

# **Radiative transfer simulations for light curves and spectra of kilonovae**

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in collaboration with

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Smaranika Banerjee (Stockholm U.),

Kyohei Kawaguchi (AEI), Kenta Hotokezaka (U. Tokyo)



# What can we learn from kilonova?

## Light curves

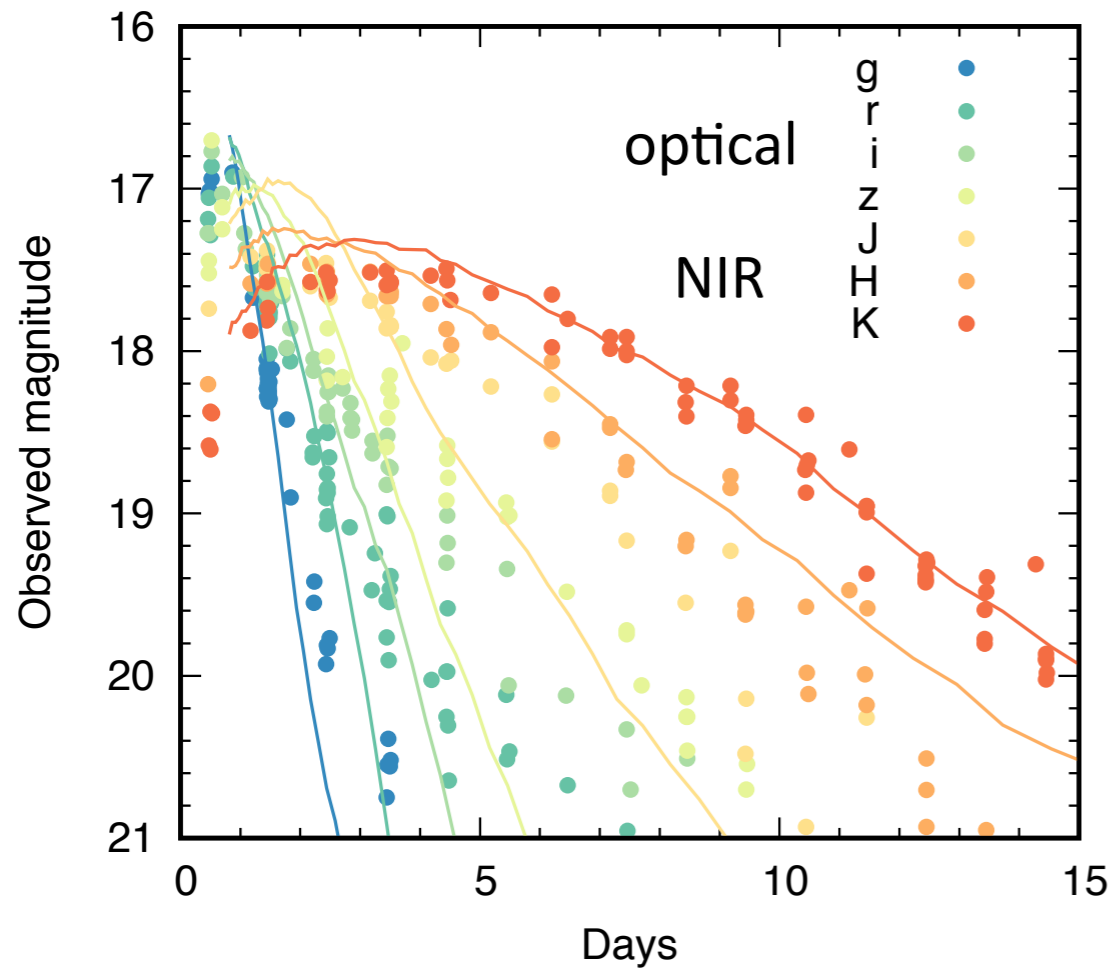


Figure from Kawaguchi+2018, 2020

Ejected mass and  
(rough) composition

## Spectra

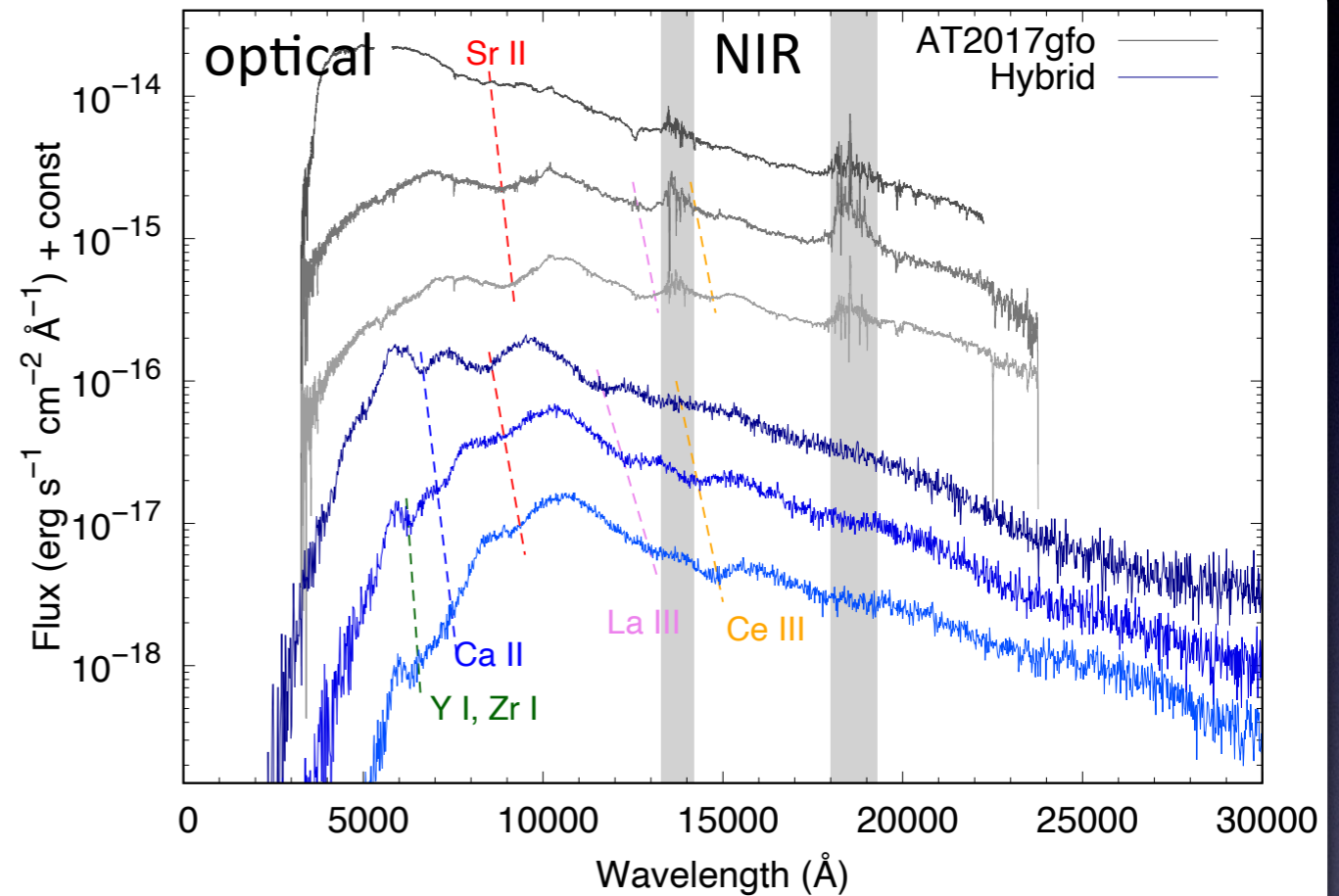


Figure from Domoto+2020,2022

Detailed composition

Origin of r-process elements  
Physics of neutron star mergers



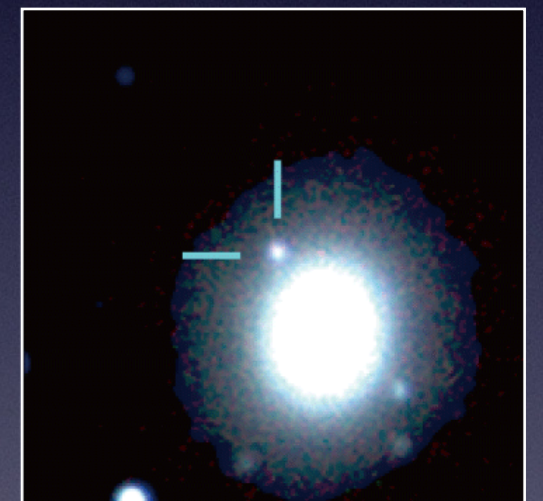
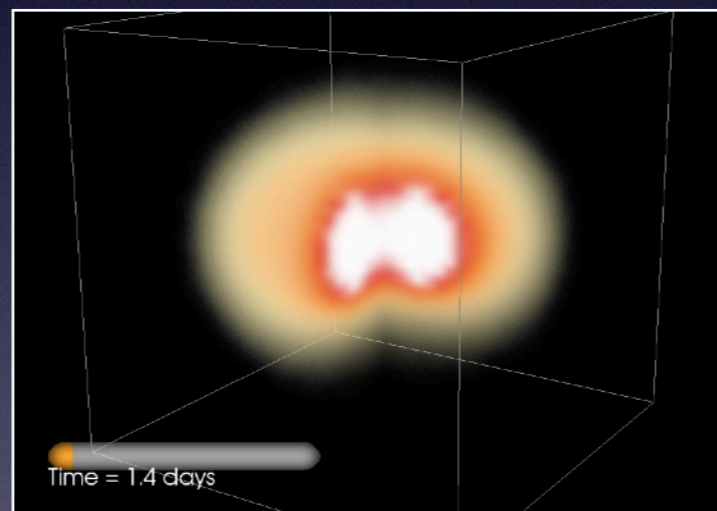
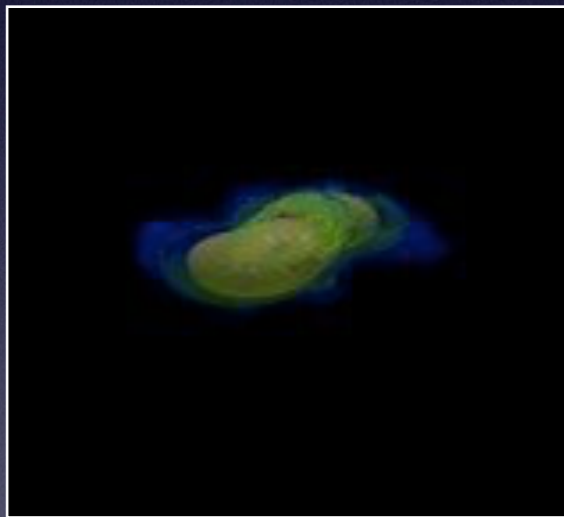
# Role of kilonova radiative transfer



