



Identification and Abundance Estimate of Heavy Elements in Kilonova Spectra

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in collaboration with

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Kyohei Kawaguchi (AEI), Gediminas Gaigalas, Laima Kitovienė, Pevel Rynkun (Vilnius U.)

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Light curves

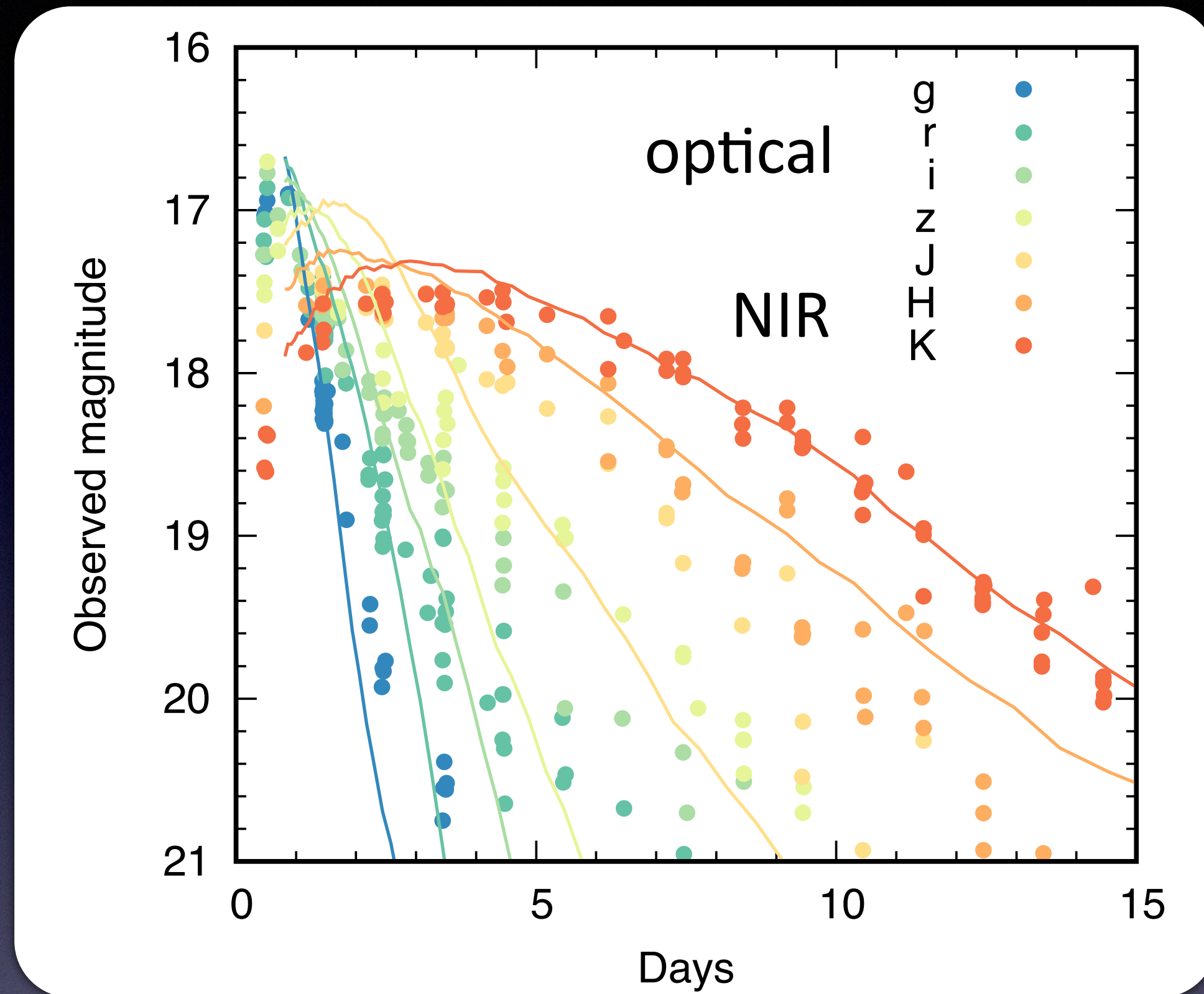


Figure from Kawaguchi+2018, 2020

Spectra

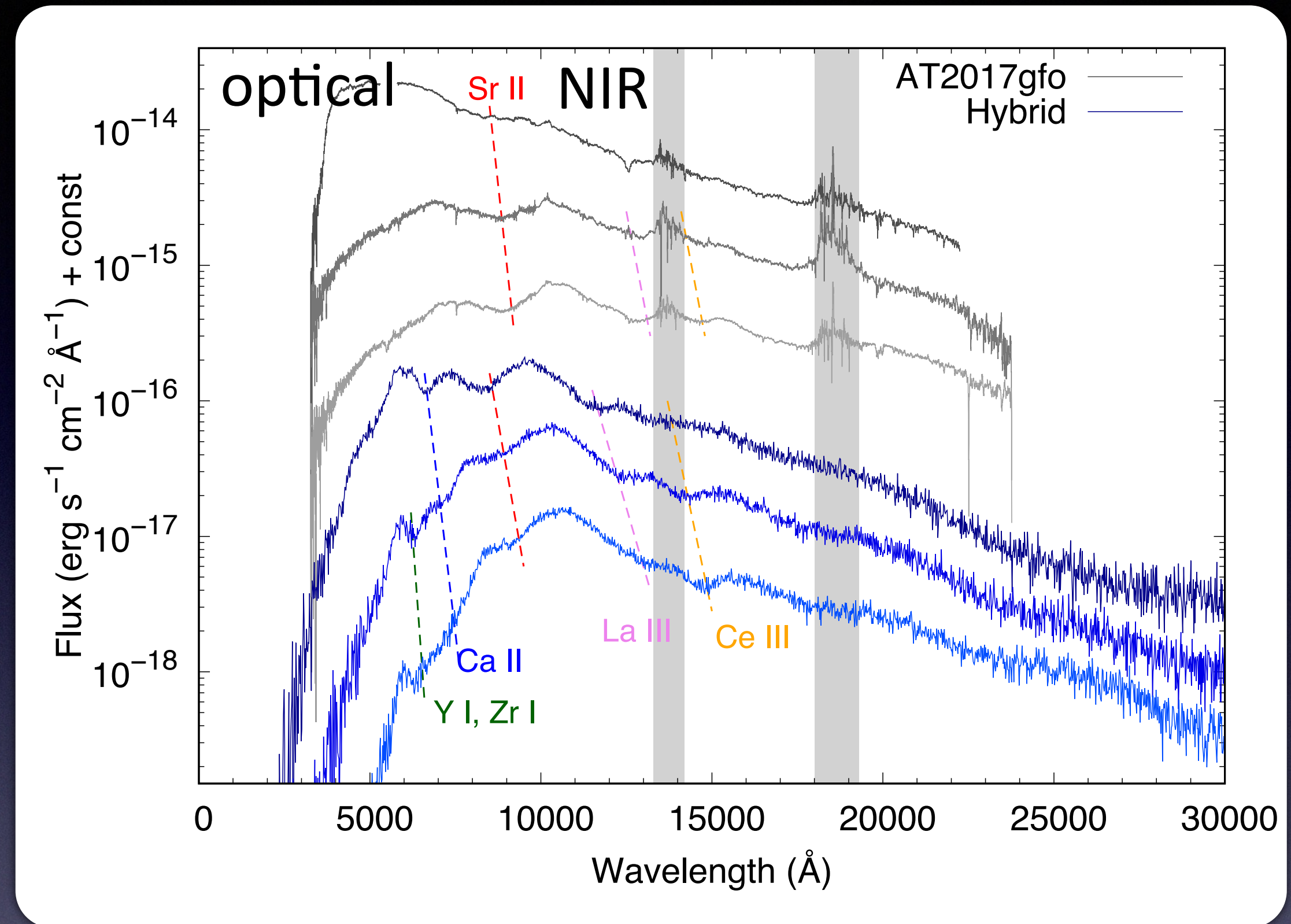


Figure from Domoto+2020,2022

What can
we learn?

Atomic
data?

Ejected mass and
(rough) composition

Opacity
(statistical properties)

Detailed elemental compositions

Accurate wavelength and
transition probability

Identification and Abundance Estimate of Heavy Elements in Kilonova Spectra

- **Element identification in kilonova spectra**
- “Experiments” with chemically peculiar stars
- Towards abundance estimates

“Minimum” atomic data for kilonovae (LTE)

Bound-bound transitions (“line”)

Friend & Castor 1983 (stellar wind), Pinto & Eastman 1993 (supernova)

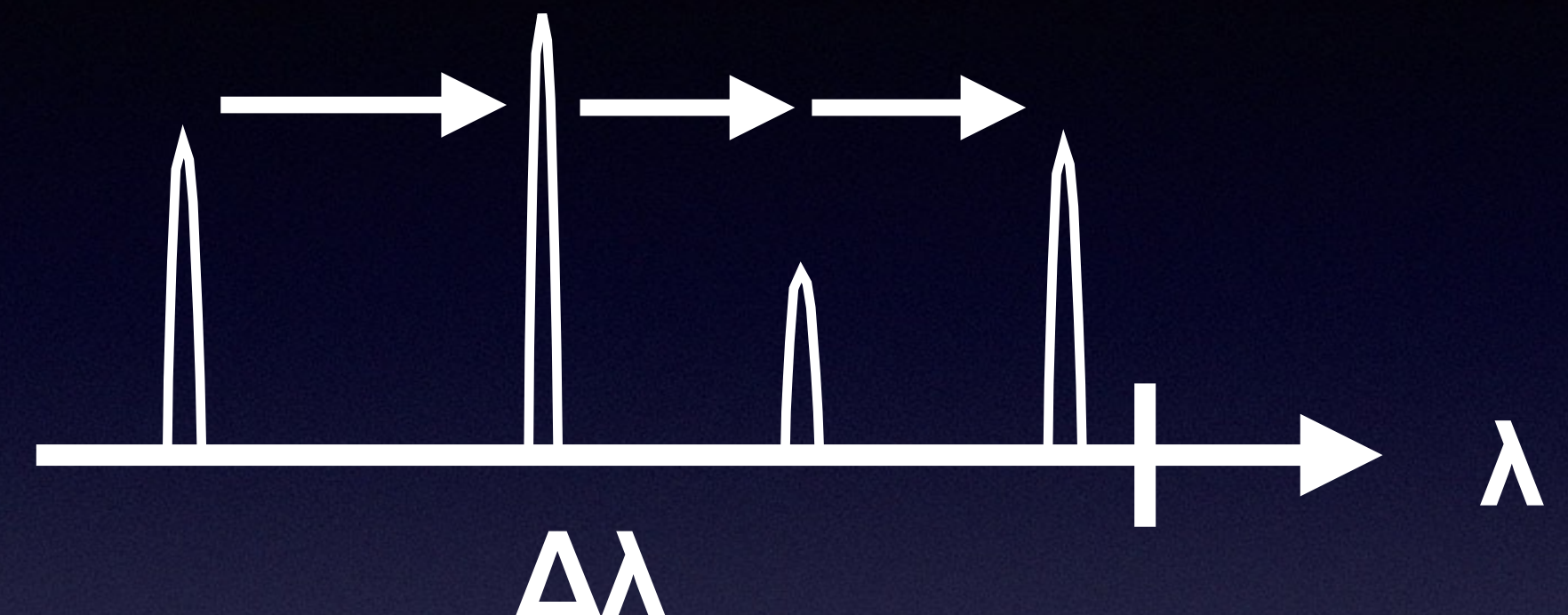
Kasen+06, Kasen+13, MT & Hotokezaka 13 (kilonova)

$$\kappa_{\text{exp}}(\lambda) = \frac{1}{ct\rho} \sum_l \frac{\lambda_l}{\Delta\lambda} (1 - e^{-\tau_l})$$

Optical depth of each line (**under LTE**)

$$\begin{aligned} \tau_l &= \int \alpha dr \\ &= \frac{\pi e^2}{m_e c} n_{i,j} t \lambda_l f_l \frac{g_l}{Z_p} e^{-\frac{E_l}{kT}} \end{aligned}$$

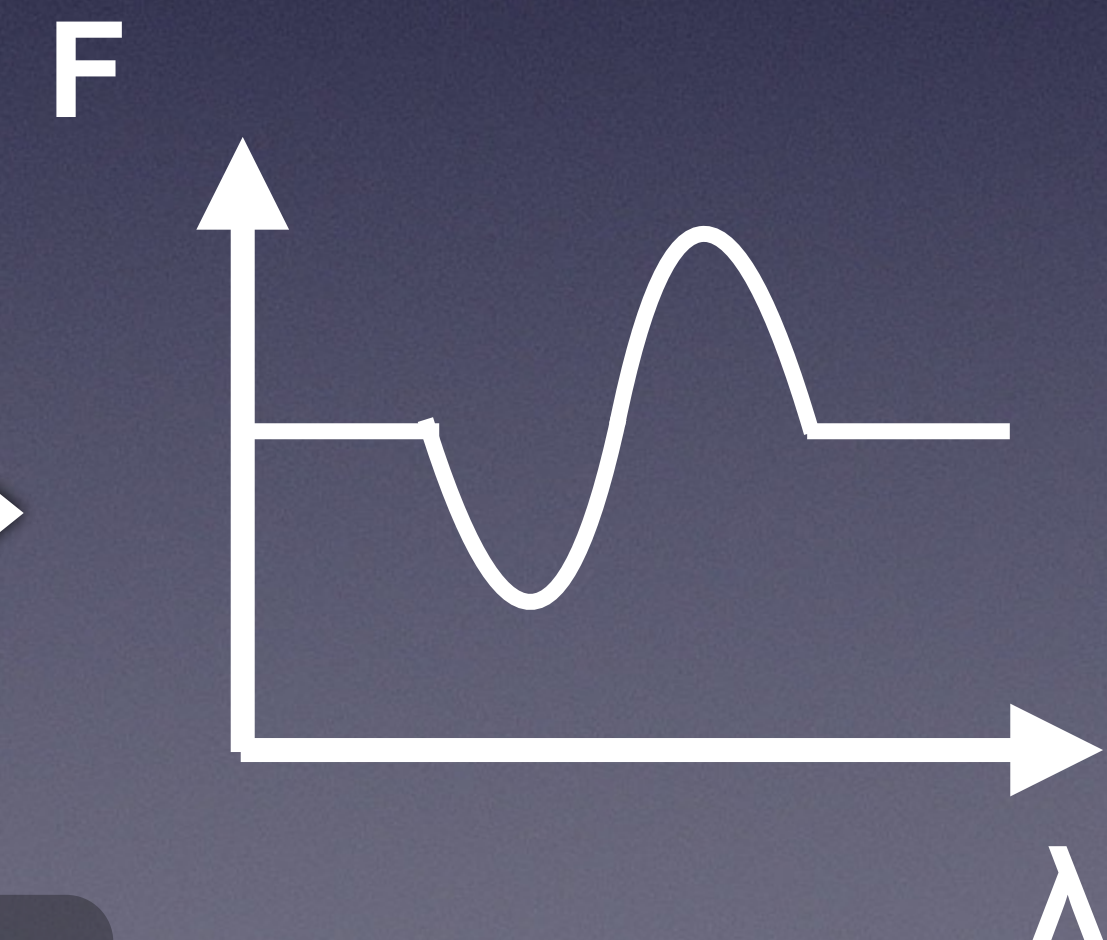
b-b opacity



Energy levels



Spectrum

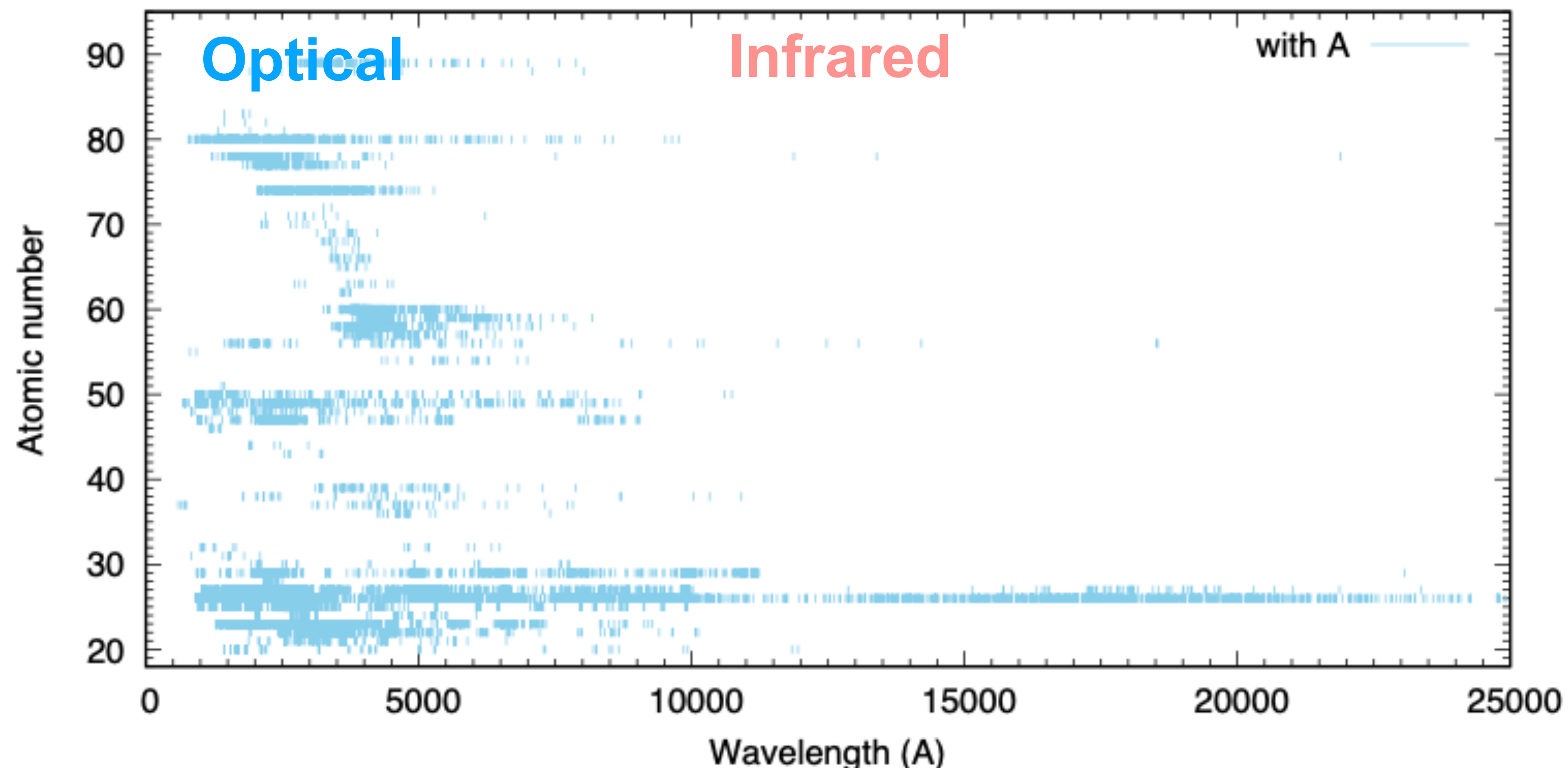


Energy levels + transition probabilities

Available atomic data

Data from the NIST database
(singly ionized)

