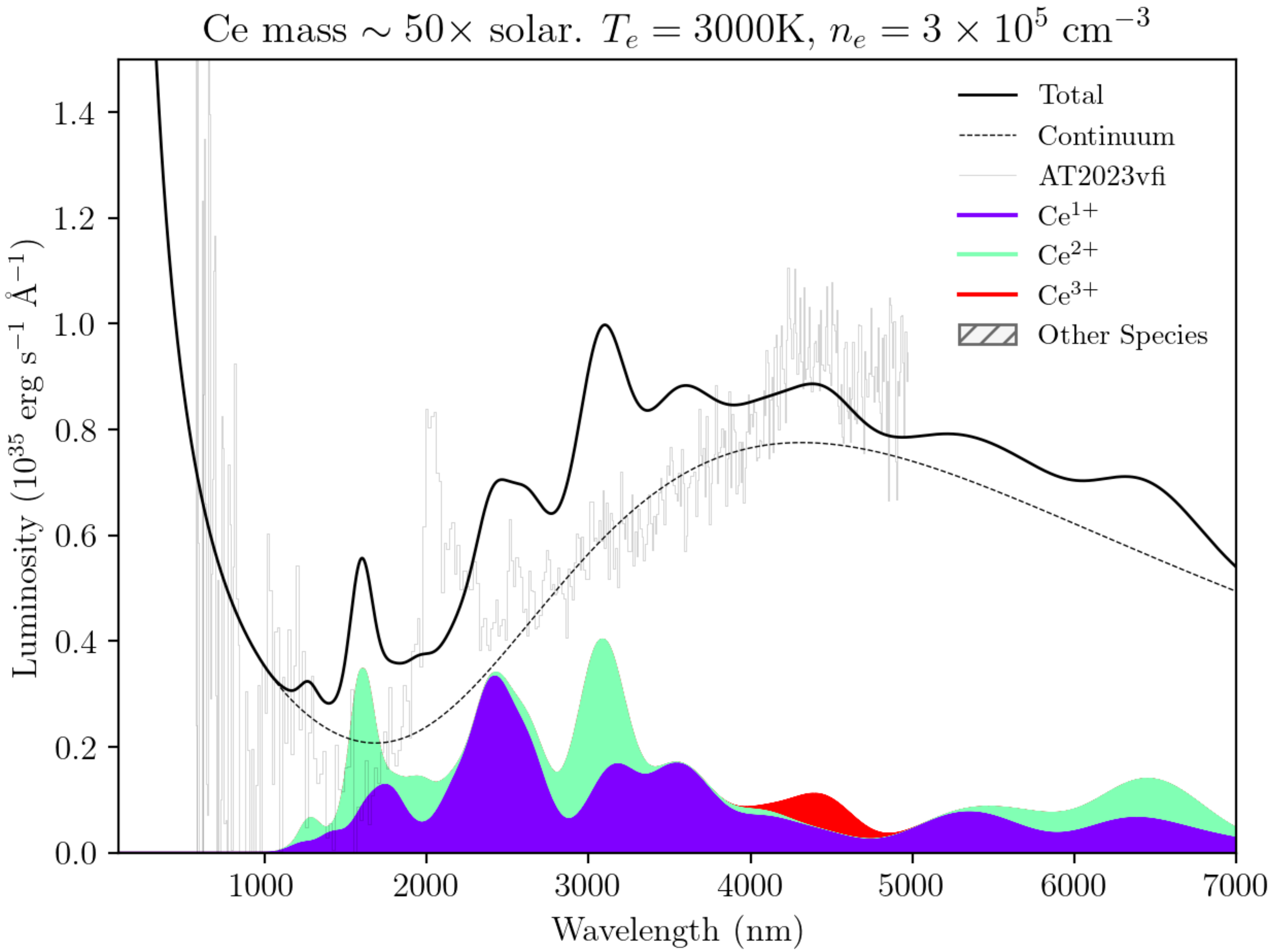


Cerium
Charge state balance

- For notable Ce emission, need super-solar abundance.