dynamical ejection  $\Rightarrow$  post-merger ejection

optically thick  $\Rightarrow$  thin

Light curves  
Spectra



<http://www.aei.mpg.de/comp-rel-astro>

MT & Hotokezaka 13

(C) NAOJ

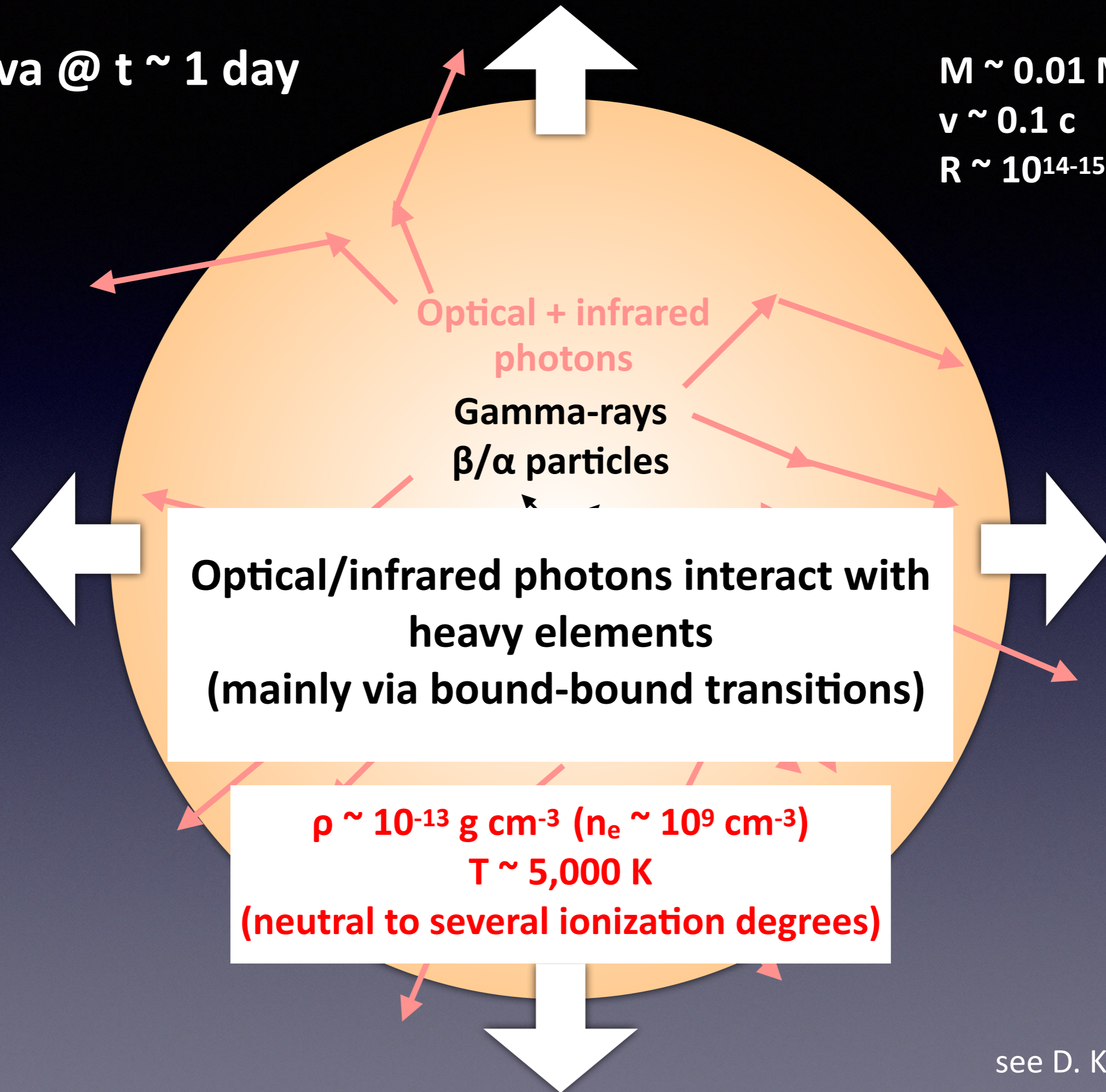
What is necessary ingredients (= atomic data)?

What is necessary for future improvement?