Transitions with known transition probability

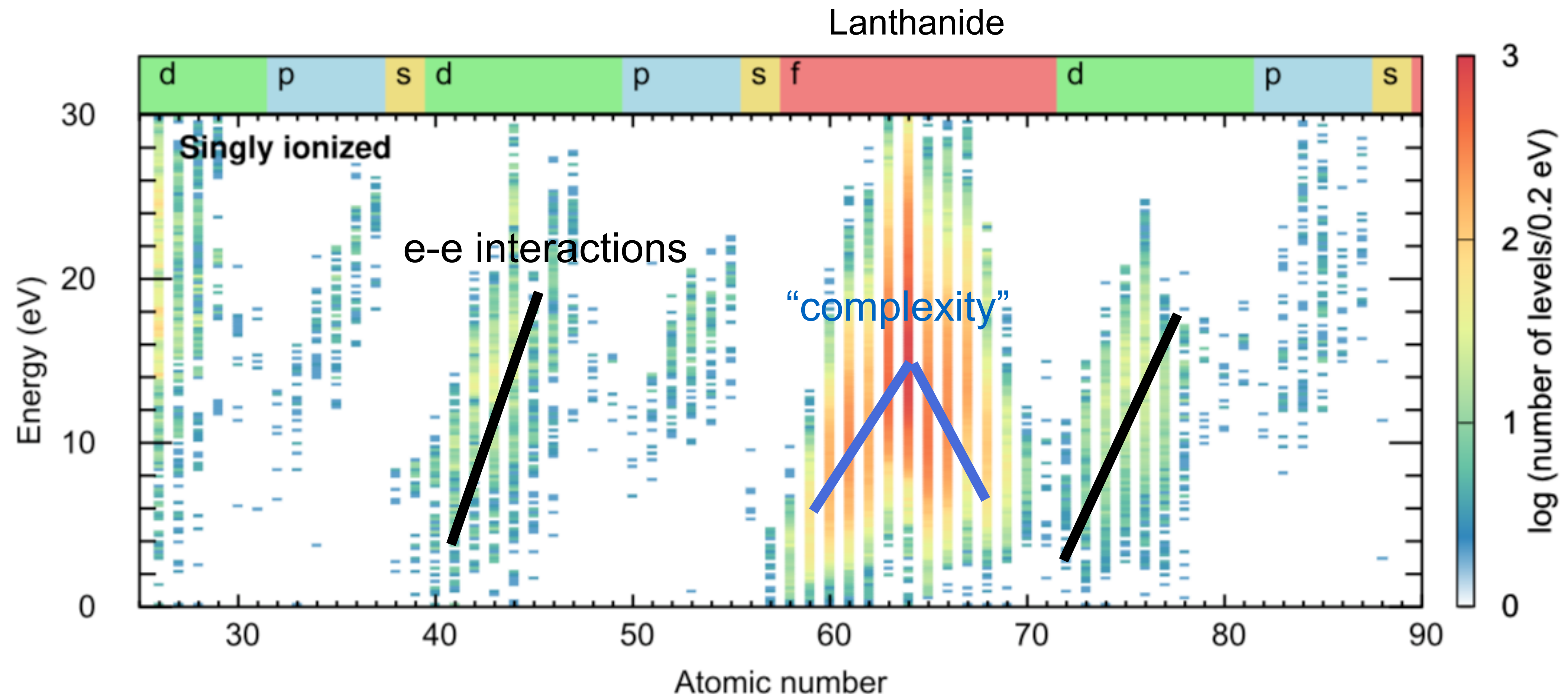


Accurate transition data are highly incomplete (in particular NIR)

Atomic structure calculations

Talks by Chris, Stephane, & Andreas

MT, Kato, Gaigalas, Kawaguchi 20 (HULLAC)
Kato, MT, et al. 24 (ver 2)
see also Fontes+20,21, Deprince+25, Flörs+26

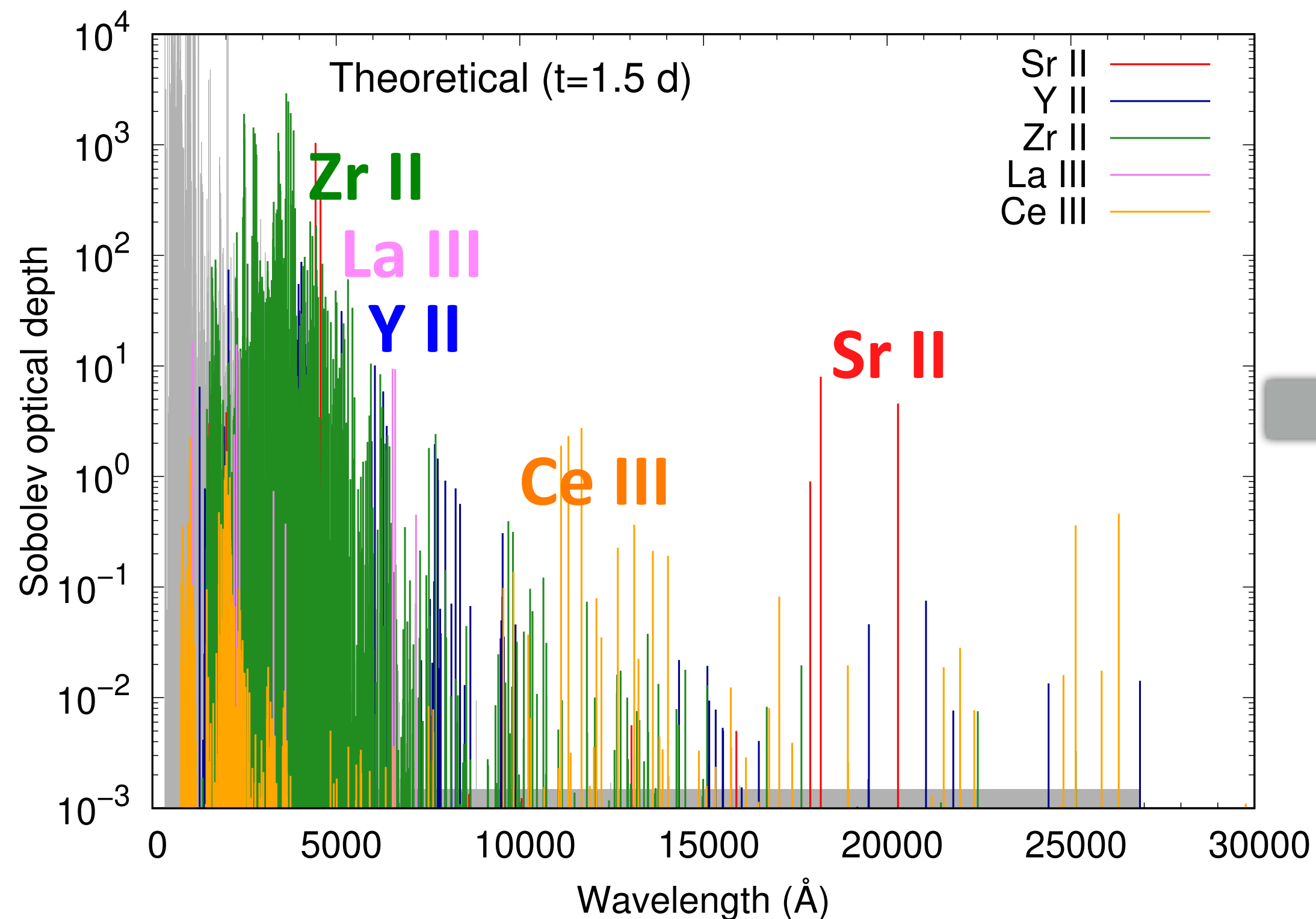


<http://dpc.nifs.ac.jp/DB/Opacity-Database/>

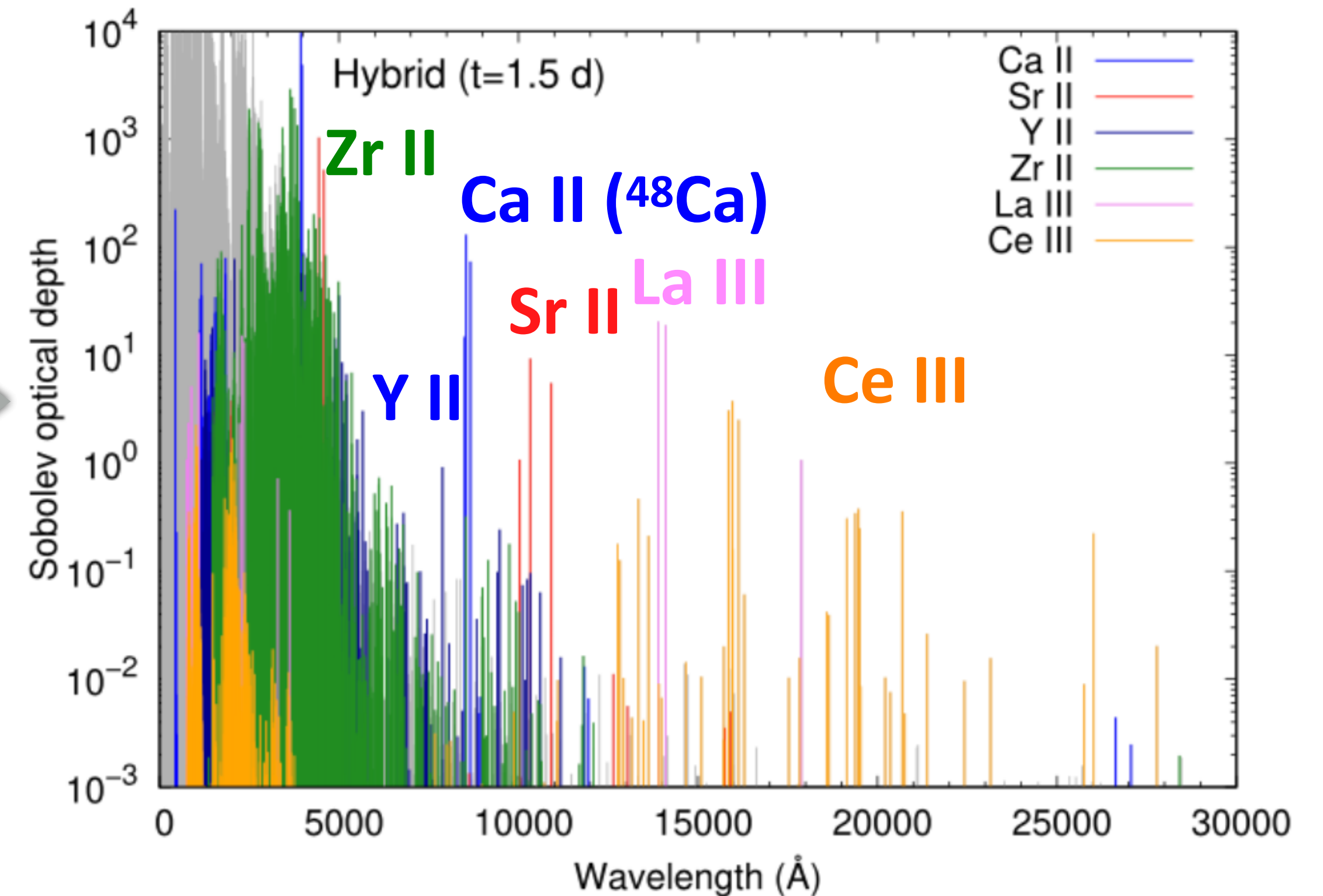
Selection of important elements

Domoto, MT, Kato+22

Theoretical data (MT+20)
(wavelengths are incorrect)



**Calibrated
for important elements**



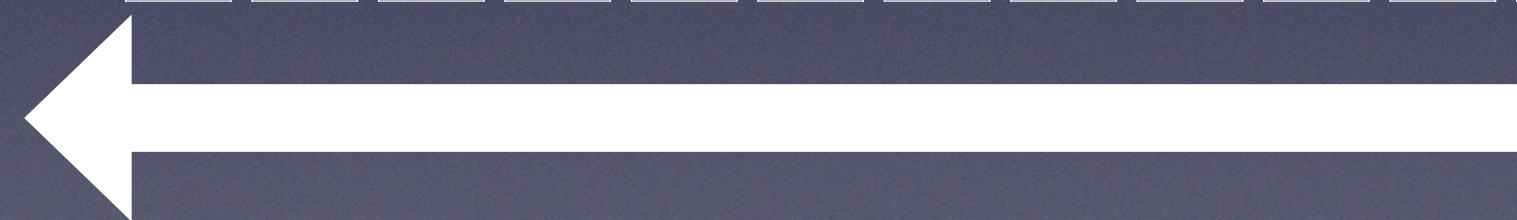
Relatively small number of elements/ions are important

Important elements for kilonova spectra

Watson+19 (Sr)
Domoto, MT, Kato+22 (La, Ce)
Sneppen & Watson 23 (Y)

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
87 Fr	88 Ra	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og	