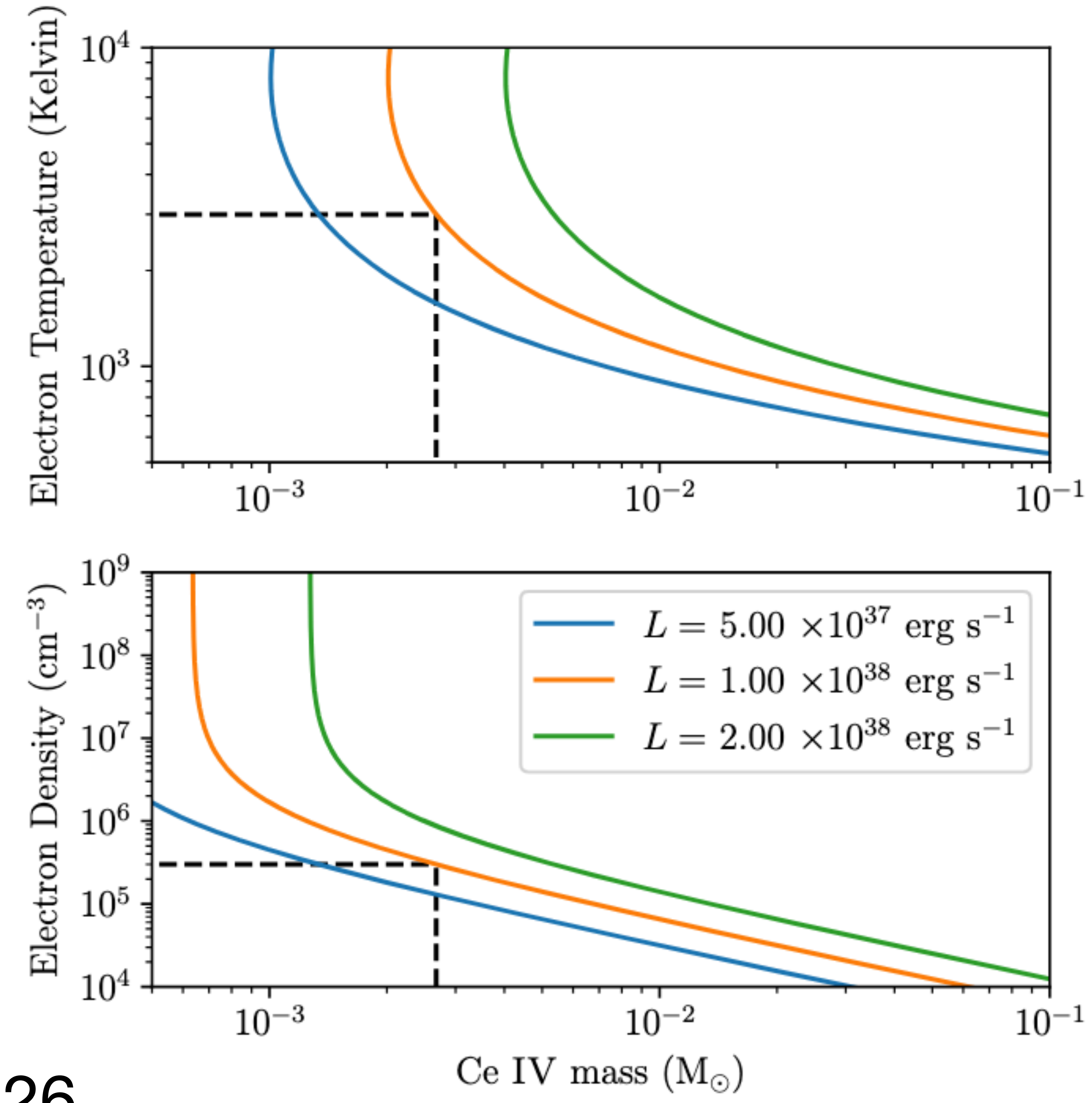


(Mulholland+26b, in prep)

Cerium

Charge state balance

- To explain the 4.5 micron emission in terms of fully Ce IV
- Need:
  - More ionization
  - $\sim 3 \times 10^{-3} M_{\odot}$ of just Ce IV
  - Seems unlikely.
- Contrast with Domoto+23, Gillanders & Flörs+26



(Mulholland+26b, in prep)