**Kilonova @ t ~ 1 day**

**M ~ 0.01 Msun**  
**v ~ 0.1 c**  
**R ~ 10<sup>14-15</sup> cm**



see D. Kasen's talk



# Radiative transfer simulations for light curves and spectra of kilonovae

- Light curves
- Spectra



# Two different demands on atomic data

## Light curves

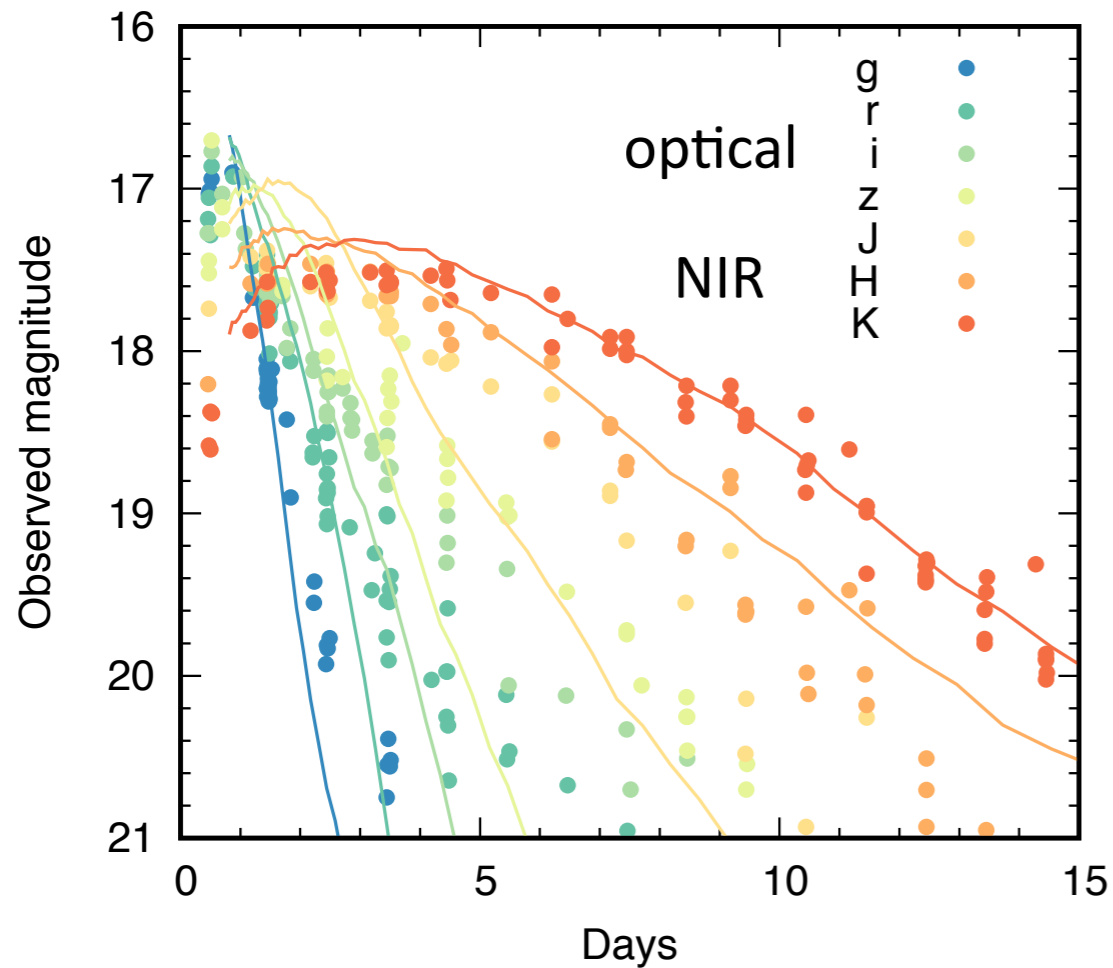


Figure from Kawaguchi+2018, 2020

**Complete** data  
for (even weak) transitions  
=> total opacity

## Spectra

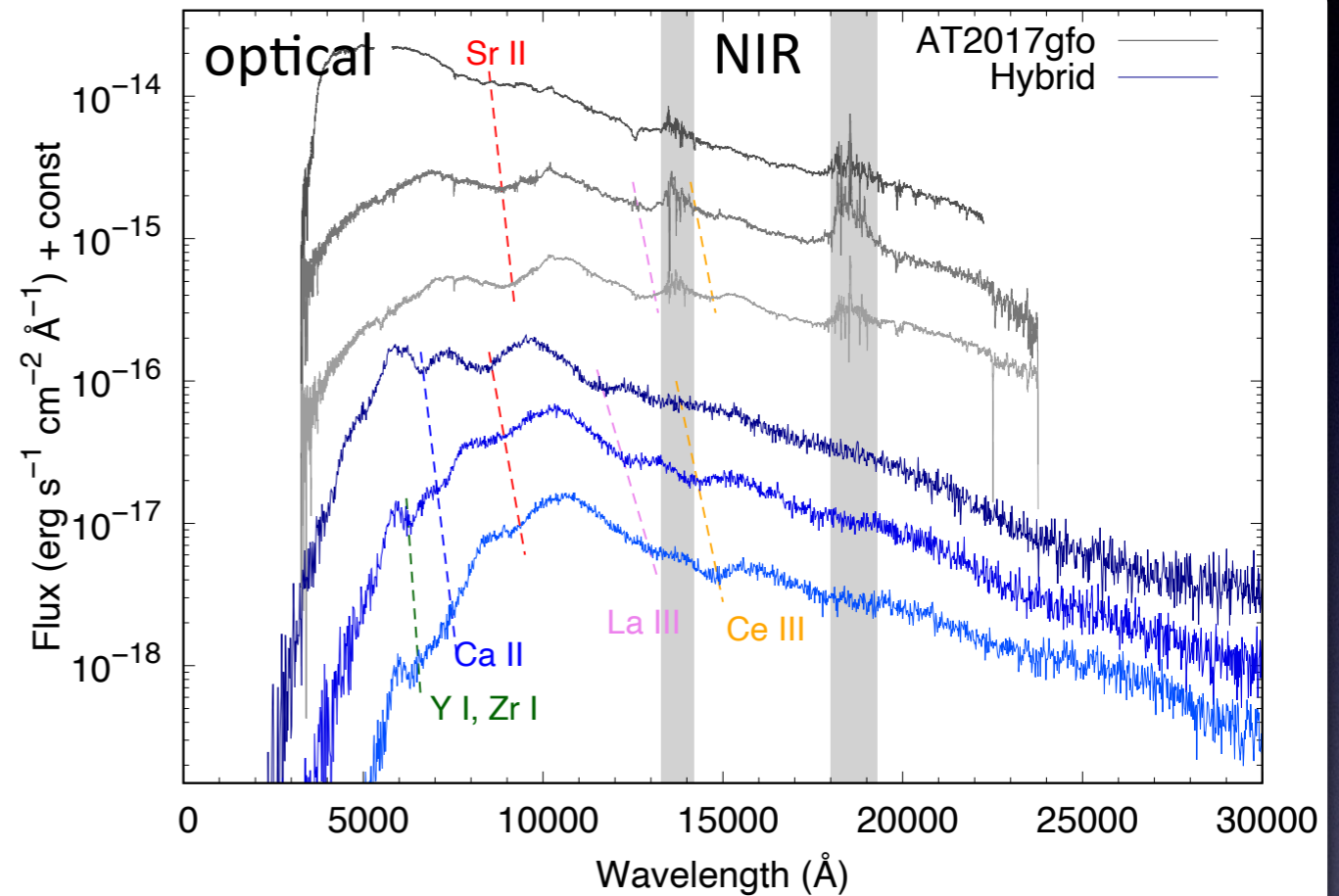


Figure from Domoto+2020,2022

**Accurate** data for  
important transitions  
=> spectral feature

see also talks by D. Kasen, C. Fryer, A. Floers, R. Ferreira da Silva, C. Fontes, S. Banerjee, P. Palmeri, ...



# “Minimum” atomic data for NS merger opacity (LTE)

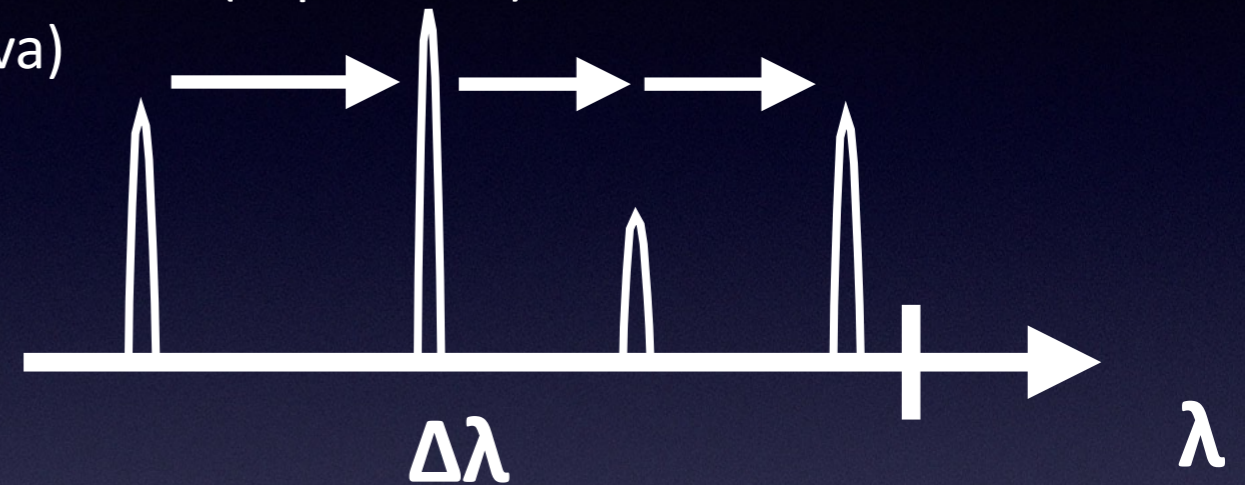
see talks by D. Kasen, Q. Pognan, K. Hotokezaka, N. Badnell for non-LTE cases

## Expansion opacity

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

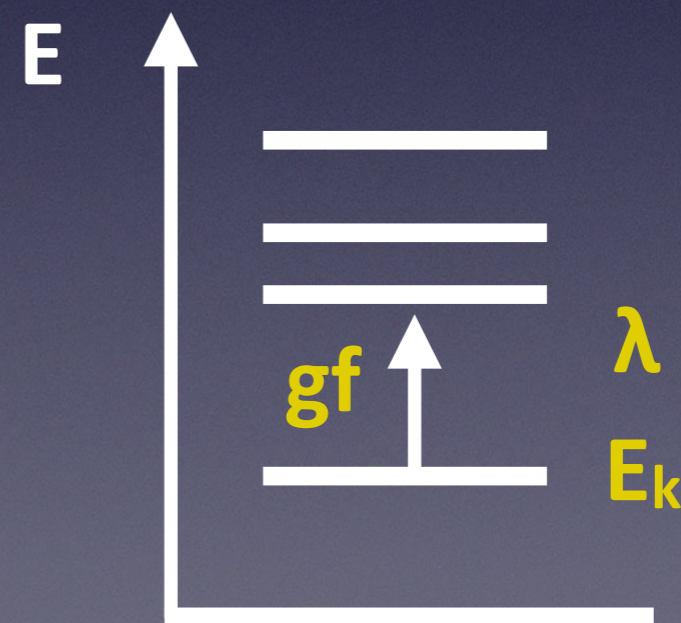
Kasen+06, Kasen+13, MT & Hotokezaka 13 (kilonova)

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



## Sobolev optical depth (homologous expansion)

$$\begin{aligned} \tau_l &= \int \alpha dr \\ &= \frac{\pi e^2}{m_e c} n_{i,j} t \lambda_l f_l \frac{g_k}{g_0} e^{-\frac{E_k}{kT}}, \end{aligned}$$



No systematic, experimentally-evaluated data



# Status of atomic calculations for kilonova

s shell

Kasen+13: Sn II, Ce II-III, Nd I-IV, Os II (Autostructure)

Fontes+17: Ce I-IV, Nd I-IV, Sm I-IV, U I-IV (LANL Suite)

Wollaeger+18: Se, Br, Zr, Pd, Te (LANL Suite)

MT+18: Se I-III, Ru I-III, Te I-III, Nd I-III, Er I-III (HULLAC, GRASP)

Kasen+17, Fontes+20: Lanthanides (I-V)

MT+20:  $Z = 26-88$  (I-IV, HULLAC)

Fontes+22: Actinides (I-IV)

p-shell

d-shell

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	57~71 La-Lu	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	89~103 Ac-Lr	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
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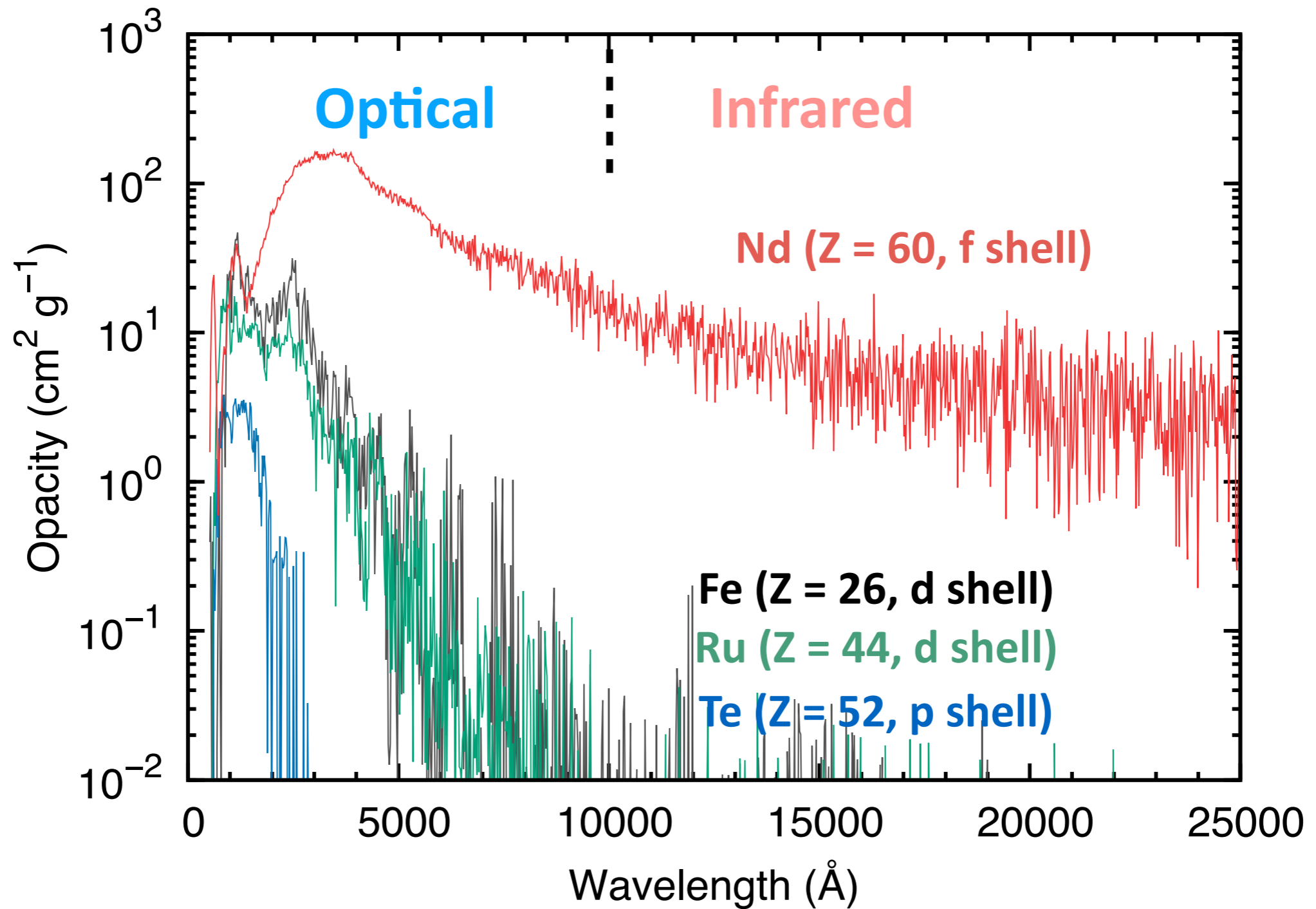
f shell