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

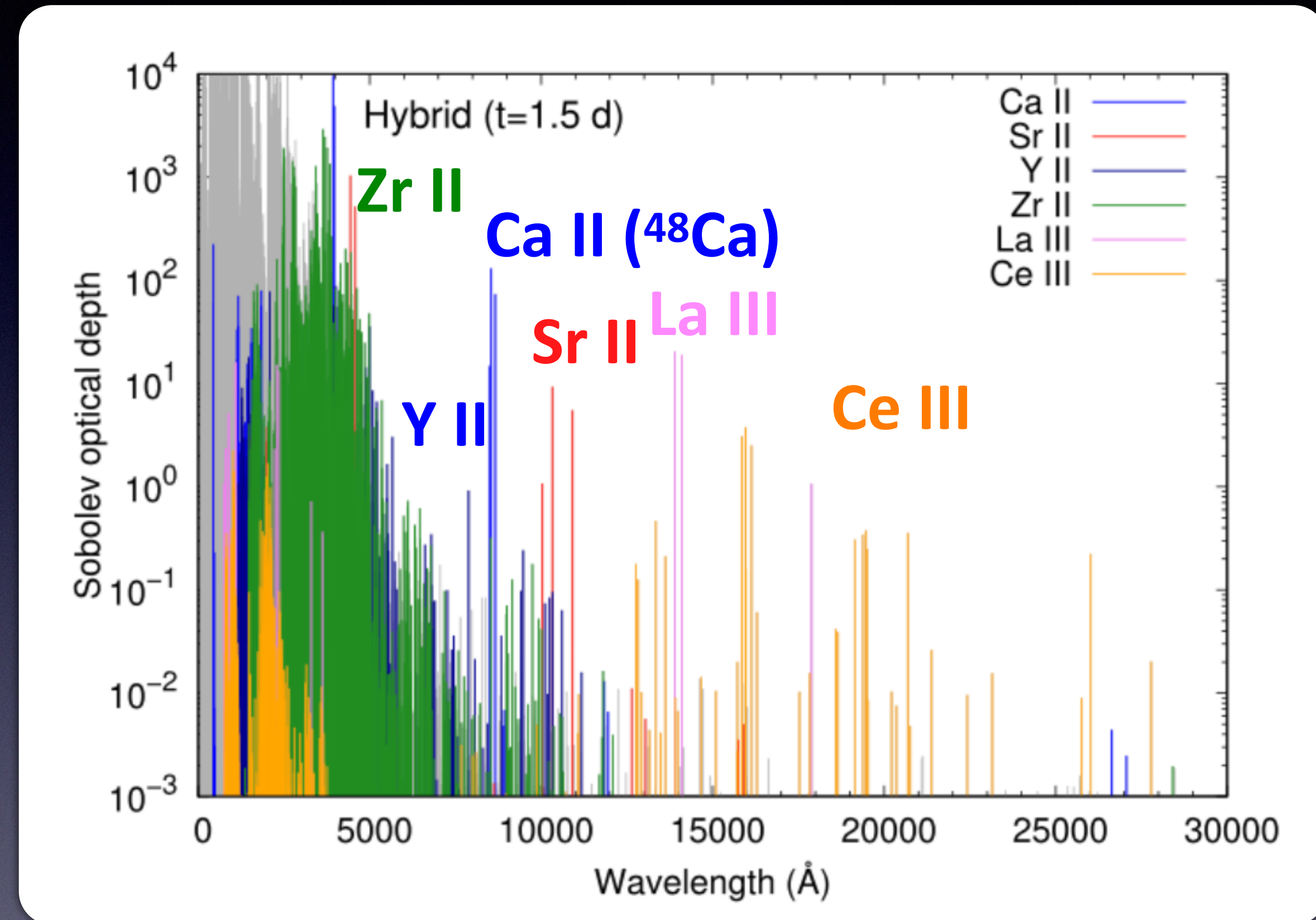


Elements with (1) low-lying energy levels

= higher population

(2) relatively simple structure = small number of transitions

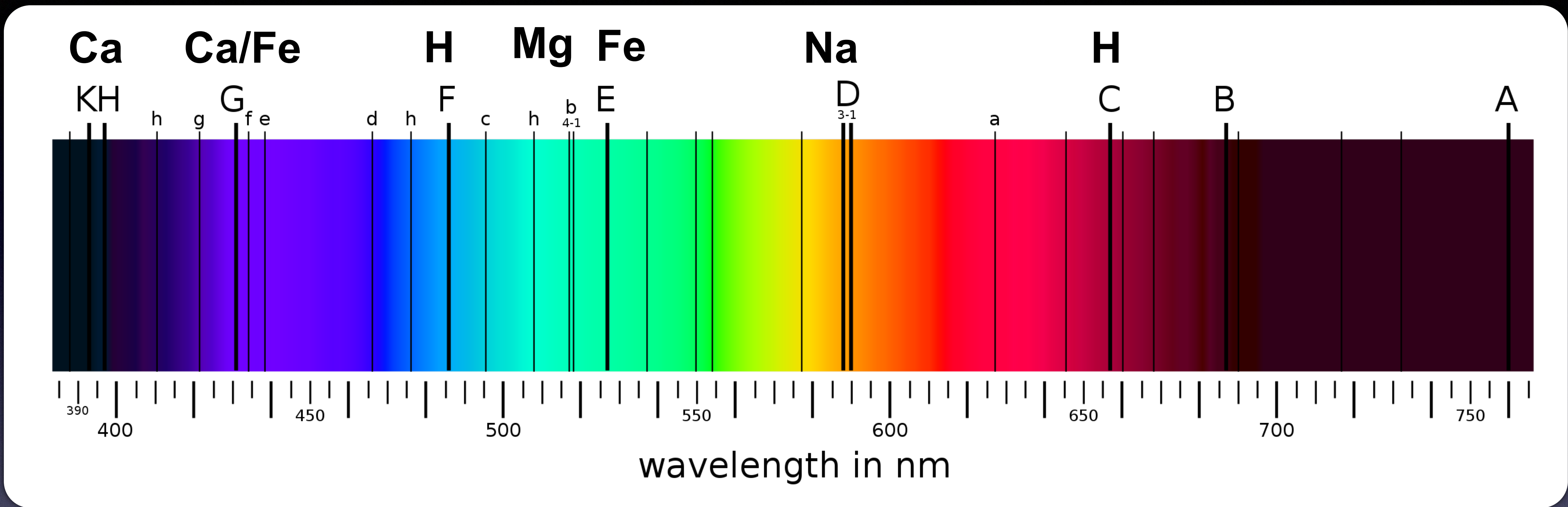
=> high transition probability (“sum rule”)



$$\tau_l = \frac{\pi e^2}{m_e c} n_{i,j} t \lambda_l f_l \frac{g_l}{Z_p} e^{-\frac{E_l}{kT}}$$

Solar spectrum

https://en.wikipedia.org/wiki/Fraunhofer_lines



Fraunhofer 1814

1 H																	2 He				
3 Li	4 Be															5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg															13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr				
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55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn				
87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og				

Kirchhoff & Bunsen 1860

CHEMICAL ANALYSIS BY SPECTRAL OBSERVATIONS.

BY
G. KIRCHHOFF AND R. BUNSEN.

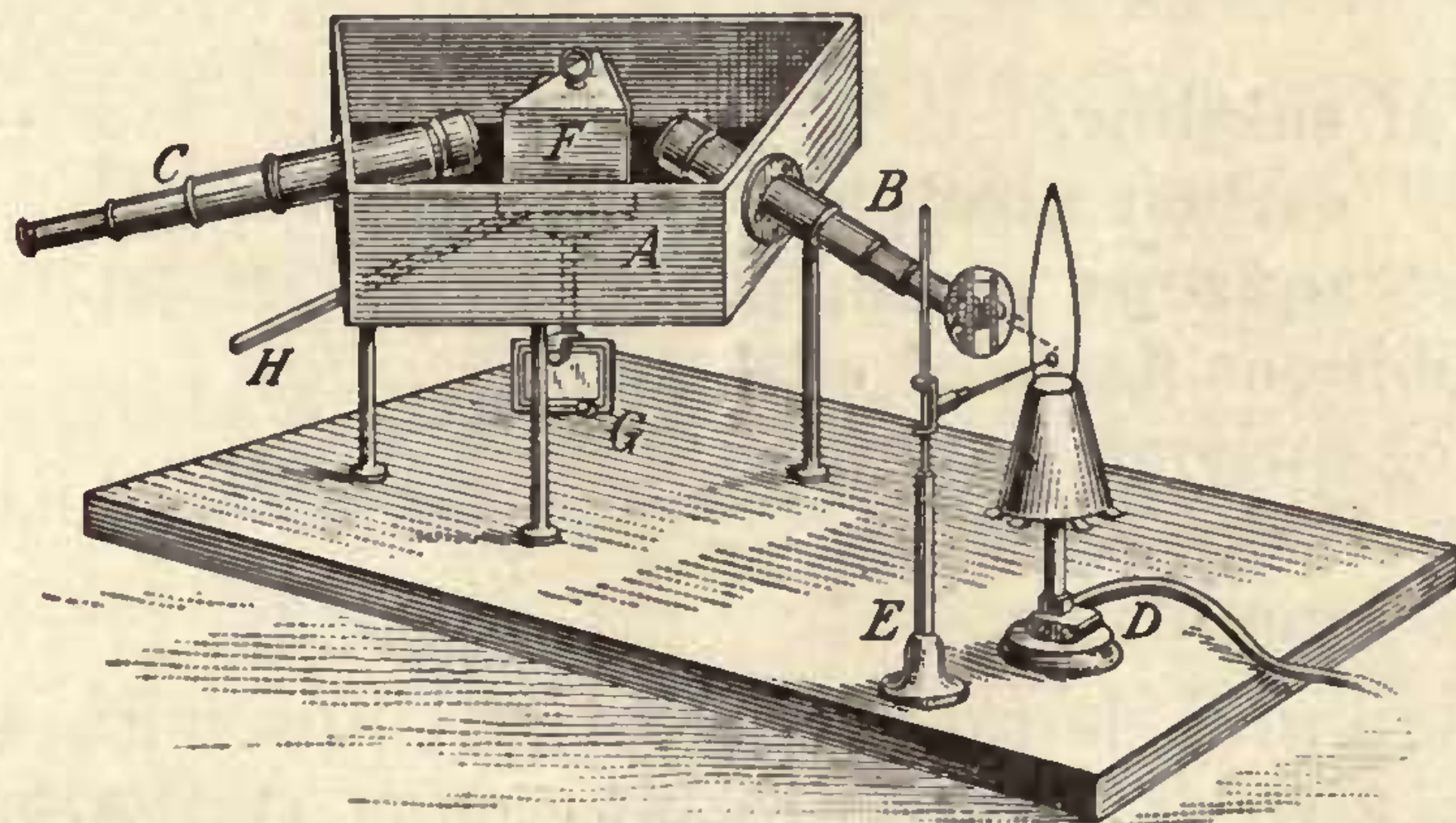


FIG. 2.

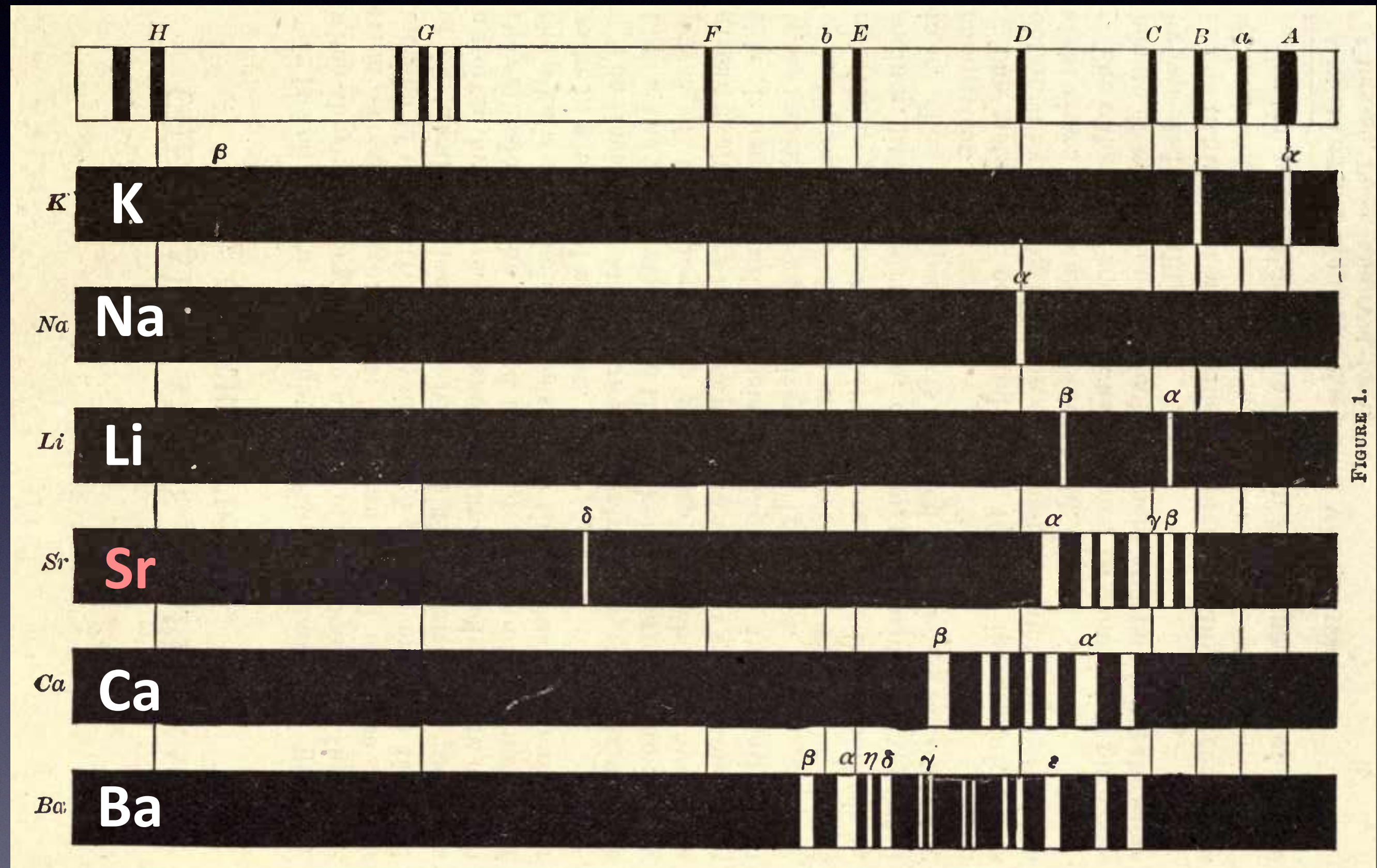


FIGURE 1.

Henry Norris Russell 1929

ON THE COMPOSITION OF THE SUN'S ATMOSPHERE¹

By HENRY NORRIS RUSSELL²

A work after the pioneering work
by Cecilia Payne 1925
(first work pointing
the H dominance in the Sun)