Cerium

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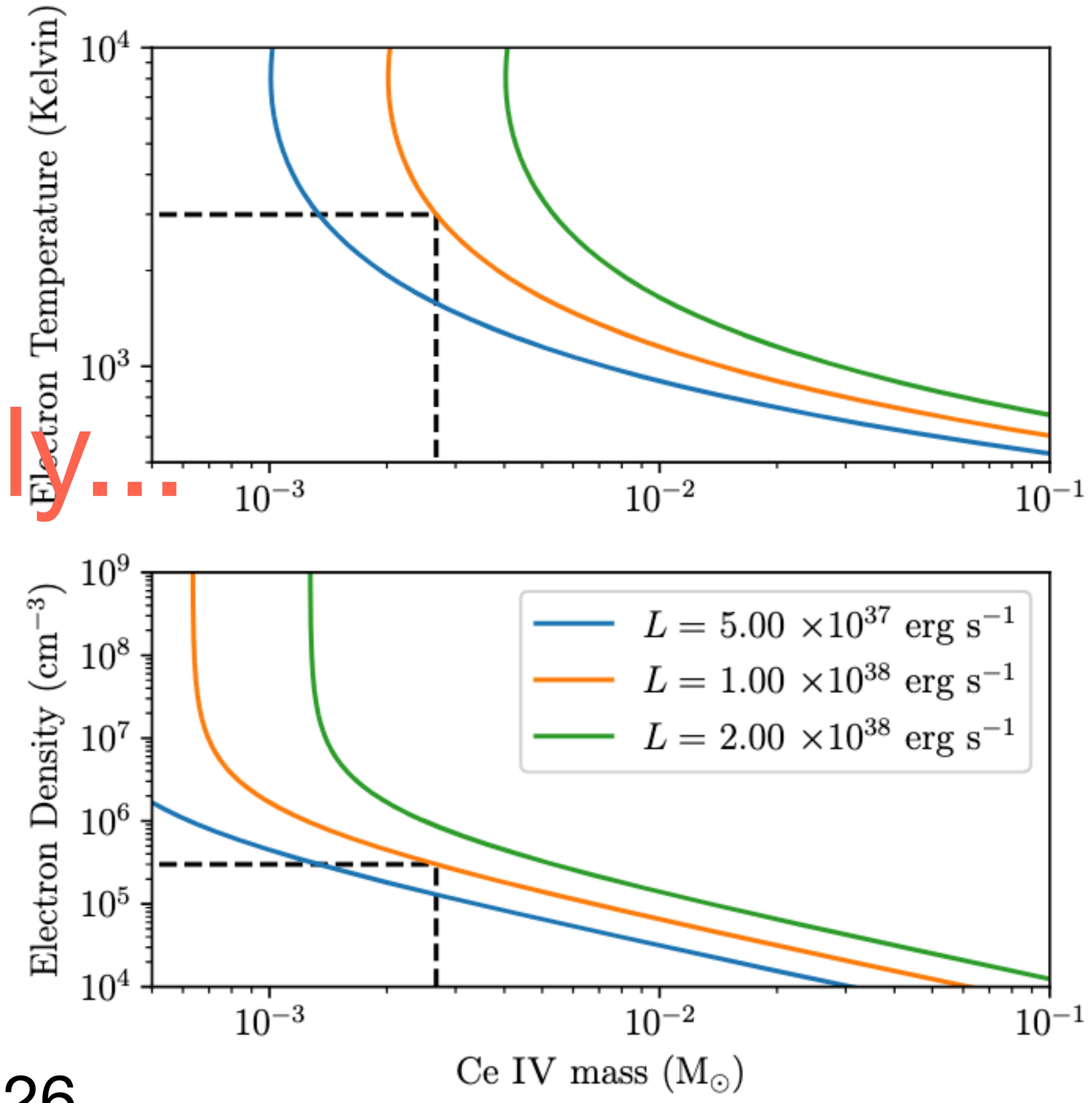
Favour Se heavily...