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
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# Bound-bound opacity

Kasen+13, MT & Hotokezaka 13,  
MT+18, 20, Fontes+20



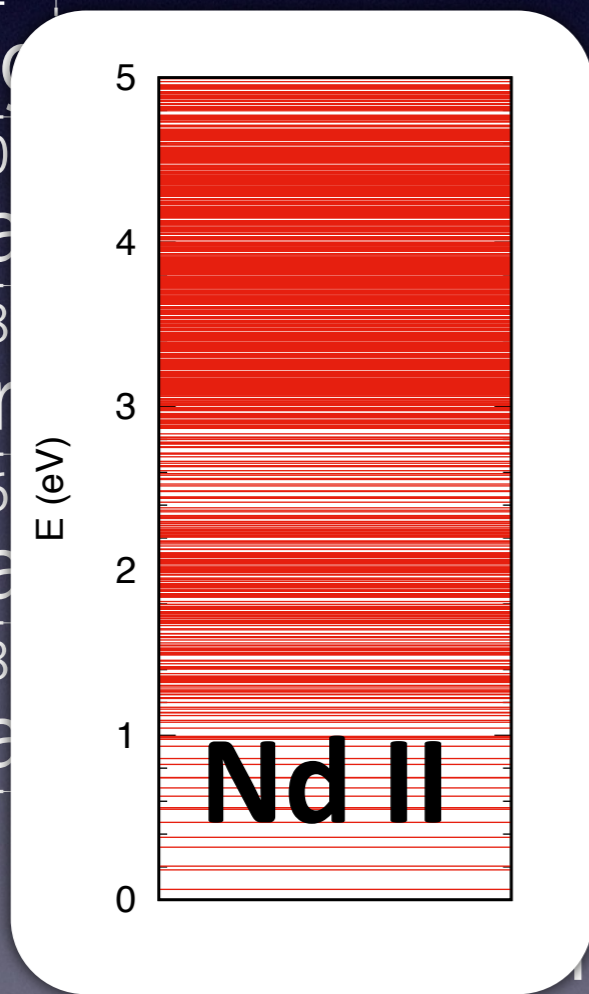


$$\lambda = \frac{hc}{\Delta E}$$

open s shell

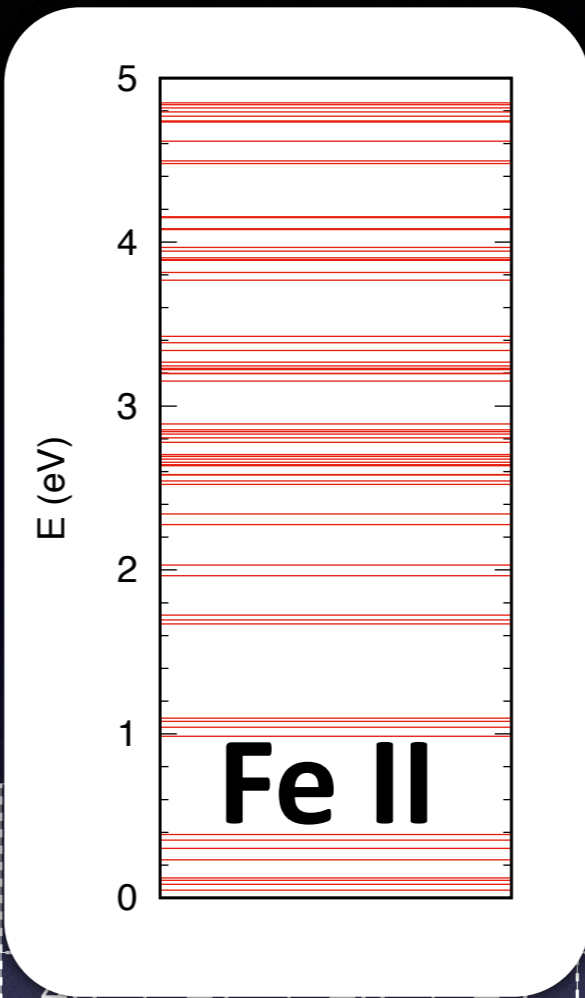
1	H		
3	Li	4	Be
11	Na	12	Mg
19	K	20	Ca
37	Rb	38	Sr
55	Cs	56	Ba
87	Fr	88	Ra

High opacity  
in infrared



open d-shell

25	Mn	26	Fe	27	Co																								
43	Tc	44	Ru	45	Rh	46	Pd	47	Ag	48	Cd	49	In	50	Sn	51	Sb	52	Te	53	I	54	Xe						
75	Re	76	Os	77	Ir	78	Pt	79	Au	80	Hg	81	Tl	82	Pb	83	Bi	84	Po	85	At	86	Rn						
107	Bh	108	Hs	109	Mt	110	Ds	111	Rg	112	Cn	113	Nh	114	Fl	115	Mc	116	Lv	117	Ts	118	Og						
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



open p-shell

6	C	7	N	8	O	9	F	10	Ne
14	Si	15	P	16	S	17	Cl	18	Ar
32	Ge	33	As	34	Se	35	Br	36	Kr
50	Sn	51	Sb	52	Te	53	I	54	Xe
82	Pb	83	Bi	84	Po	85	At	86	Rn
114	Fl	115	Mc	116	Lv	117	Ts	118	Og