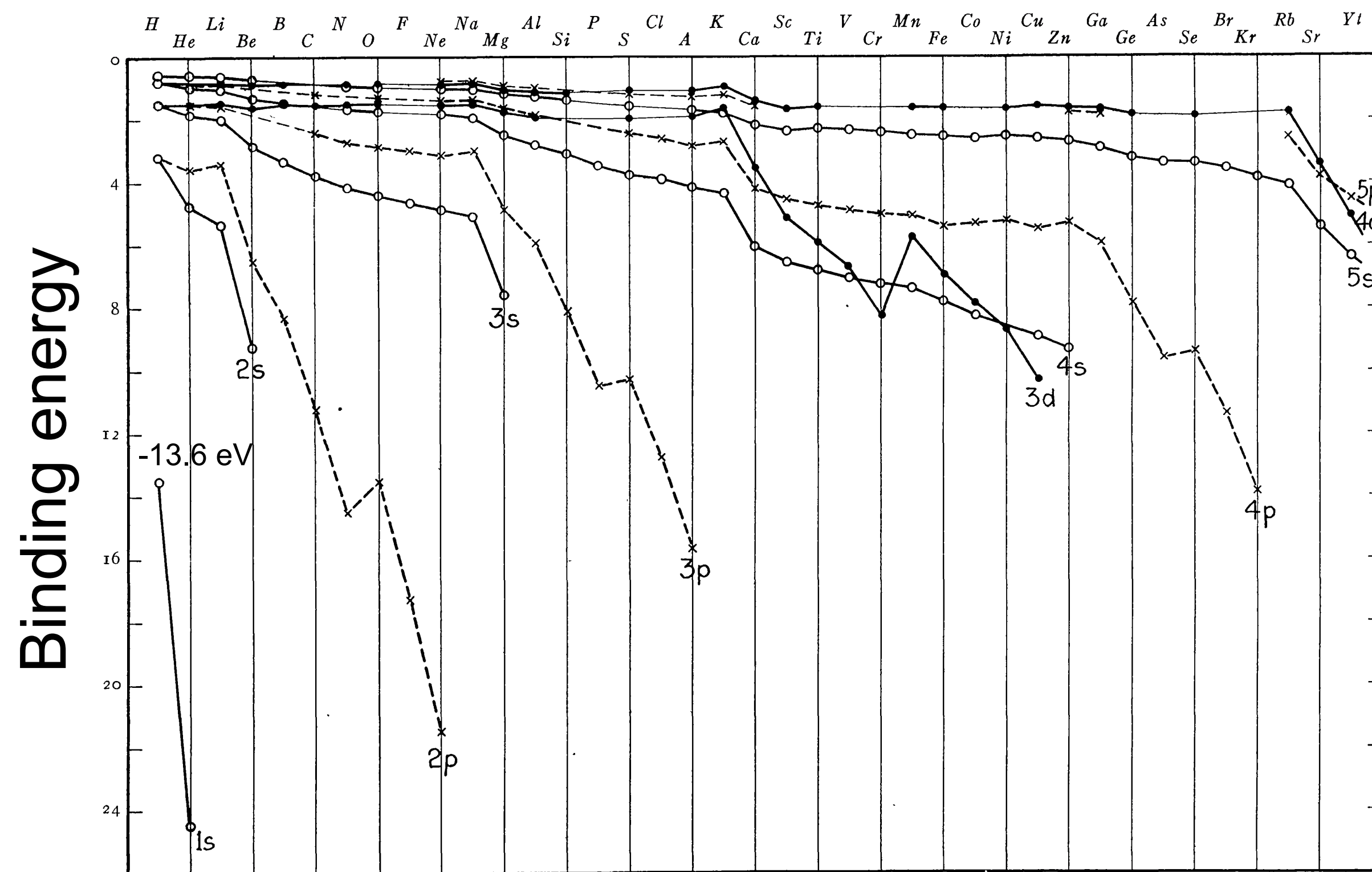


FIG. 1.—Energy of binding of electrons: neutral atoms

Atomic number

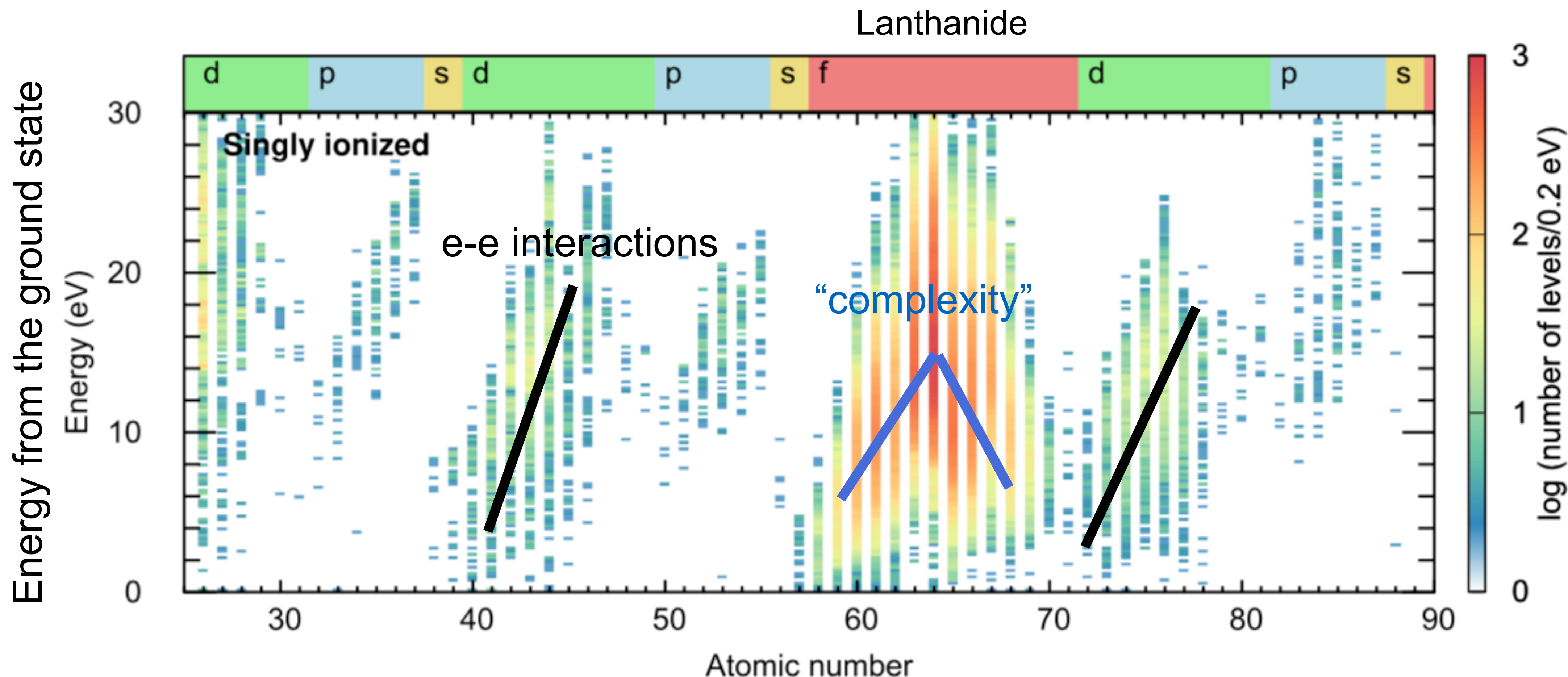
Lists of these lines, in the various arc spectra, are given in Table V. The lines marked with an asterisk have been recorded by De Gramont² or Meggers and Kiess³ as *raies ultimes*, which actually persist in the manner described. Most of the rest are of too short wave-length to have been observed by them, but are undoubtedly of the same nature. Table VI gives similar data for spark spectra. The arrangement for the short periods differs slightly in order to bring spectroscopically similar terms into the same line.

These tables confirm the conclusions which were drawn from the general structure of the spectra. The most persistent arc lines of almost all the metals lie within the region accessible in the sun, while those of the non-metals are without exception out of range. Conditions for detecting the spark lines astrophysically are favorable only for the metals in the earlier parts of the successive periods—for Be, Ca to V, Sr to Cb, Ba, La, and probably several of the rare earths, and finally for Ra.

**“earlier parts of the successive periods”
= left side of the periodic table**

Atomic structure calculations

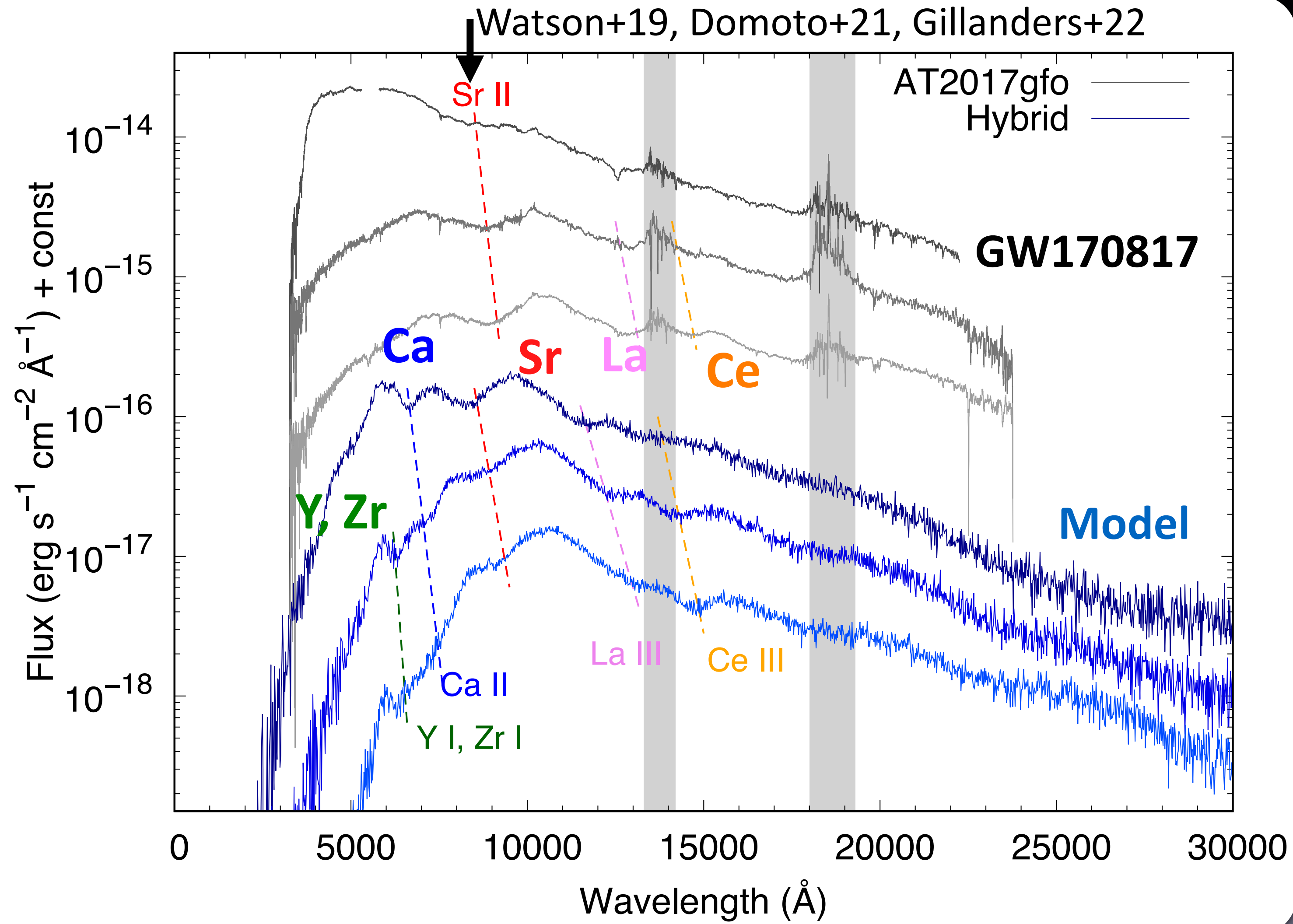
MT, Kato, Gaigalas, Kawaguchi 20 (HULLAC)
Kato, MT, et al. 24 (ver 2)
see also Fontes+20,21, Deprince+25, Flörs+26



<http://dpc.nifs.ac.jp/DB/Opacity-Database/>

Line identification in NIR wavelength

Domoto+22
see also Gillanders+24

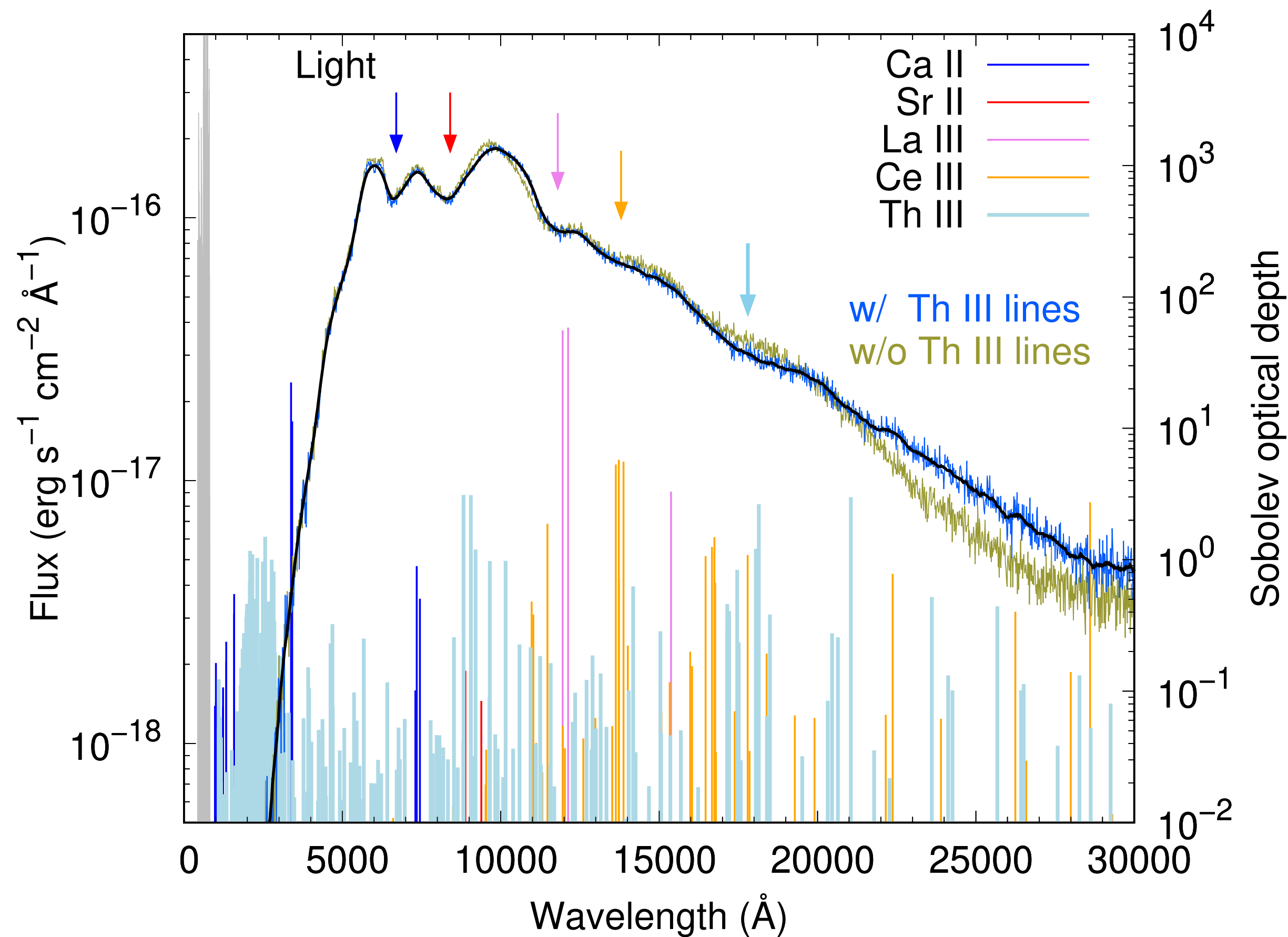


La III (Z=57) and Ce III (Z=58)

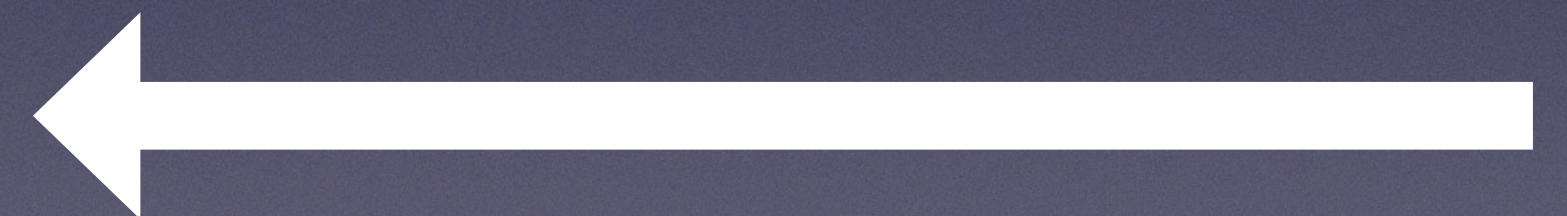
Th (Z=90): Heaviest detectable element?

see talks by Camilla and Alex
(for metal poor stars)

Domoto+25, see also Pognan+25



1 H																	2 He	
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	
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		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr		



Hope for future observations with HST/JWST

Identification and Abundance Estimate of Heavy Elements in Kilonova Spectra

- Element identification in kilonova spectra
- “Experiments” with chemically peculiar stars
- Towards abundance estimates

Road to the line identification

“Candidate”

(1) **Wavelength match**

(w/ reasonable Doppler shift)

Need transition wavelengths

(2) **Strong lines are expected**

(abundances, ionization, excitation, ...)

Need transition probabilities

(3) **Uniqueness**

No other line can produce the same feature

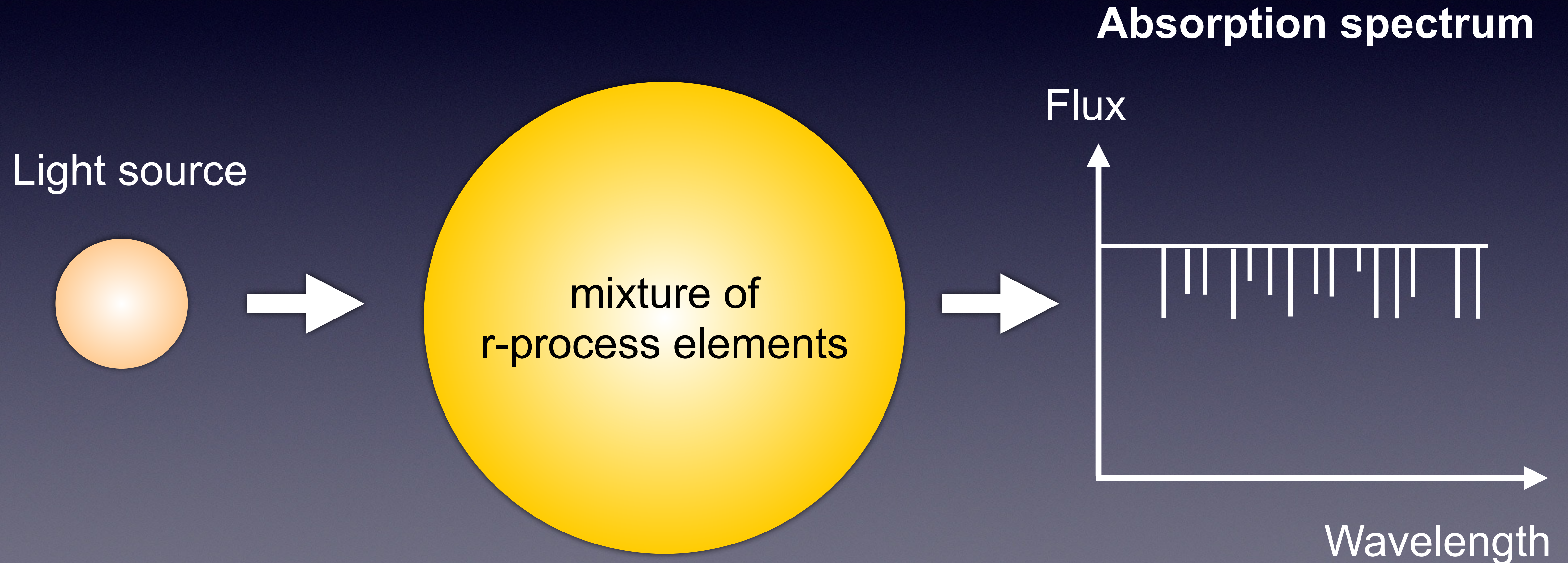
Need data of strong transitions all the elements

“Unique identification”

How to test the uniqueness of the line identification??