(Mulholland+26b, in prep)

Cerium

Charge state balance

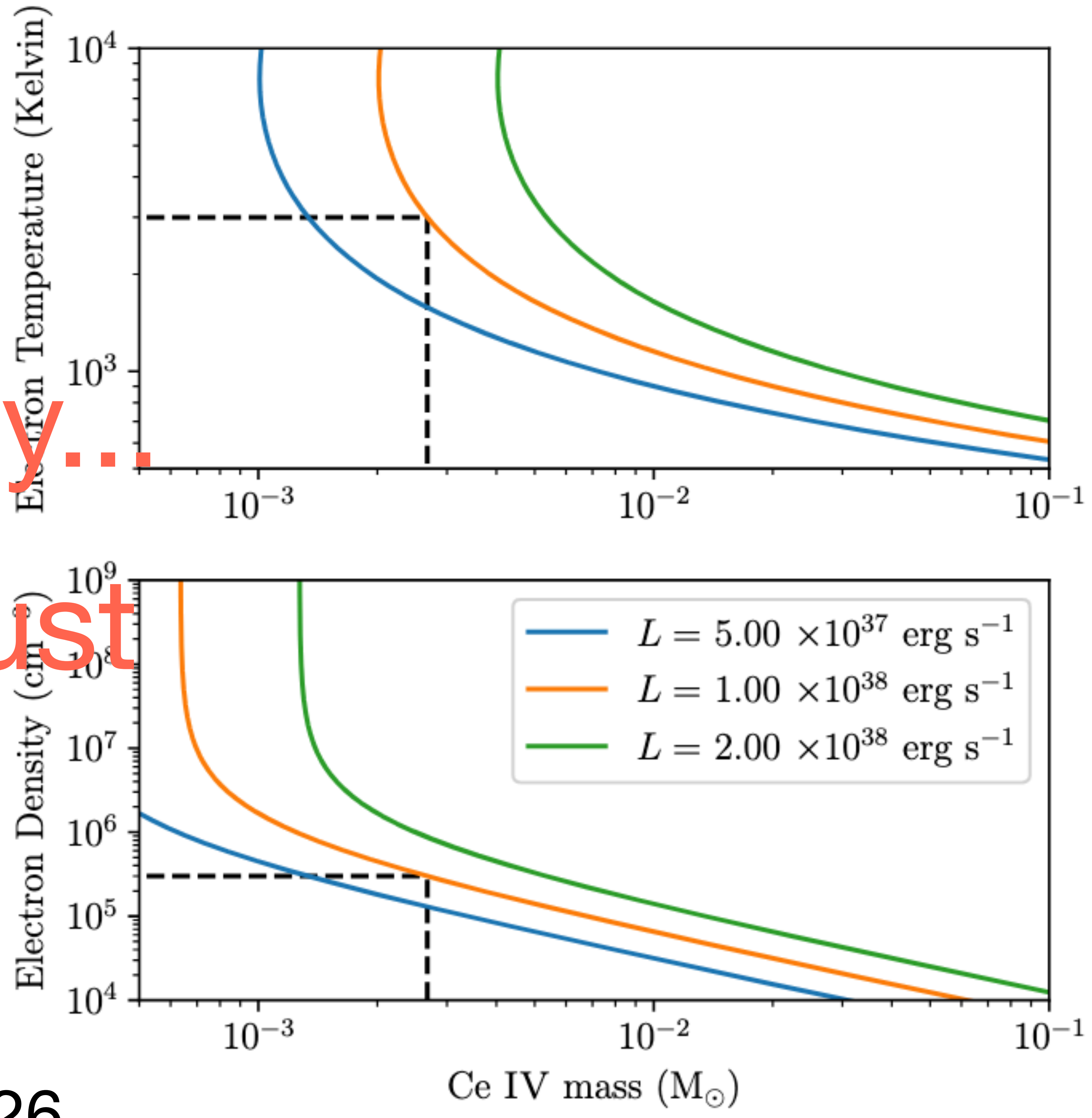
- To explain the 4.5 micron emission in terms of fully Ce IV

Favour Se heavily...