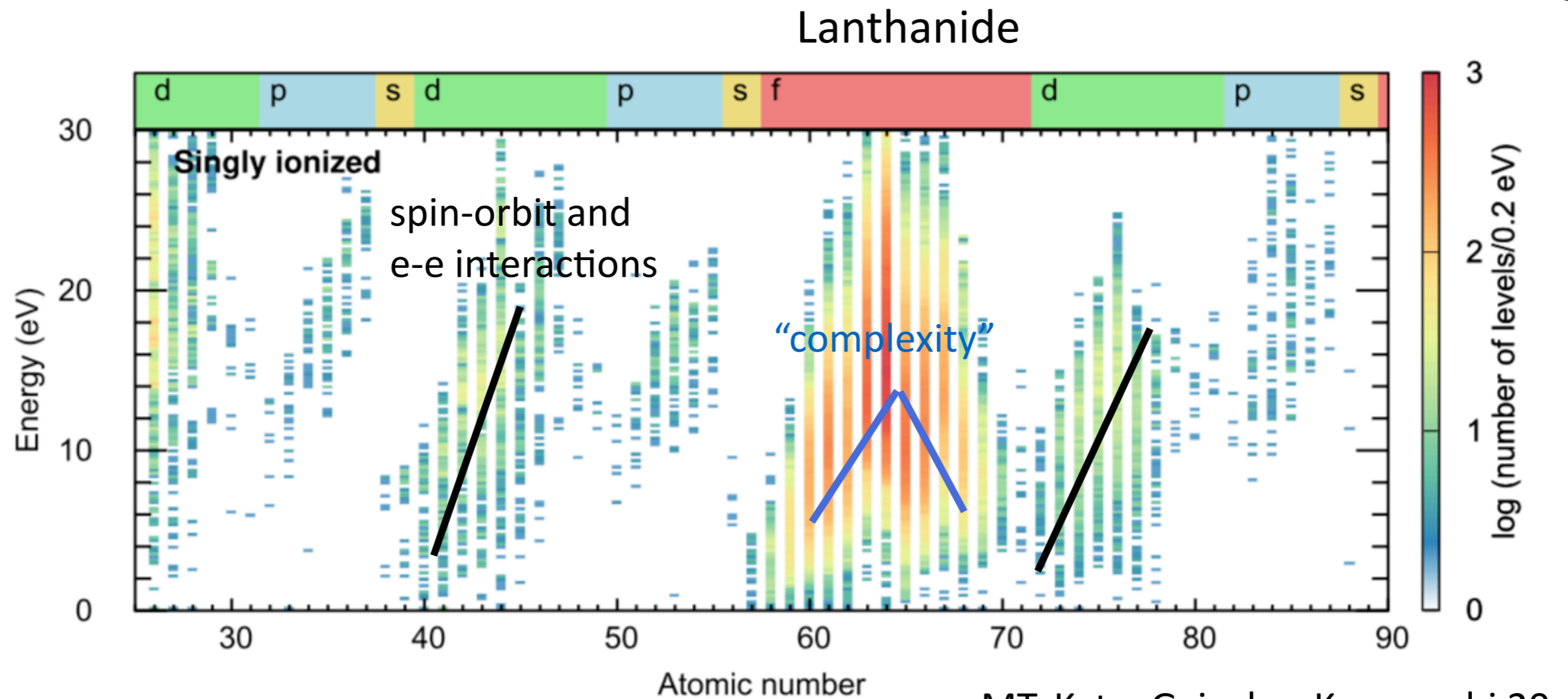
open f shell



# Energy level distribution

All the data are available at  
<http://dpc.nifs.ac.jp/DB/Opacity-Database/>

calculated with HULLAC code

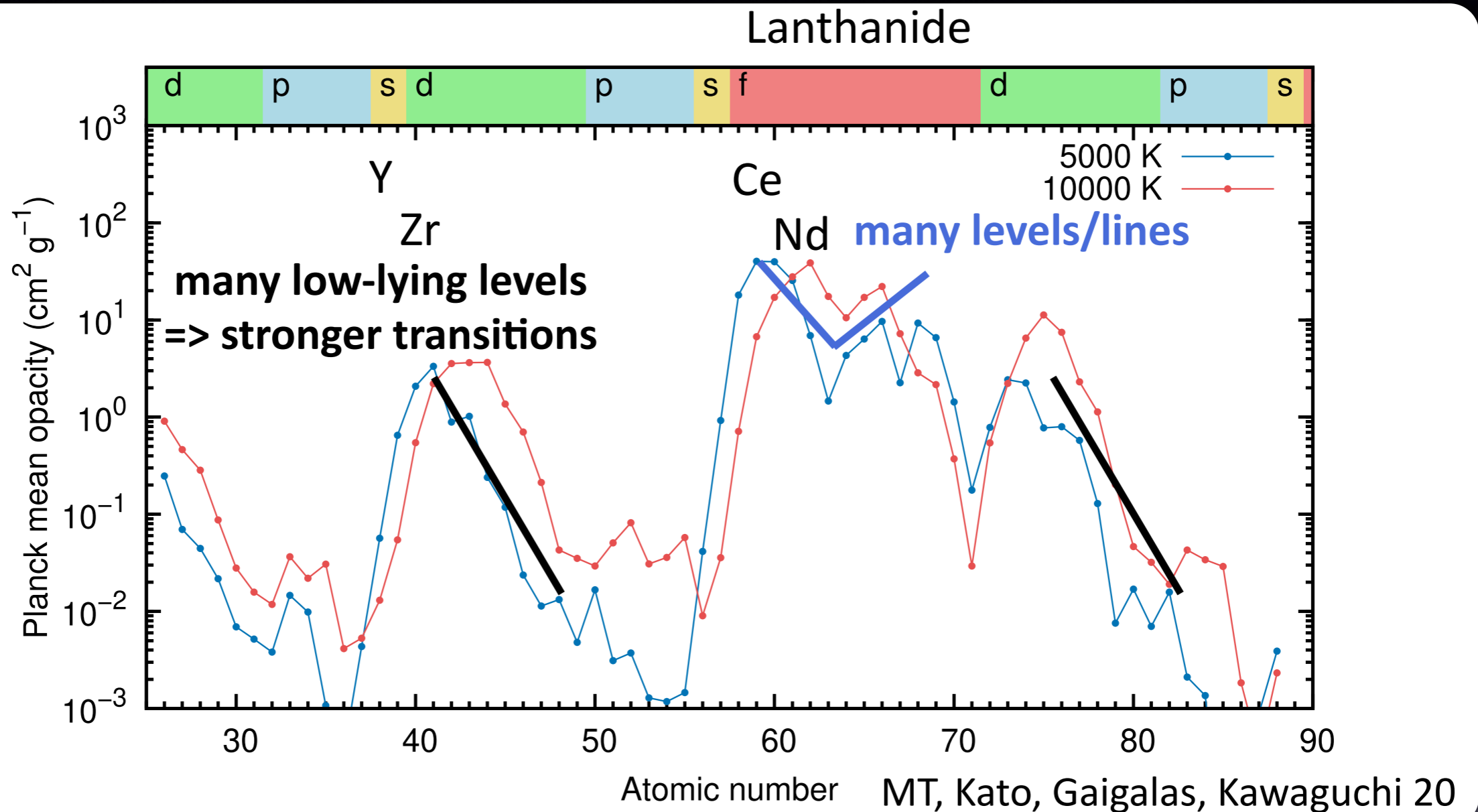


MT, Kato, Gaigalas, Kawaguchi 20



# Opacity (Planck mean)

All the data are available at  
<http://dpc.nifs.ac.jp/DB/Opacity-Database/>



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

$$\tau_l = \frac{\pi e^2}{m_e c} n_{i,j} t \lambda_l f_l \frac{g_k}{g_0} e^{-\frac{E_k}{kT}}$$



# Understanding the impact of accuracy in atomic calculations

see Gaigalas+19 for Nd (see also Floers+23)

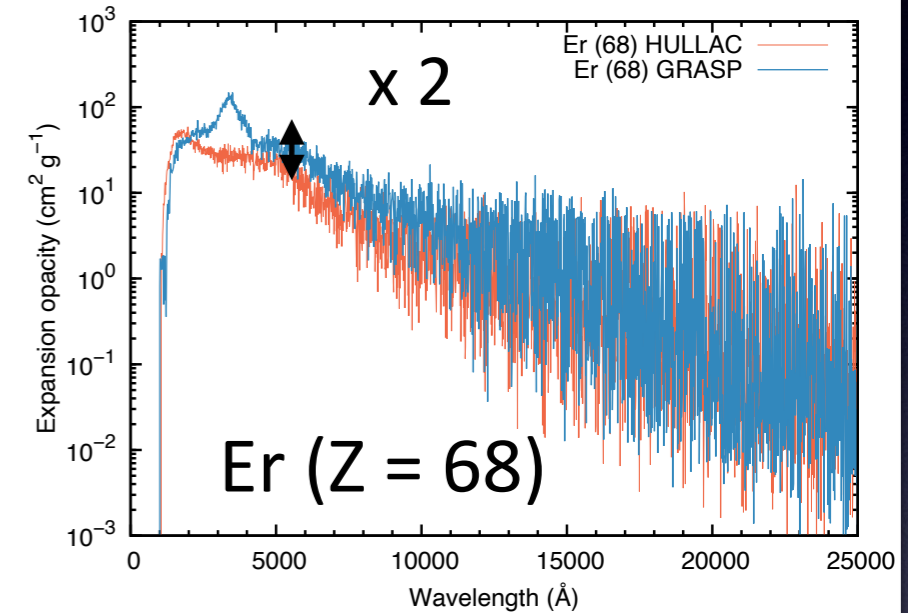
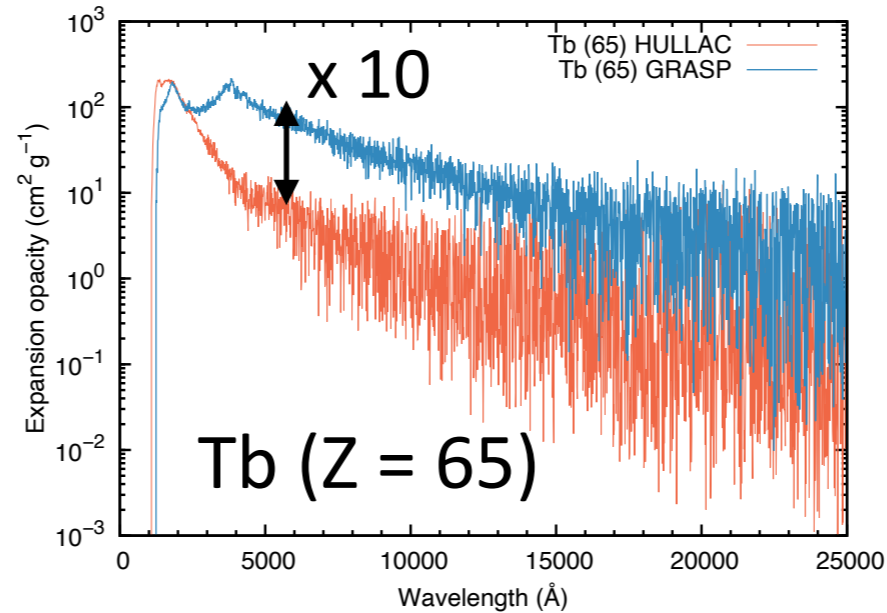
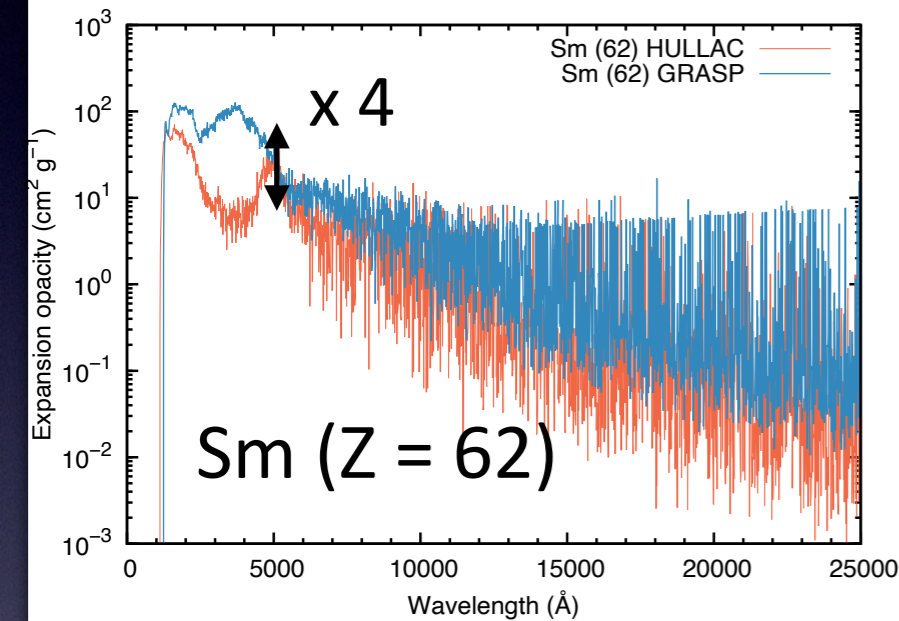
## Singly ionized lanthanides