The best spectroscopic experiment...

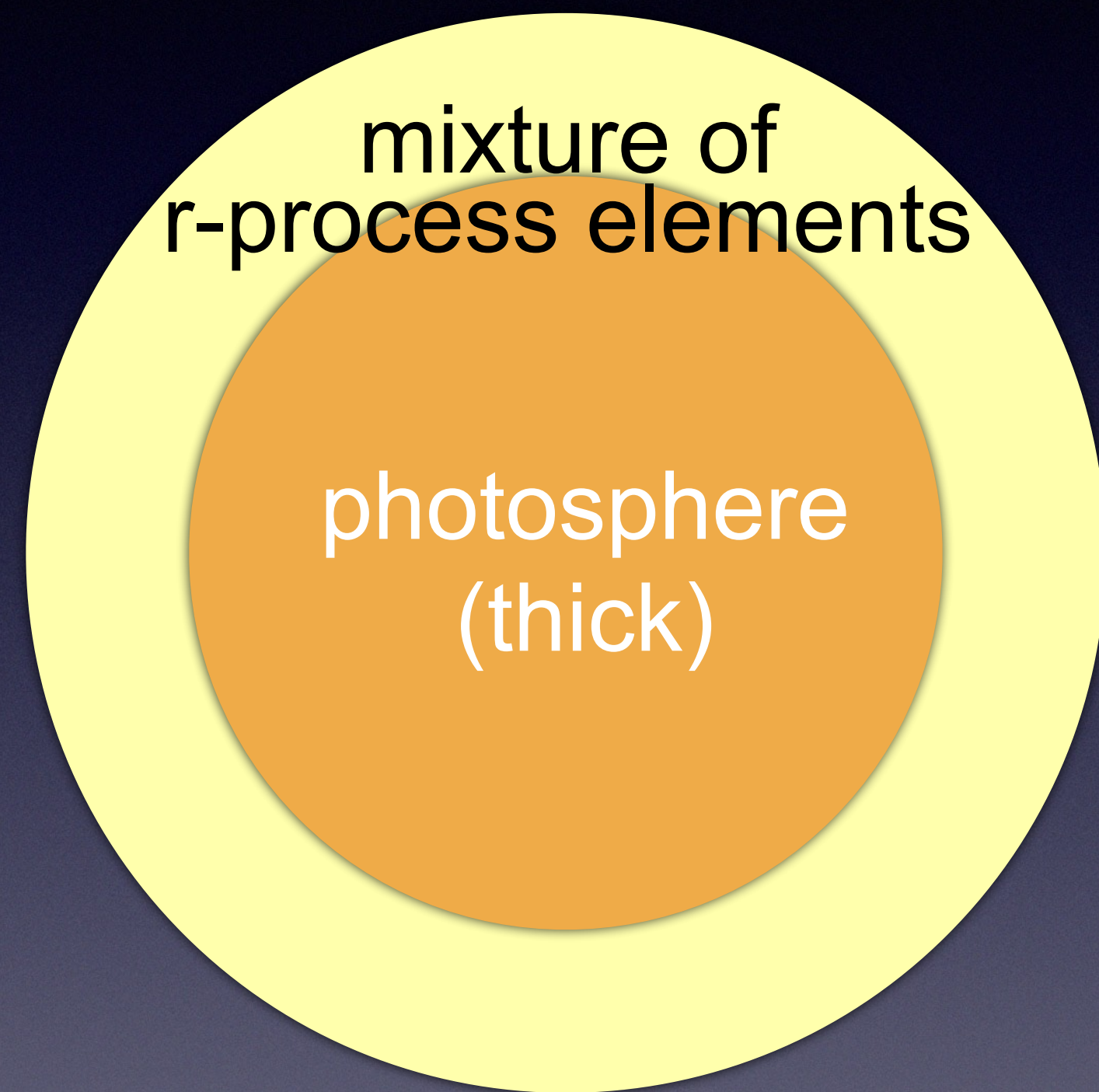
- $T \sim 5,000 \text{ K}$, $\rho \sim 10^{-15} \text{ g cm}^{-3}$ ($n \sim \rho / A m_p \sim 10^7 \text{ cm}^{-3}$)
- Heavy elements dominated plasma



“Experiments” with chemically peculiar stars

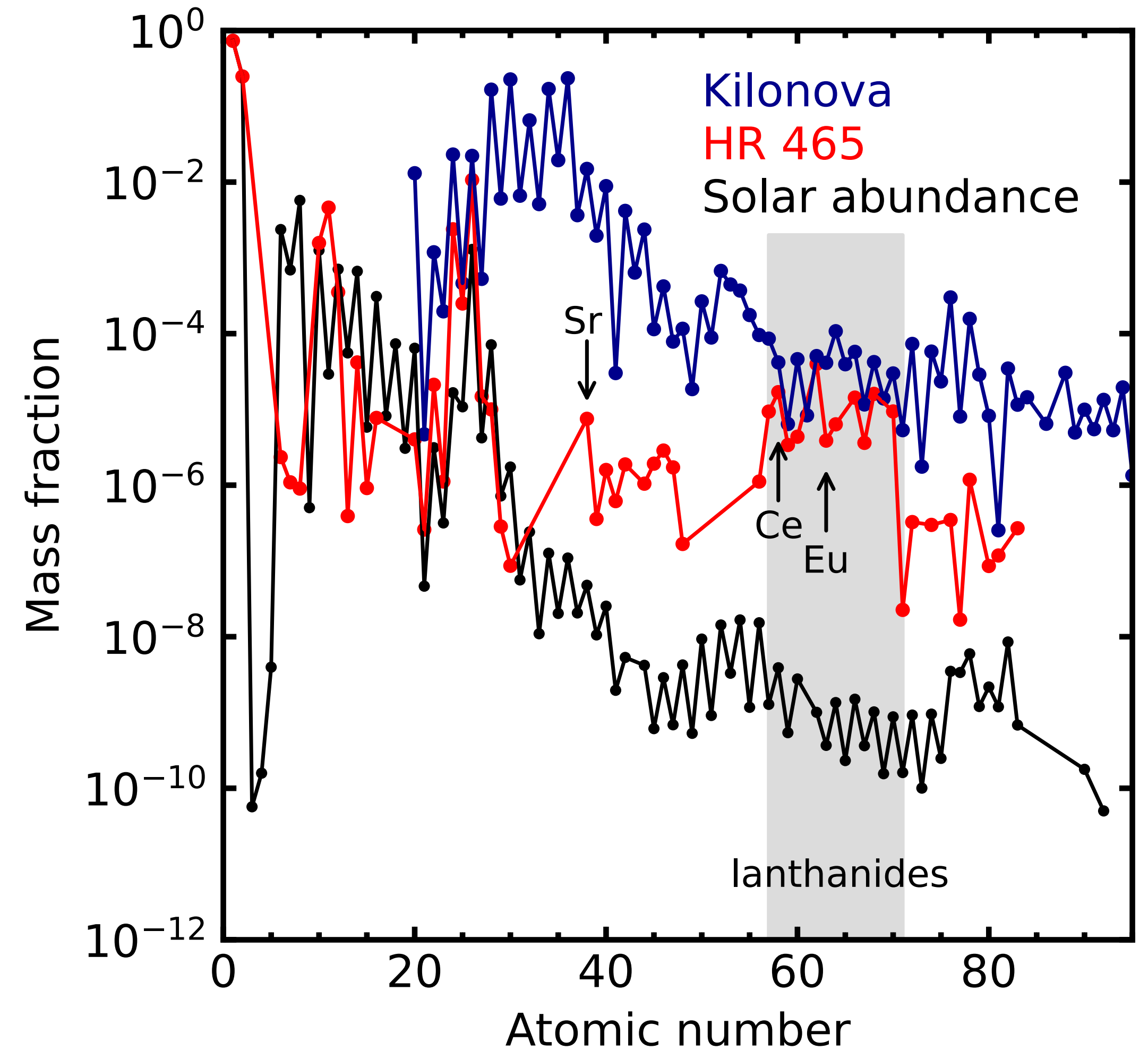
MT, Domoto, Aoki et al. 2023

absorption feature



HR 465

$[\text{Fe}/\text{H}] \sim +1.0$, $[\text{Eu}/\text{H}] \sim +4.0$

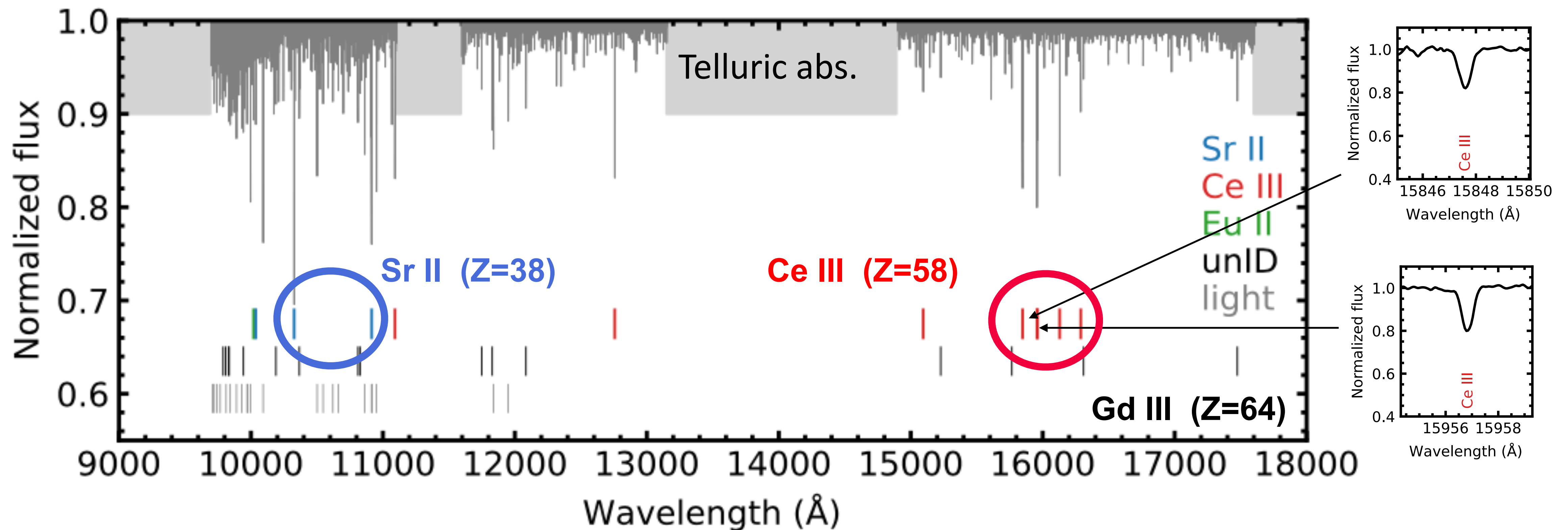


Similar lanthanide abundances (and ionization degrees) with NS merger

NIR spectrum of chemically peculiar star

MT, Domoto, Aoki+23 (Ce)

Subaru/IRD (R ~ 70,000)



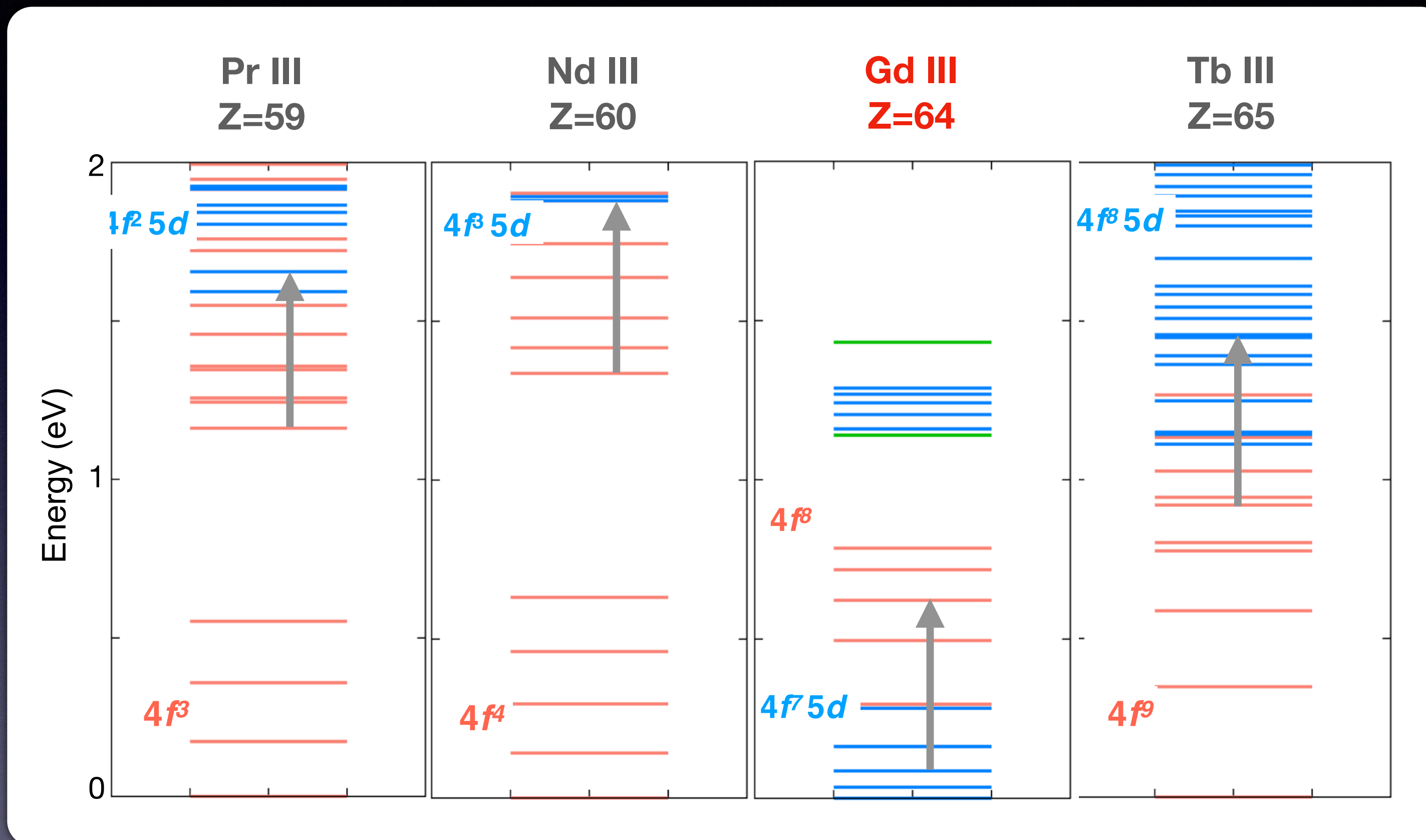
Strongest lines = Sr II, Ce III, and **Gd III** (La III is not covered)

No other comparably strong lines = uniqueness of the identification

An interesting exception: Gd ($Z=64$)

see also Gillanders+24,
Collins+26 (atomic data by Flörs+26)