- Need:

Maybe its just dust

  - More ionization
  - $\sim 3 \times 10^{-3} M_{\odot}$ of just Ce IV
  - Seems unlikely.
- Contrast with Domoto+23, Gillanders & Flörs+26

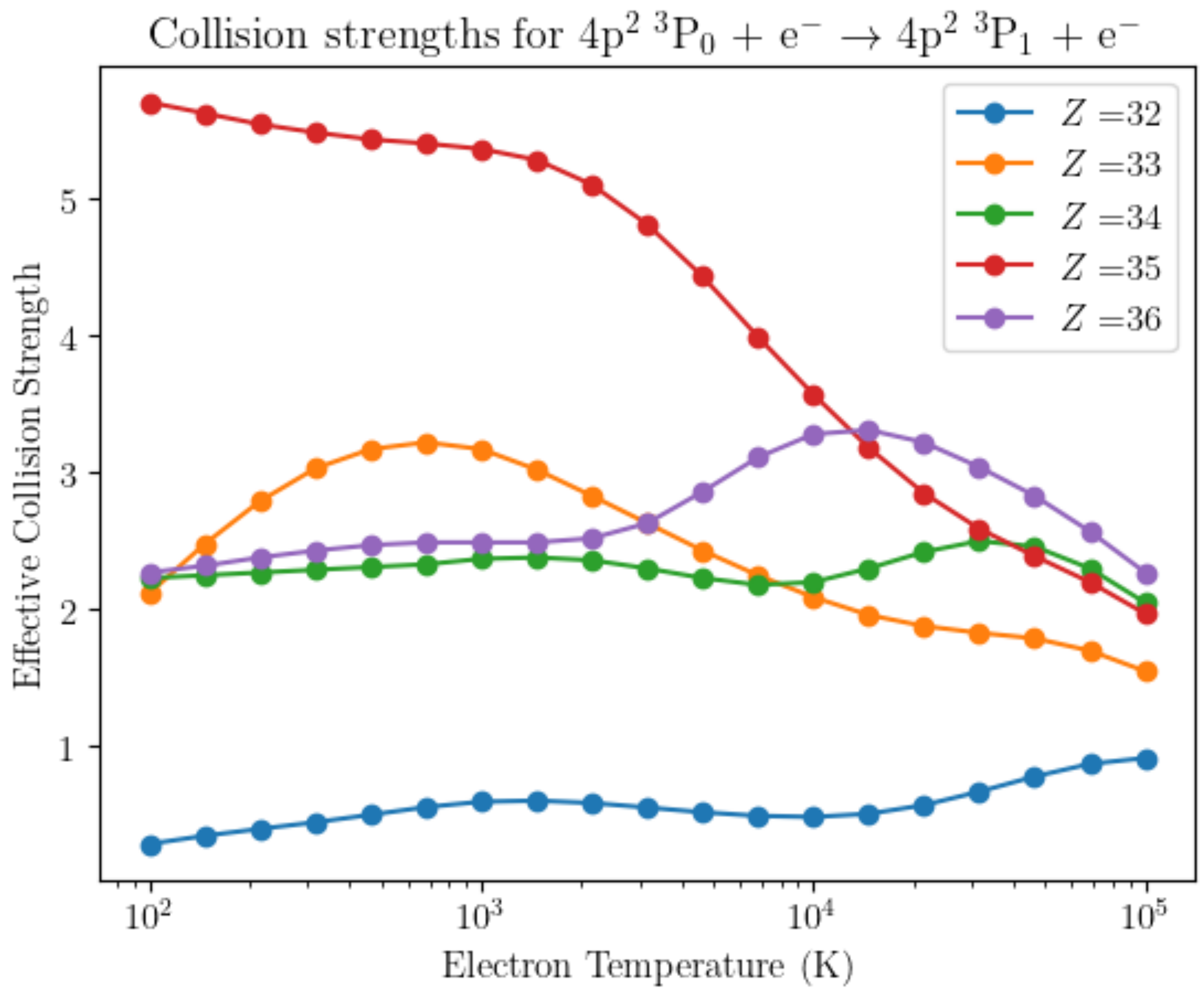


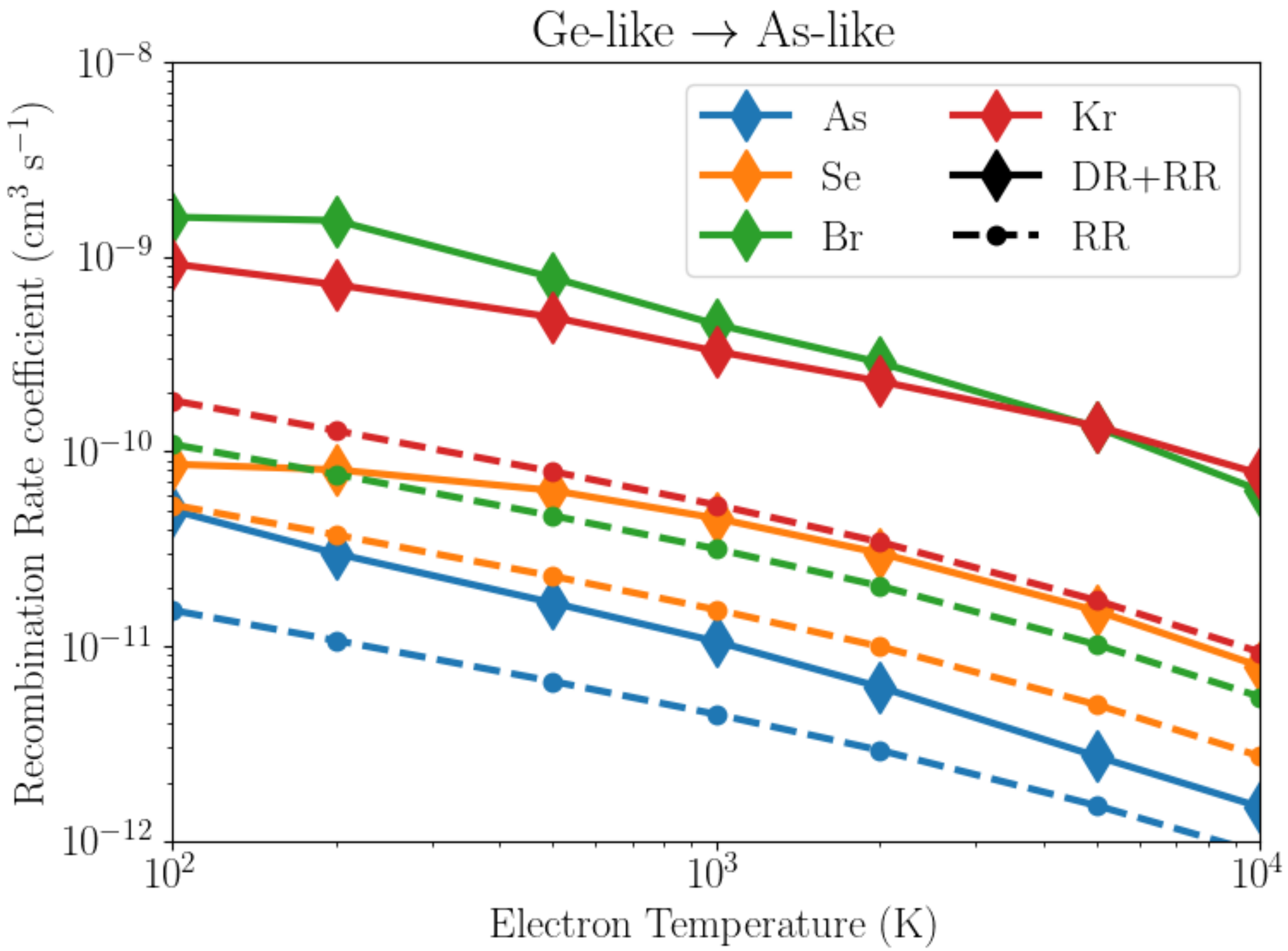
(Mulholland+26b, in prep)