GRASP (Radziute+20, 21)

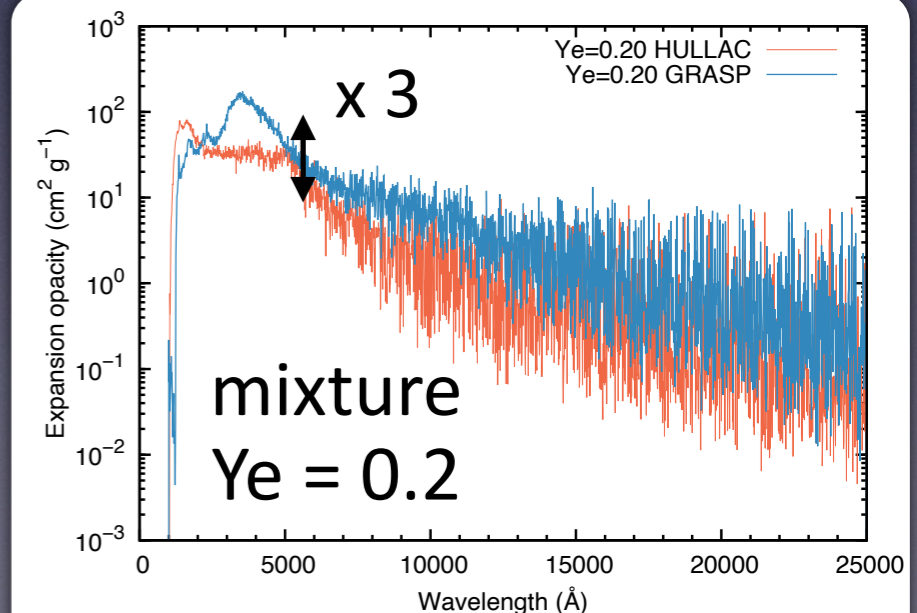
see P. Jonsson's talk

HULLAC (Tanaka+20)

T = 5000 K



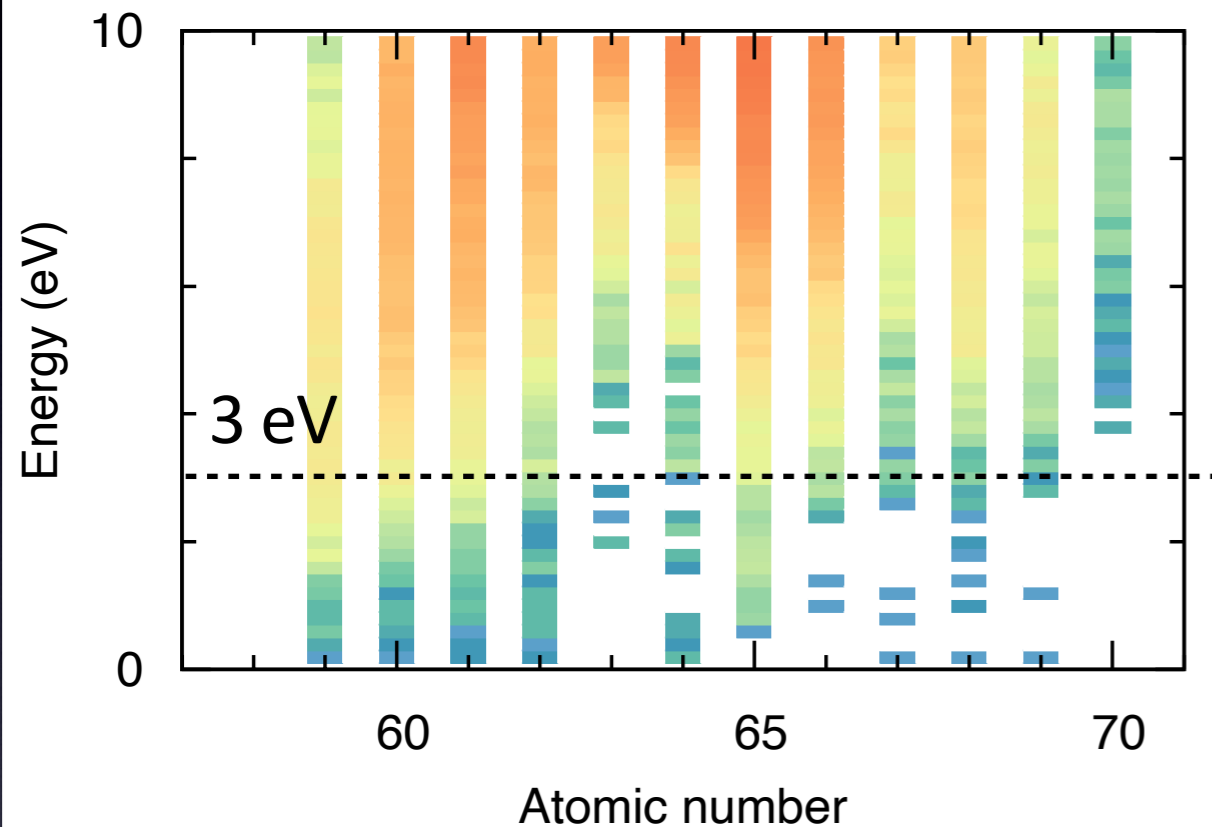
Largest difference in the most complex ions