Rahmouni, MT, Domoto+25



$4f^7 5d$ (4f half closed) has lower energy than $4f^8$



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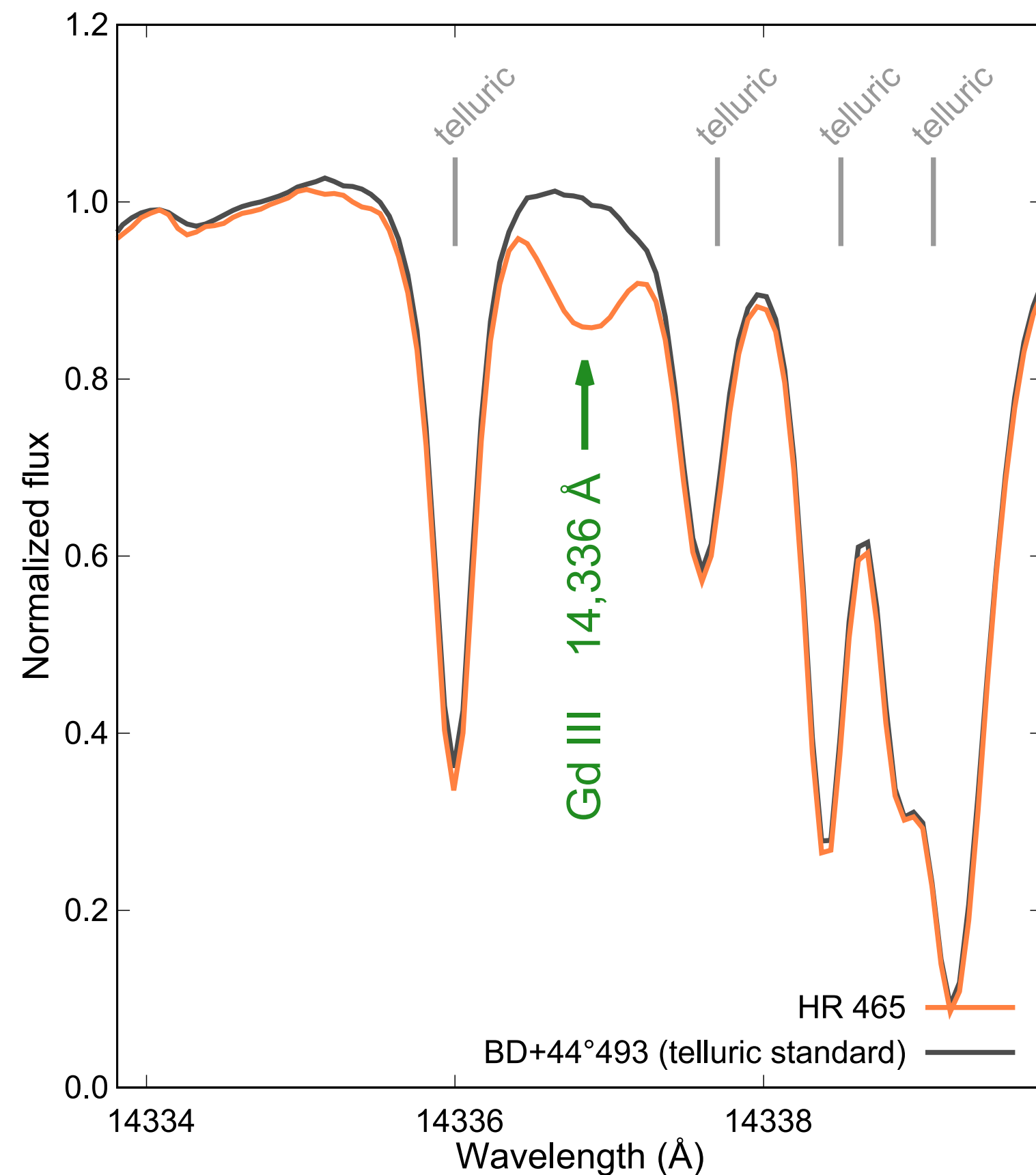


Importance of Gd features (Z=64)

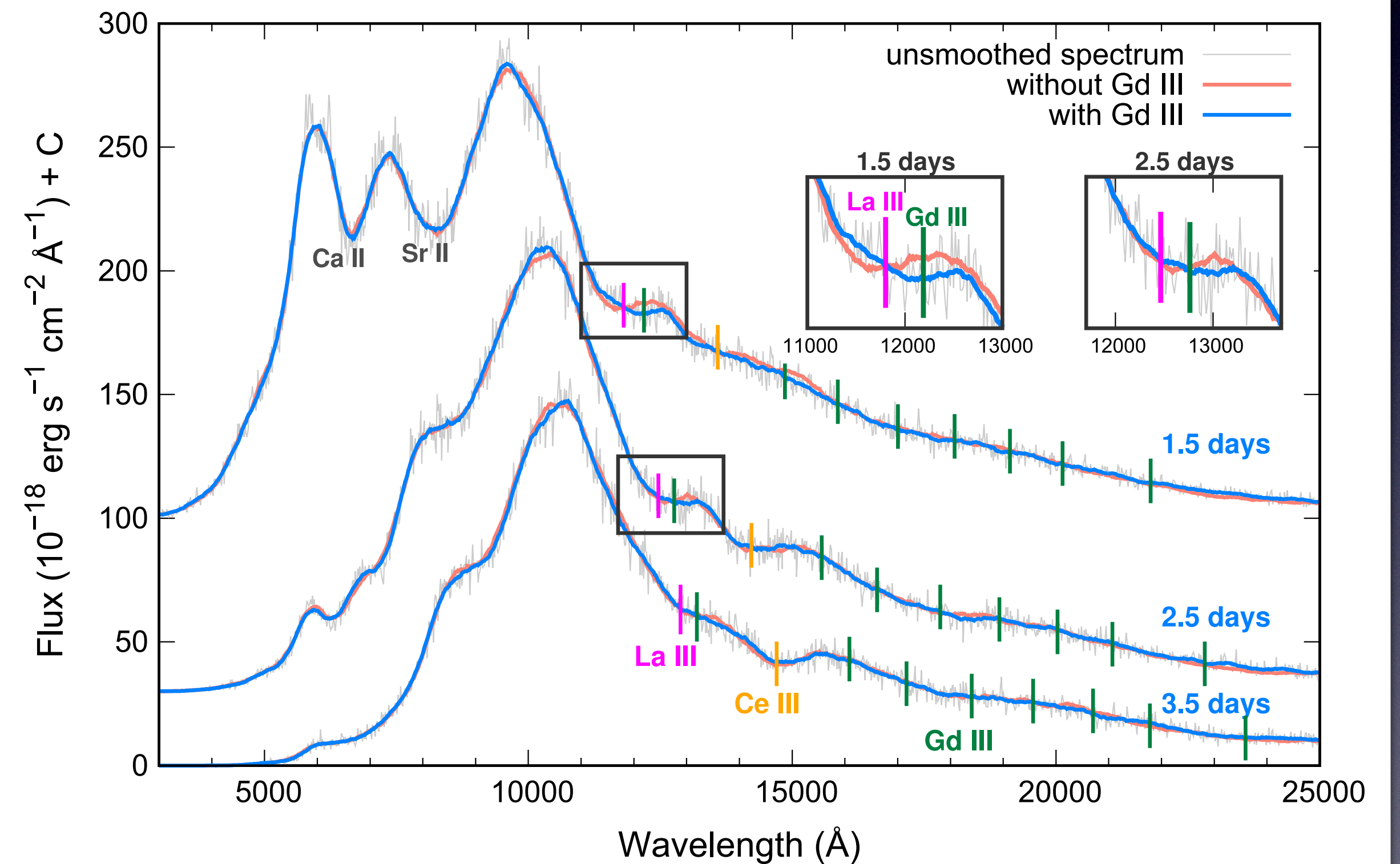
Rahmouni, MT, Domoto+25

see also Gillanders+24,
Collins+26 (atomic data by Flörs+26)

Chemically peculiar star

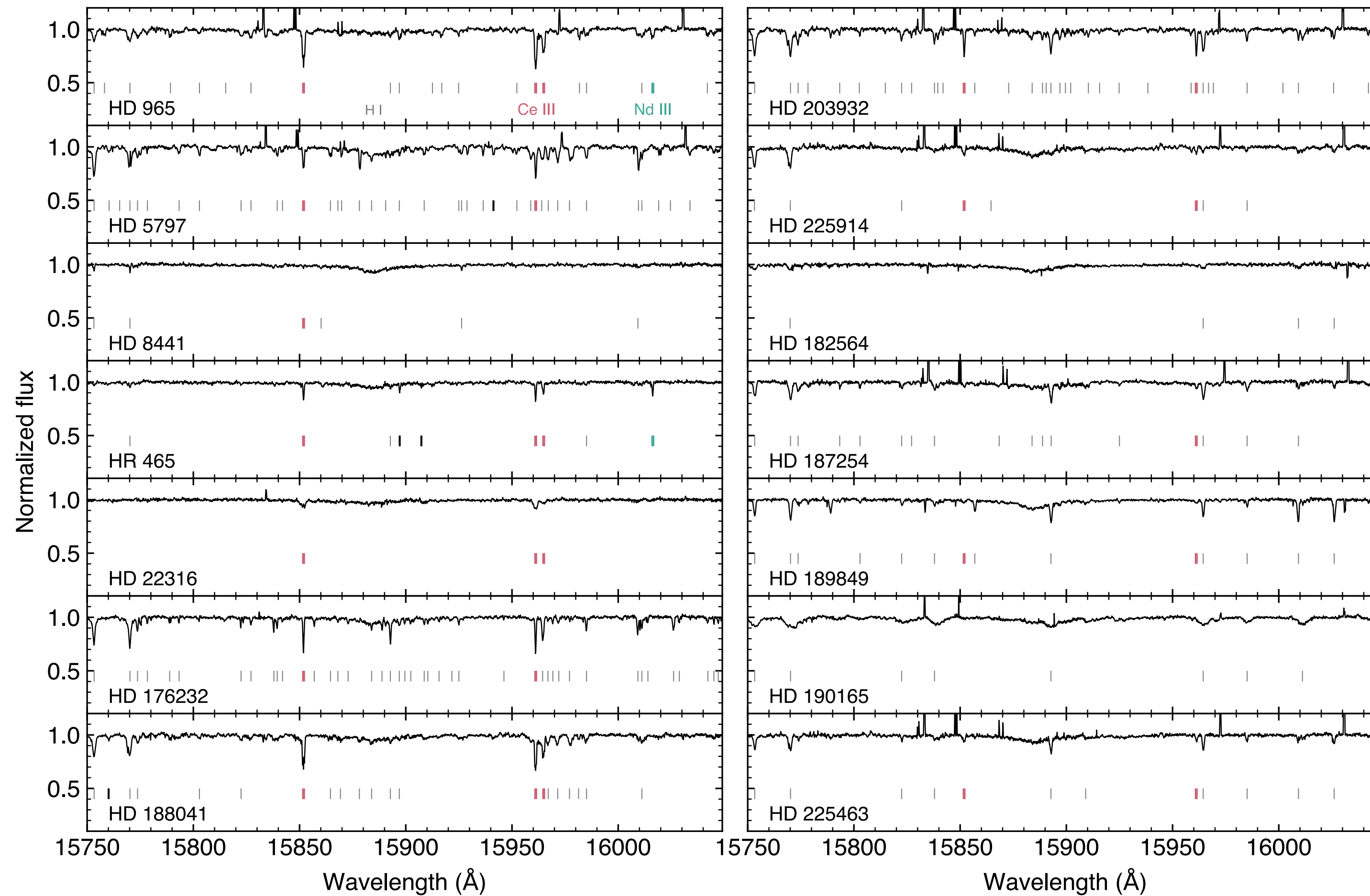


Kilonova



NIR spectra of 13 more chemically peculiar stars

Domoto, MT+ submitted



* Eu II and Gd III
Half-filled 4f + 1 electron

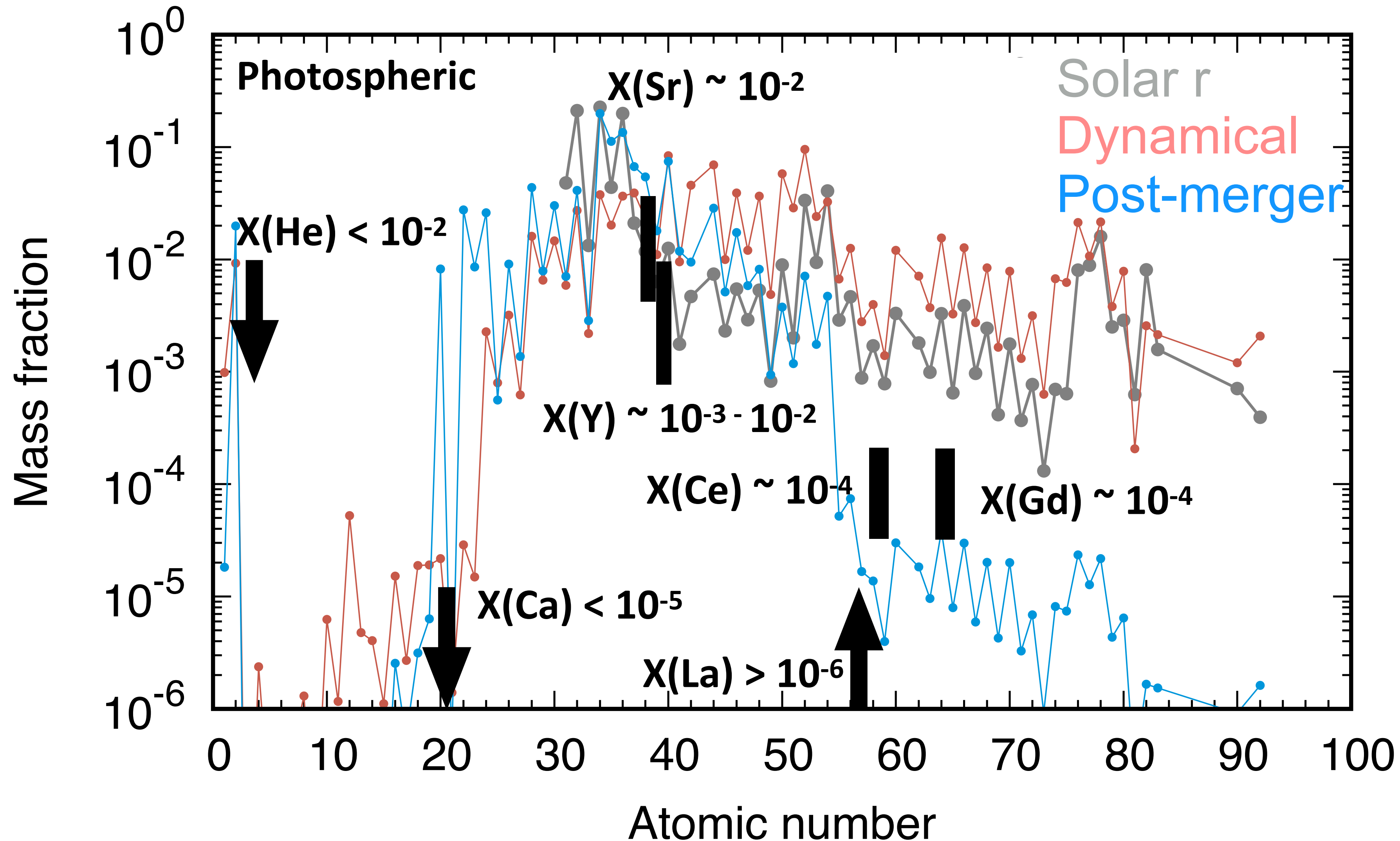
Strongest: Sr II, Ce III, and Gd III
Other (weaker) candidates: Eu II and Nd III

Identification and Abundance Estimate of Heavy Elements in Kilonova Spectra

- Element identification in kilonova spectra
- “Experiments” with chemically peculiar stars
- Towards abundance estimates

Constraints on nucleosynthesis (photospheric spectra)

Photospheric phase: Sr (Watson+19), Sr, Ca (Domoto+21), La, Ce (Domoto+22),
Y (Sneppen+23), Gd (Rahmouni+25), He (Sneppen+24, NLTE)