4. Wider first peak

Z = 31 - 36

Atomic data



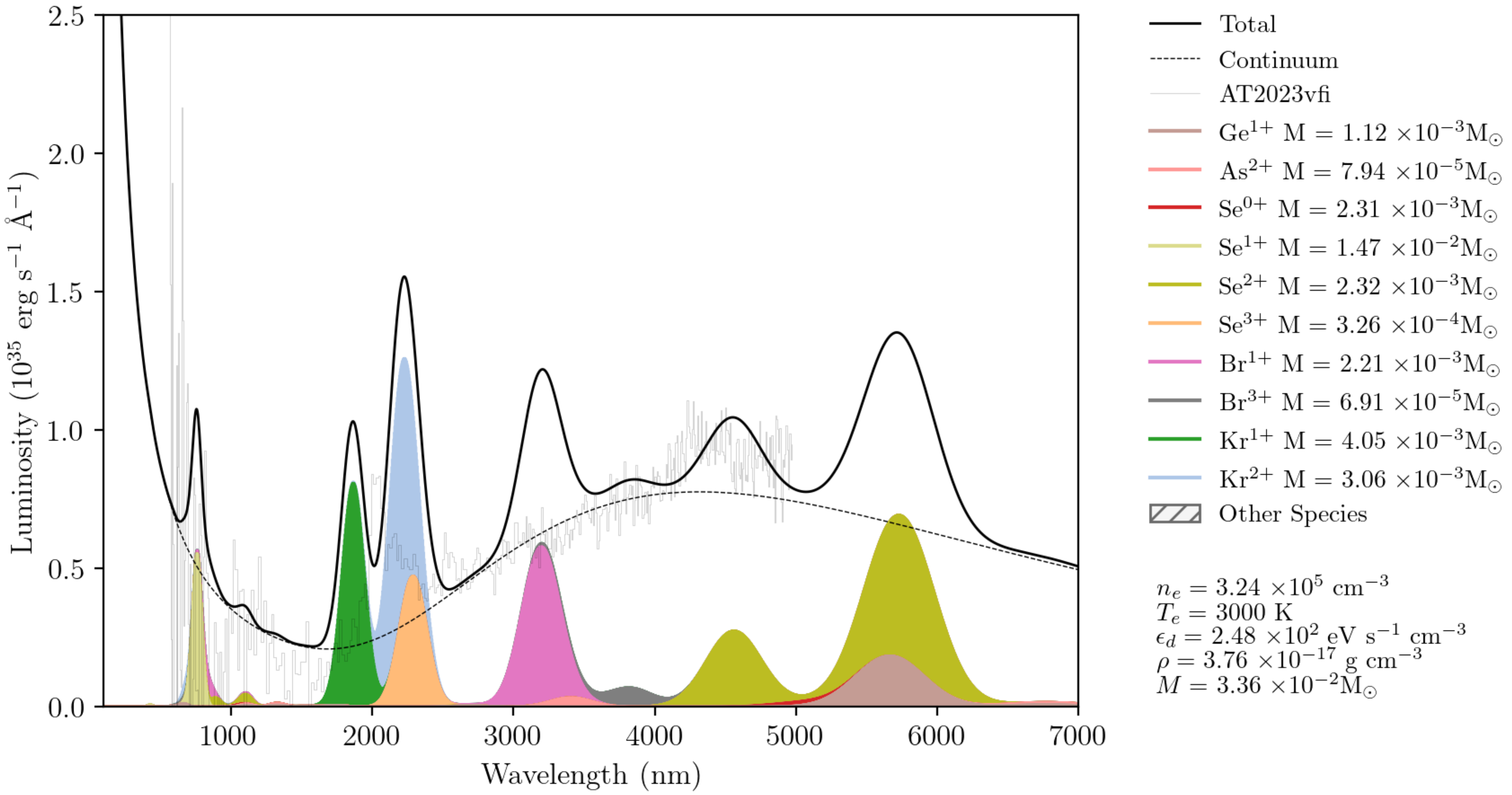


- EIE using DARC R-matrix (Mulholland+26c, in prep)
- RR and DR using AUTOSTRUCTURE

Z = 31 - 36

Modelling

- Simple CRM will allow for parameter space exploration of deposition, temperature density.
- Br very difficult to suppress in II and IV states - 3D RT needed.
- Se III interesting - difficult to suppress Se IV. Cf Jerkstrand+26



(Mulholland+26c, in prep)

Conclusions

- Collision data produced for Te I - V, Ce II - IV, Ga - Kr.
- Analytic formula good, but use with caution - or scale according to its atomic structure
- Te IV may not be crazy to consider at 1.08 μm in RT models.
- Ce will be difficult to track to the nebular phase,without much larger production.
- Simple CRMs good for OOM estimate - but more sophisticated RT needed,
- Simple atomic structure of the first R-process peak elements may guide spectral identification.

Appendix: Ce Recombination Rates

- ~ 1 dex disagreement
- Perhaps John's talk will tell us more