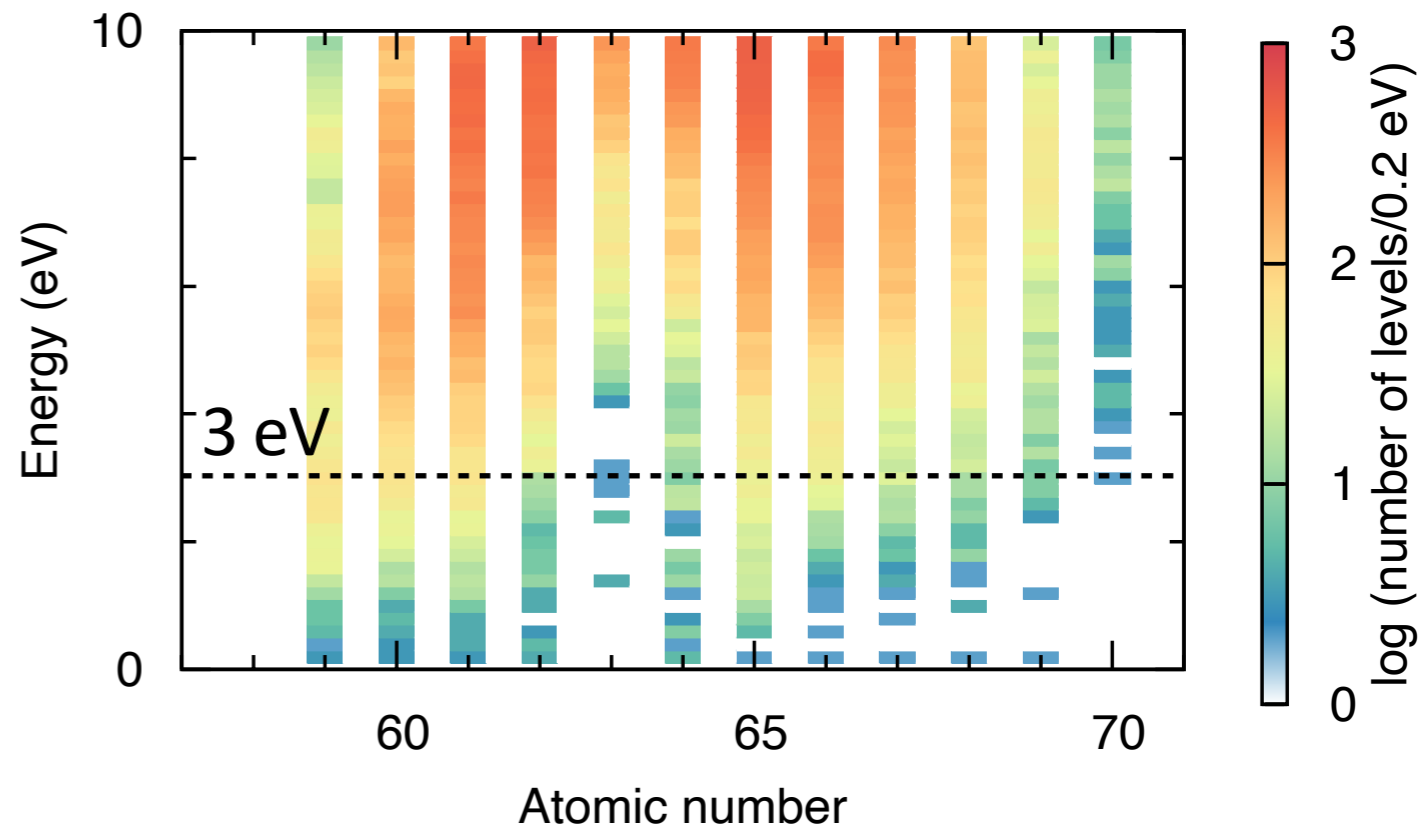


# Energy level distributions

## HULLAC



## GRASP

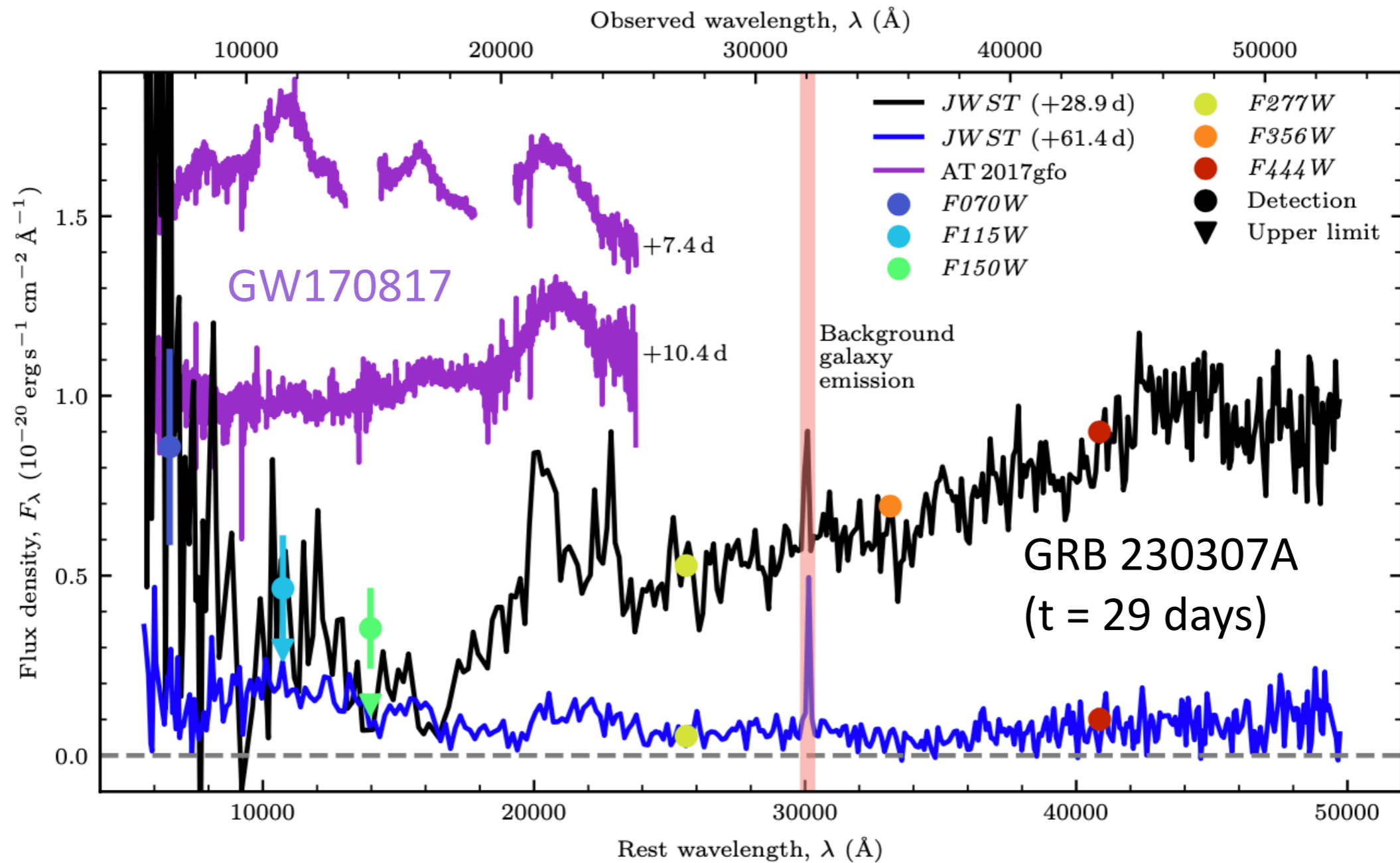


**HULLAC results tend to show upward energy level distribution**  
(Main difference is in  $4f^n 5d 6s$  configurations)



# Kilonova in GRB230307A?

Levan+23, Gillanders+23



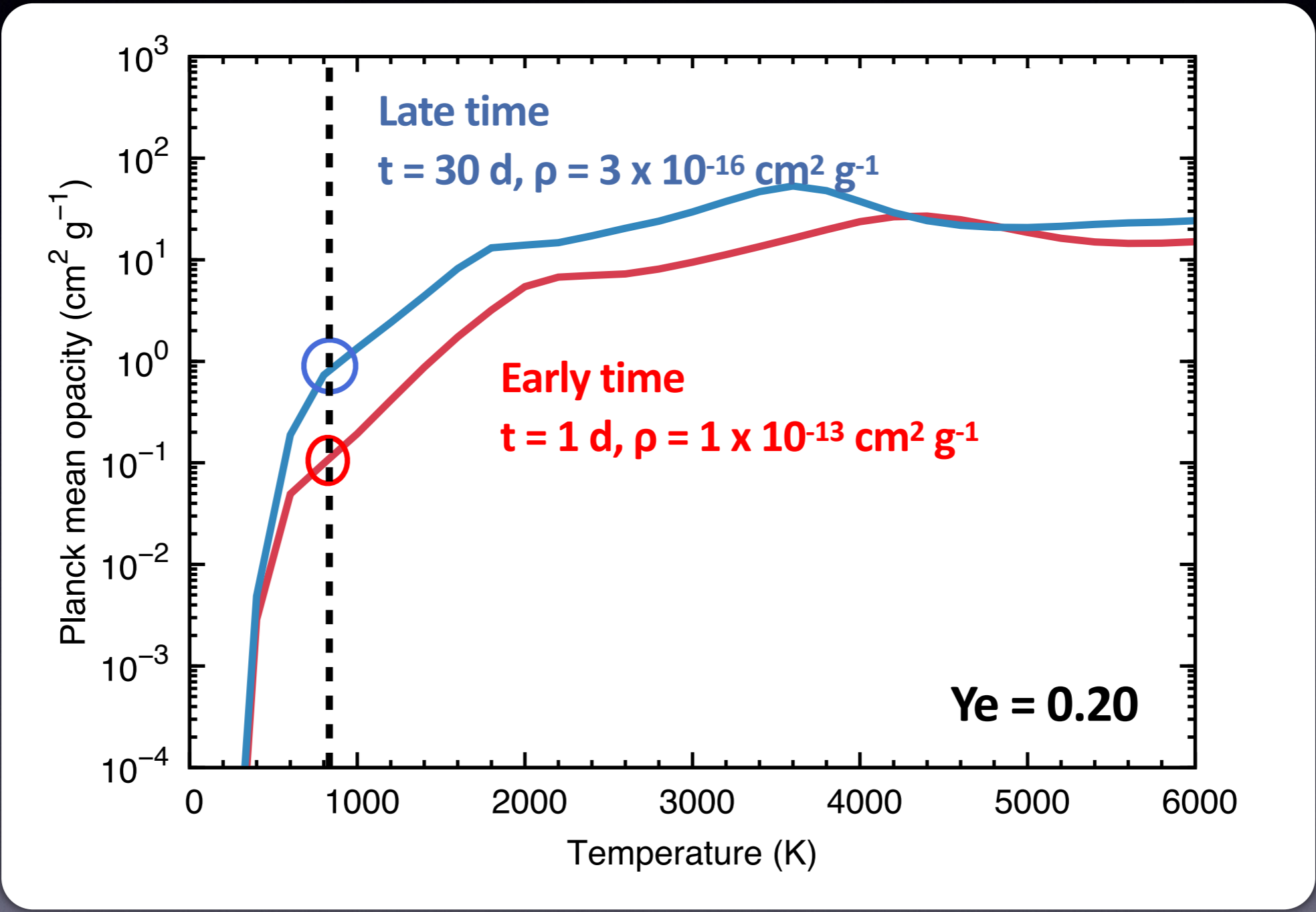
$\kappa > \sim 5 \text{ cm}^2 \text{ g}^{-1}$  to keep the photosphere



# High opacity at late time?

$$\tau_l = \frac{\pi e^2}{m_e c} n_{i,j} t \lambda_l f_l \frac{g_k}{g_0} e^{-\frac{E_k}{kT}}$$

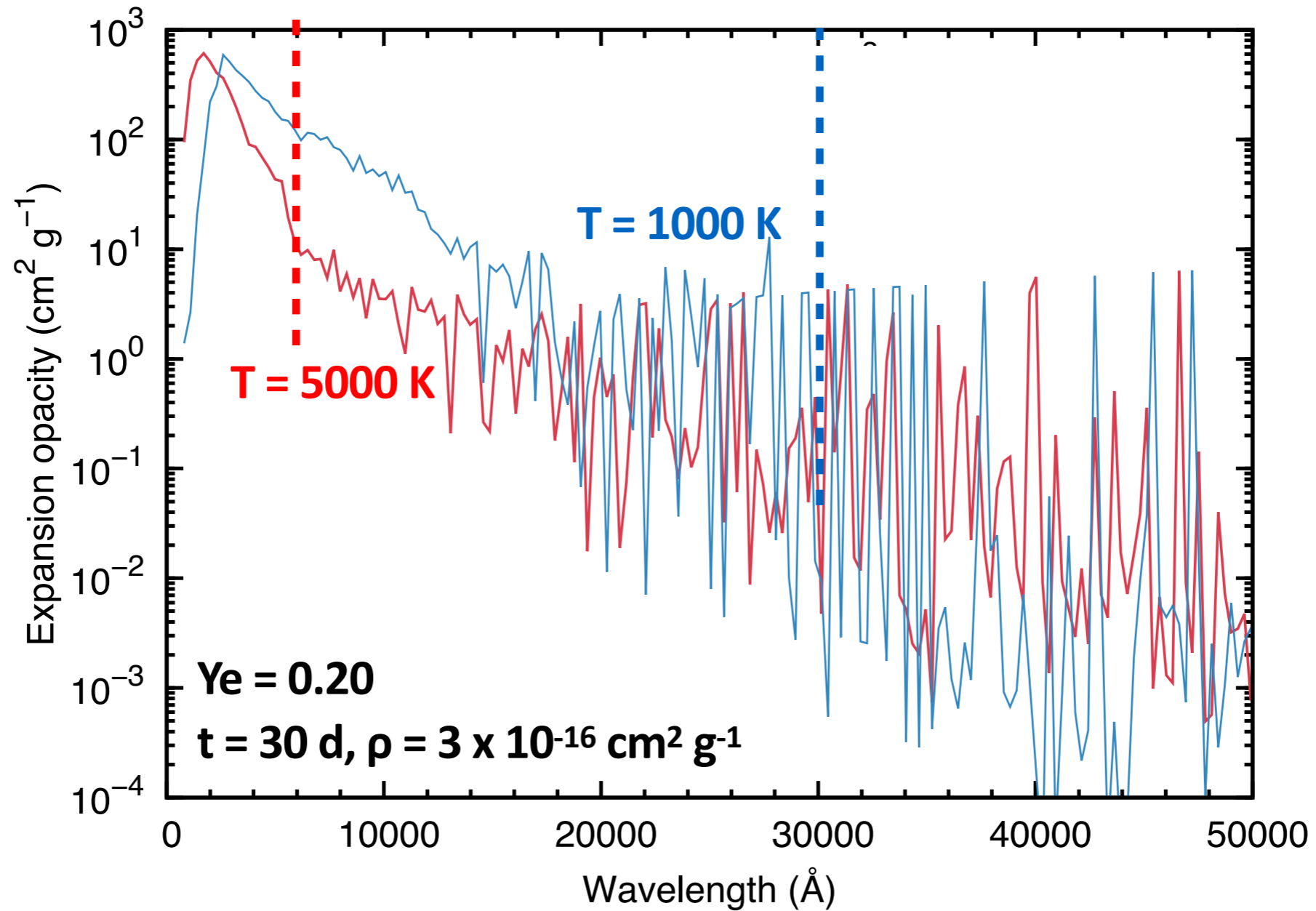
$$\kappa_{\text{exp}}(\lambda) = \frac{1}{ct\rho} \sum_l \frac{\lambda_l}{\Delta\lambda} (1 - e^{-\tau_l})$$