X(lanthanides)
 $\sim 10^{-3} ??$

see also Gillanders+26

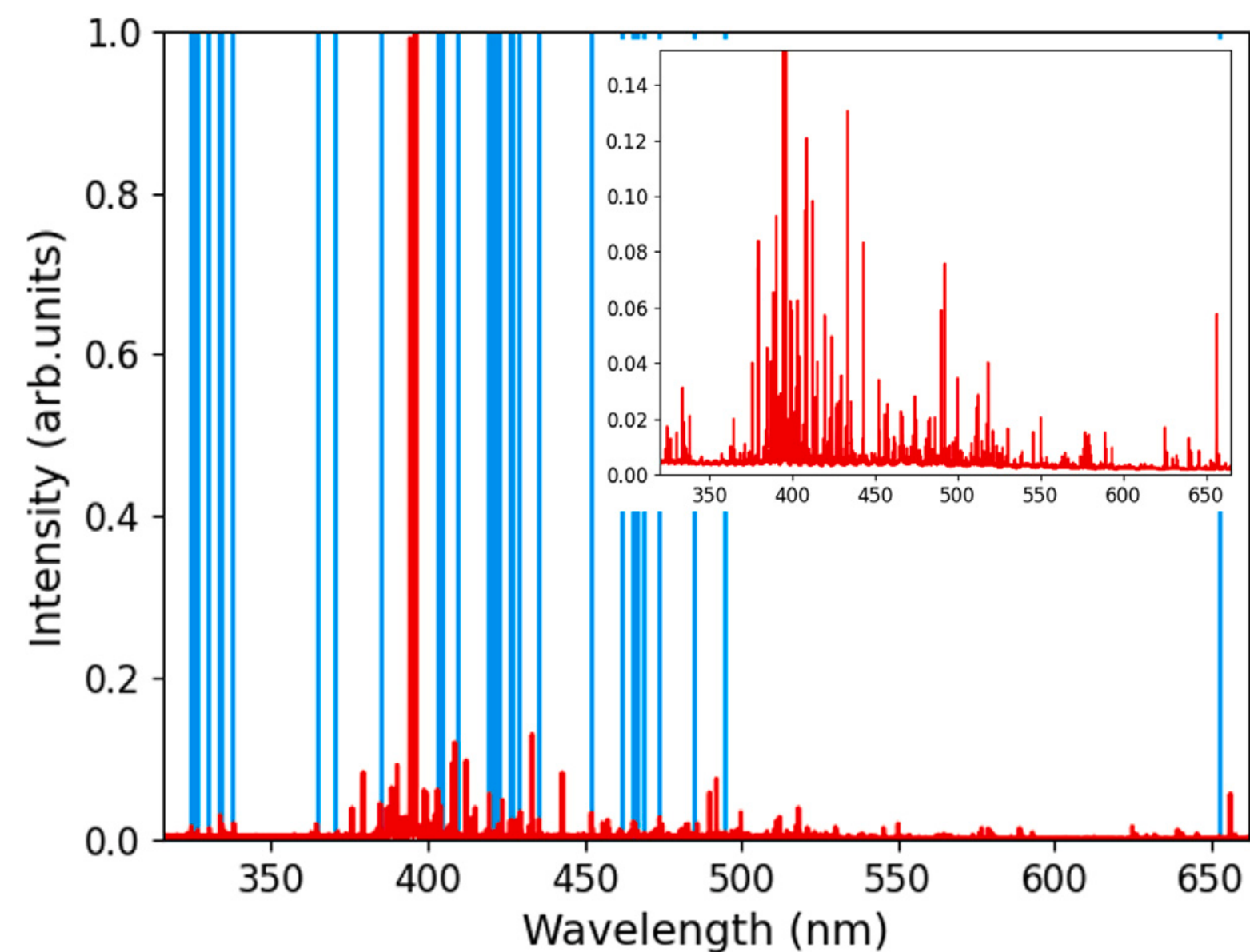
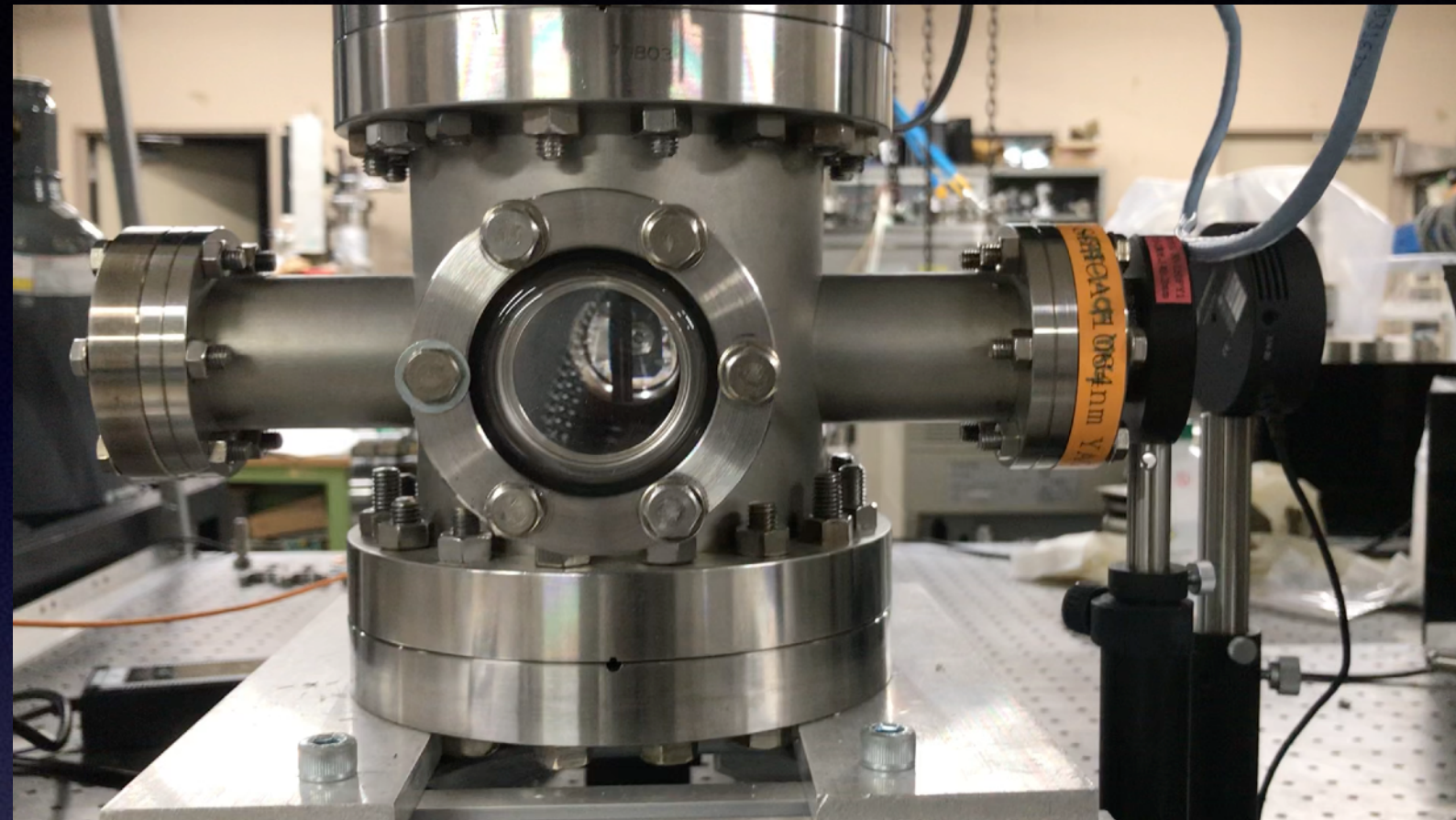
Model by Fujibayashi+23
SFHo 135-135
(mass fraction is
normalized for each
component)

Toward accurate abundance estimate

- | | |
|---|--------------------------------------|
| 1. (Experimental) atomic data | Talks on Thursday |
| 2. Plasma (non-LTE) modeling | Talks on Wednesday |
| 3. Nebular phase spectra ($\sim$ total mass) | Talks in the following session today |

1. Spectroscopic experiments

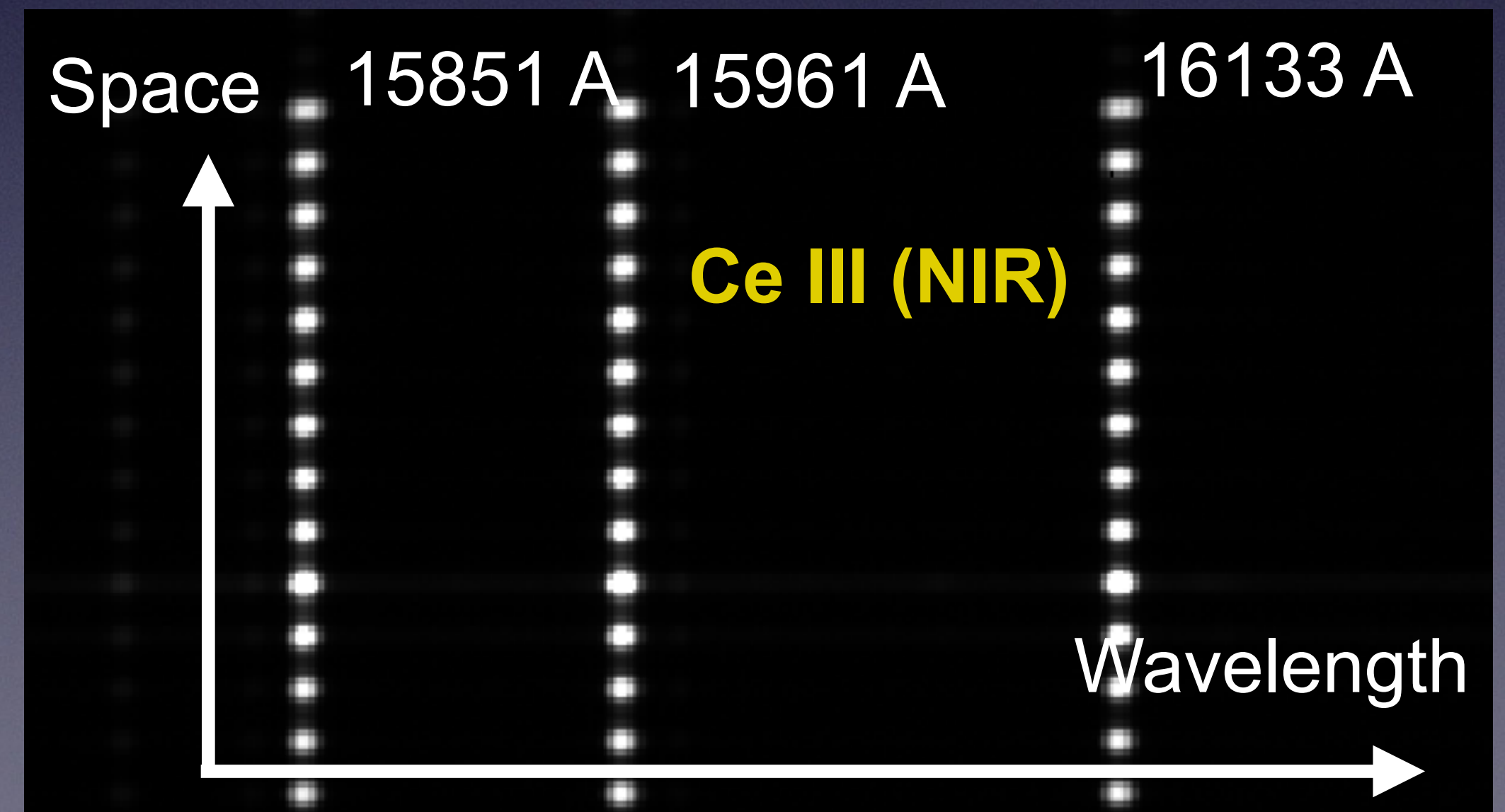
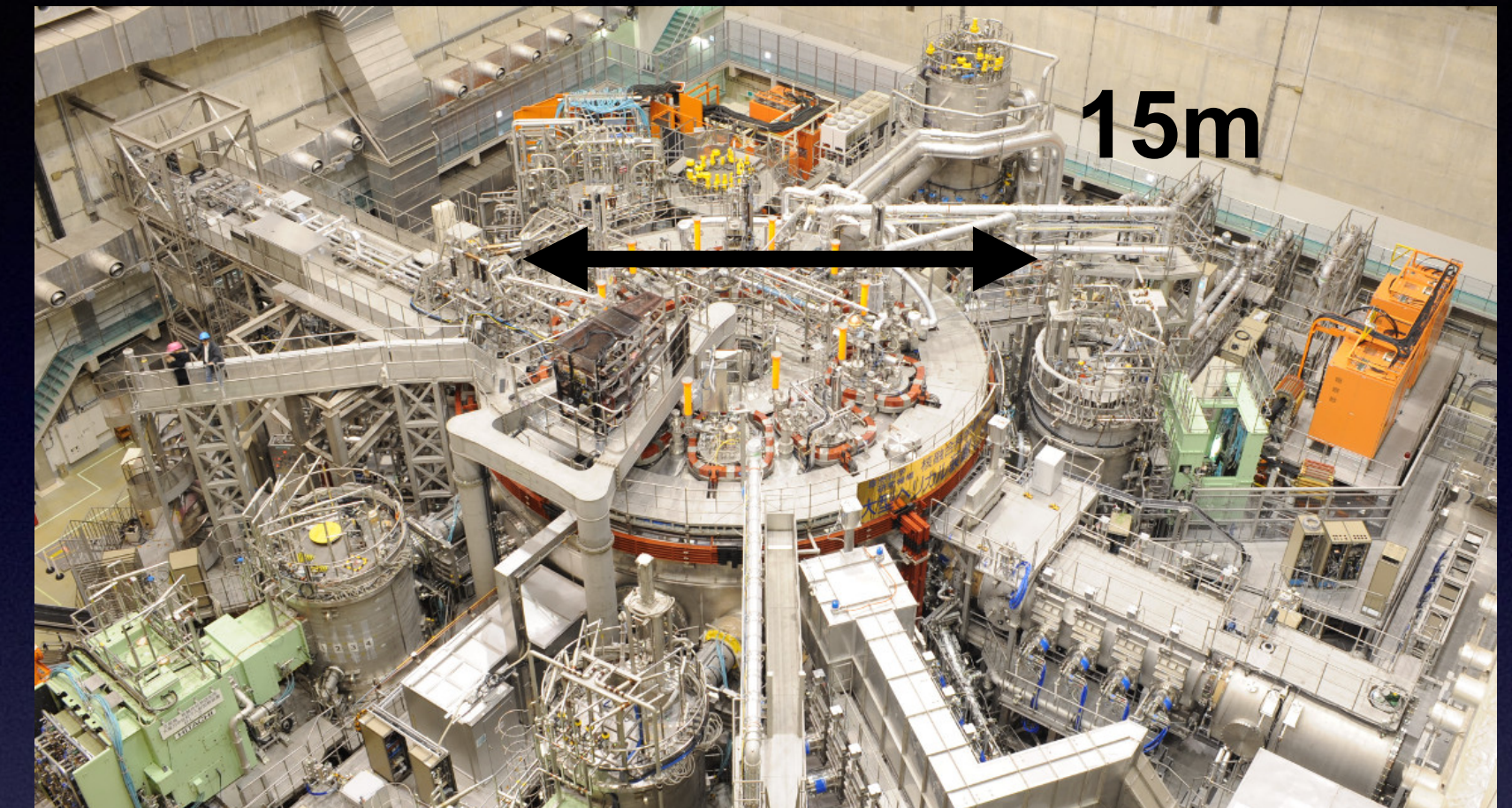
Laser induced breakdown



Kodangil, Domoto, MT+2024

Kodangil, MT, Kato+2025

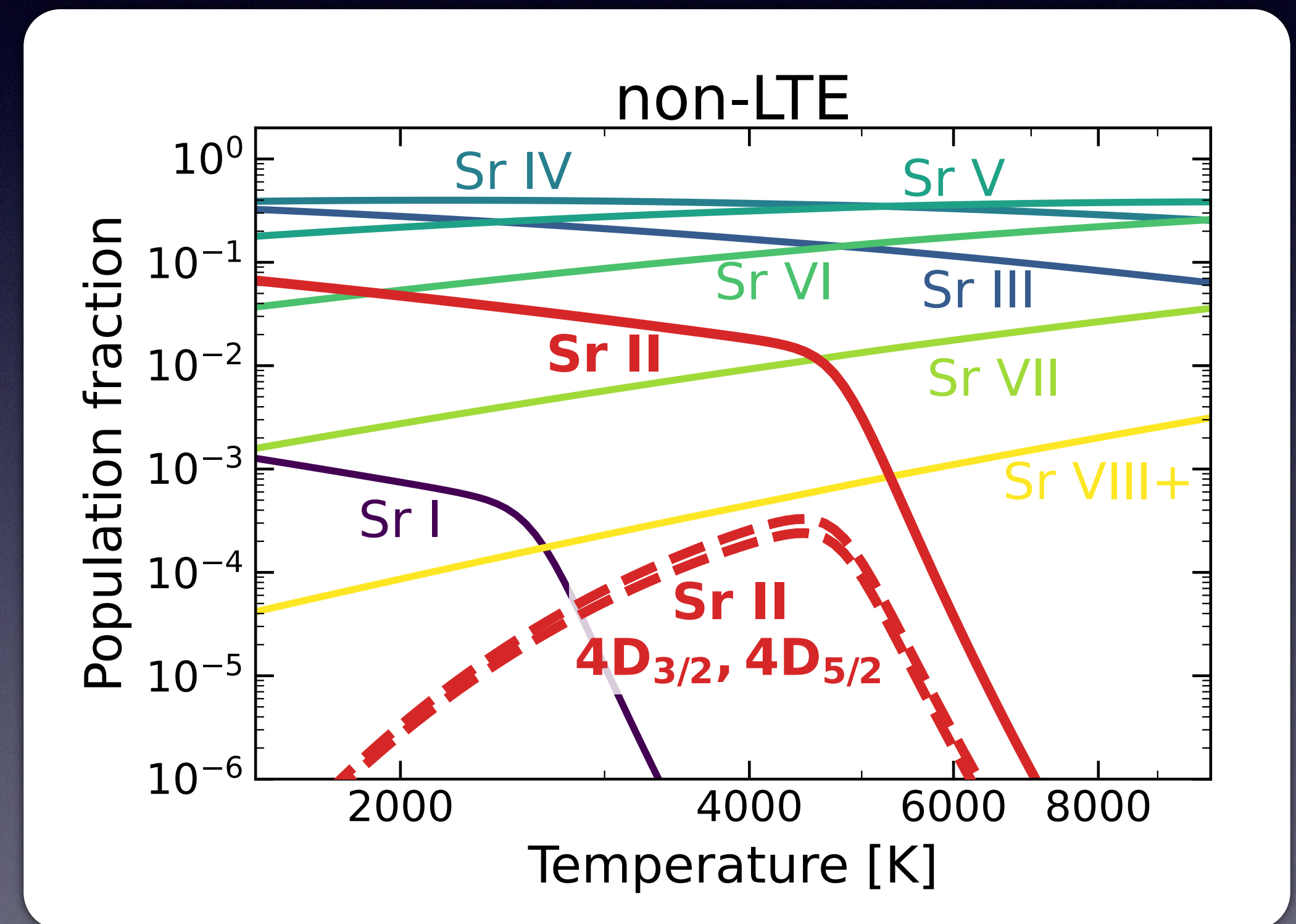
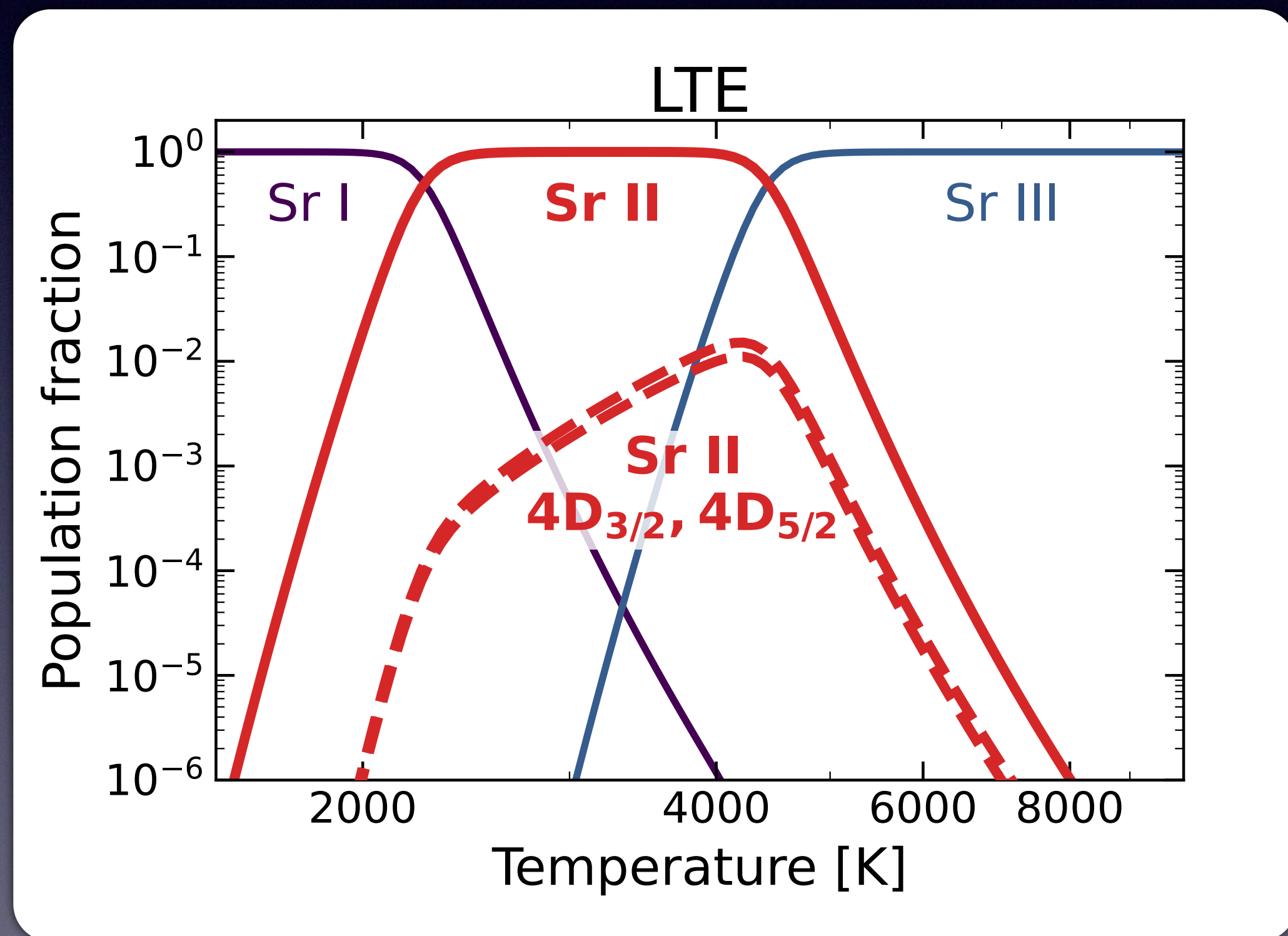
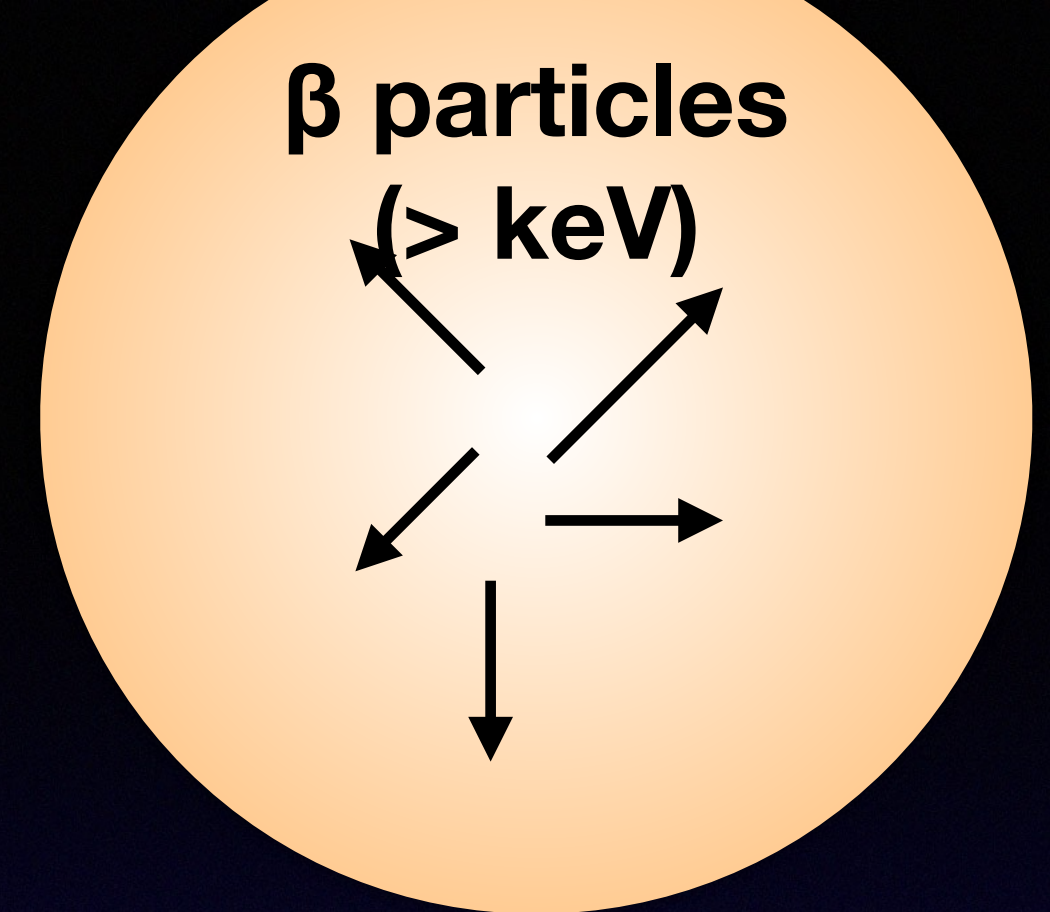
Fusion plasma



2. Non-LTE plasma modeling

Ionization by non-thermal electrons
Traumi+22, Brethauer+26, Arya+26

Chiba, MT+ 26 (arXiv:2604.05703)



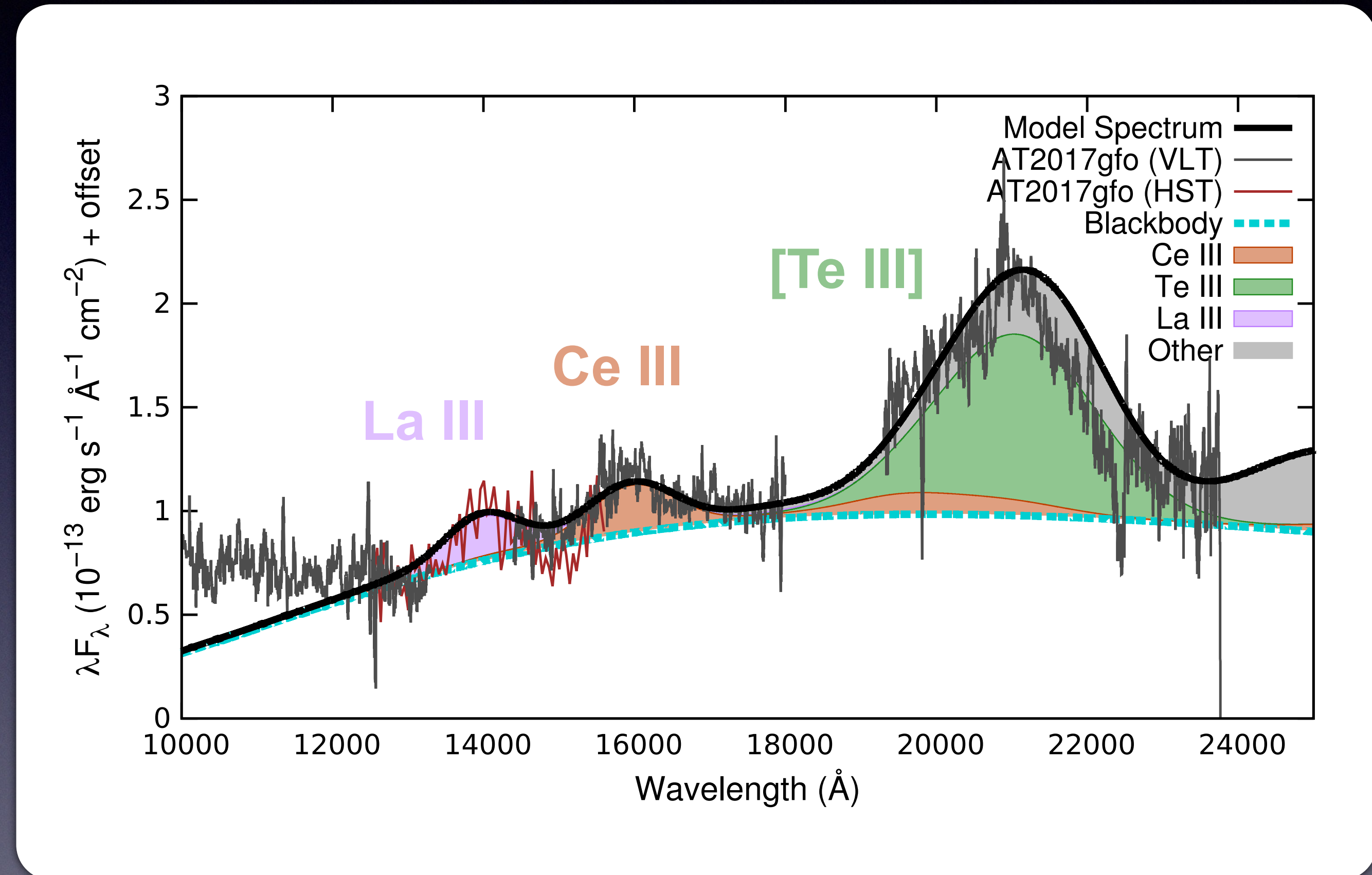
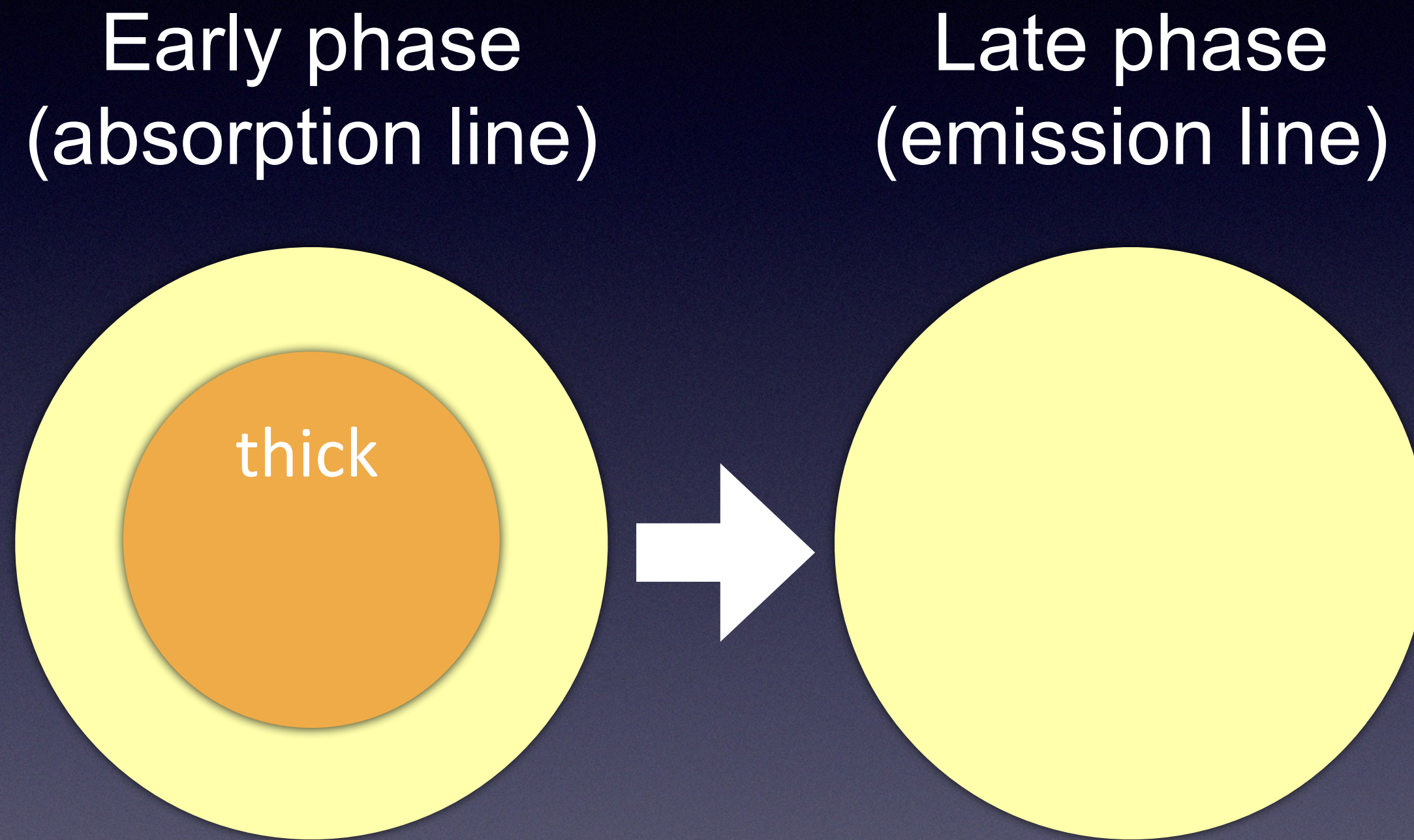
$X(\text{Sr}) \sim 10^{-2}$ (consistent with the Solar ratio)

see Aayush's talk

3. Abundance estimates in nebular spectra

Better probe of total mass

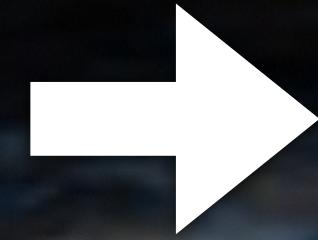
Rahmouni+ in prep.



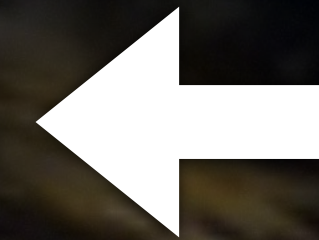
see Andreas's talk

Summary & future

Theory



Atomic data



Experiments

Ab-initio calculations
for selected important ions

NIR spectroscopy
Lifetime measurements

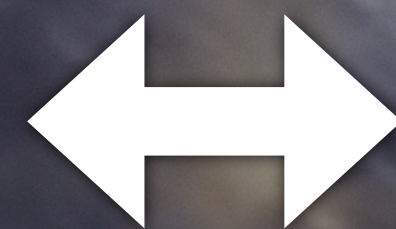
Lessons from stars



Radiation transfer

Merger
simulations

End-to-end
simulations



Non-LTE modeling
Nebular spectra

+ r-process in
core-collapse SNe

Kilonova observations

GW events + GRBs