$\kappa > \sim 5 \text{ cm}^2 \text{ g}^{-1}$  at  $t = 30\text{d}$  is difficult with  $T \sim 800 \text{ K}$  (under LTE)



# High opacity at late time?



**Non-LTE  $\Rightarrow T \sim 5,000 \text{ K}$ ?  
Optical photons can still be absorbed**



# Radiative transfer simulations for light curves and spectra of kilonovae

- Light curves
- Spectra



# Two different demands on atomic data

## Light curves

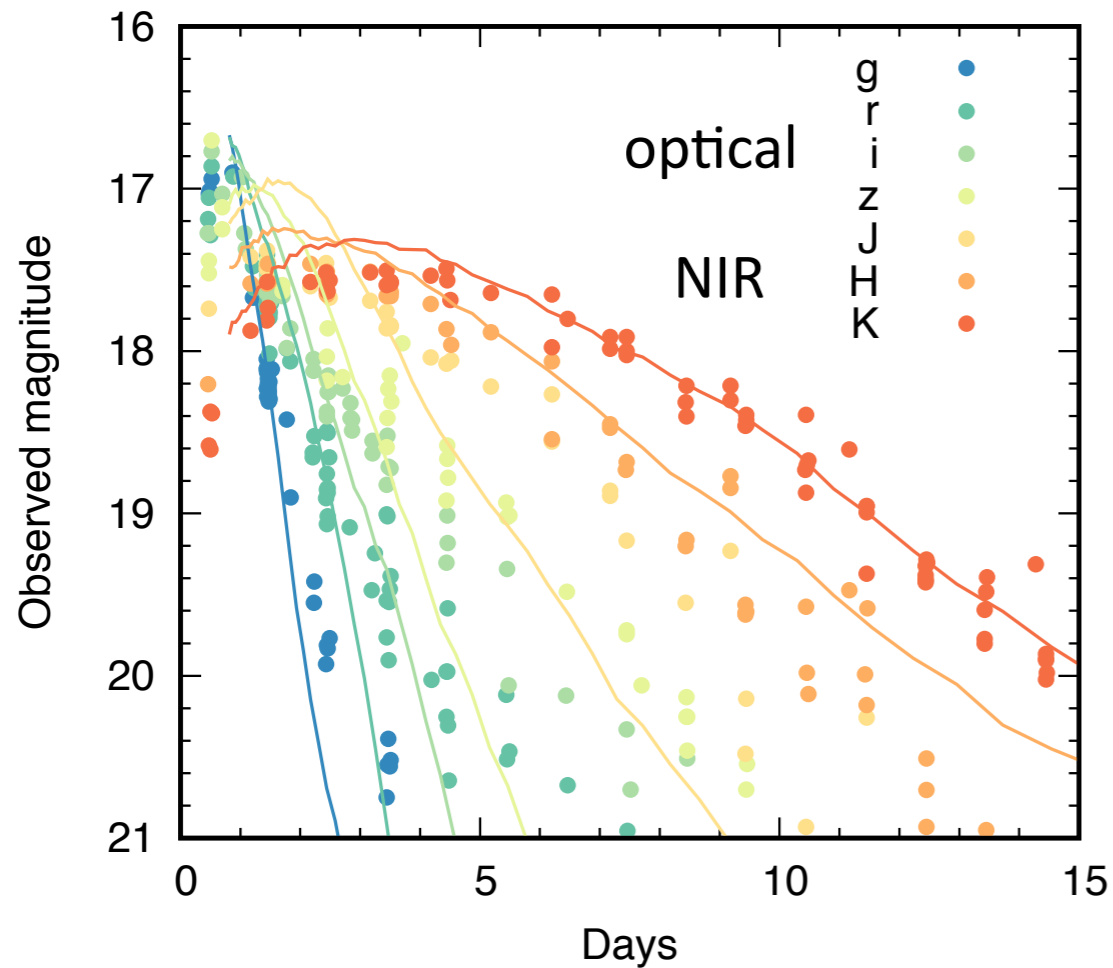


Figure from Kawaguchi+2018, 2020

**Complete** data  
for (even weak) transitions  
=> total opacity

## Spectra

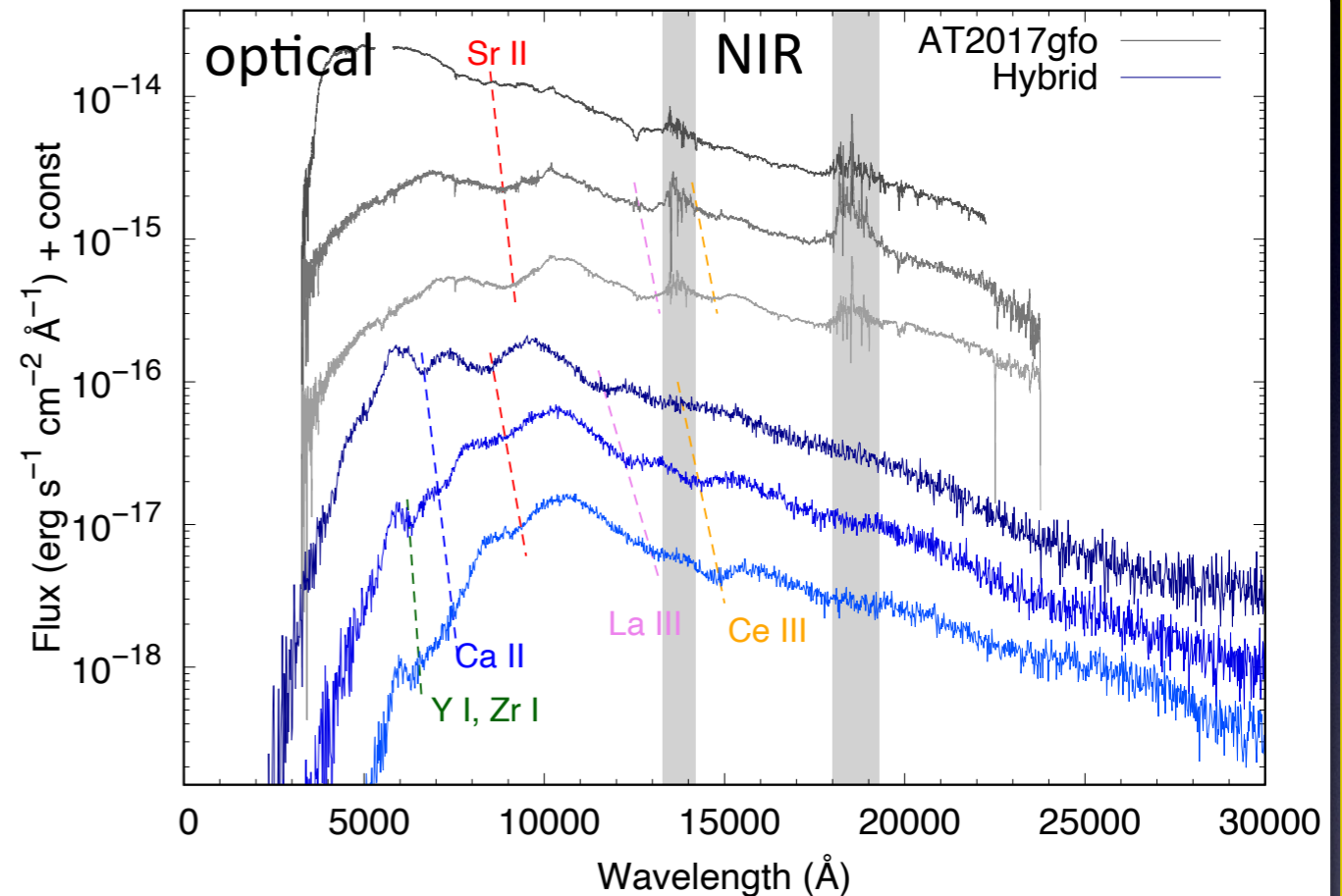


Figure from Domoto+2020,2022

**Accurate** data for  
important transitions  
=> spectral feature

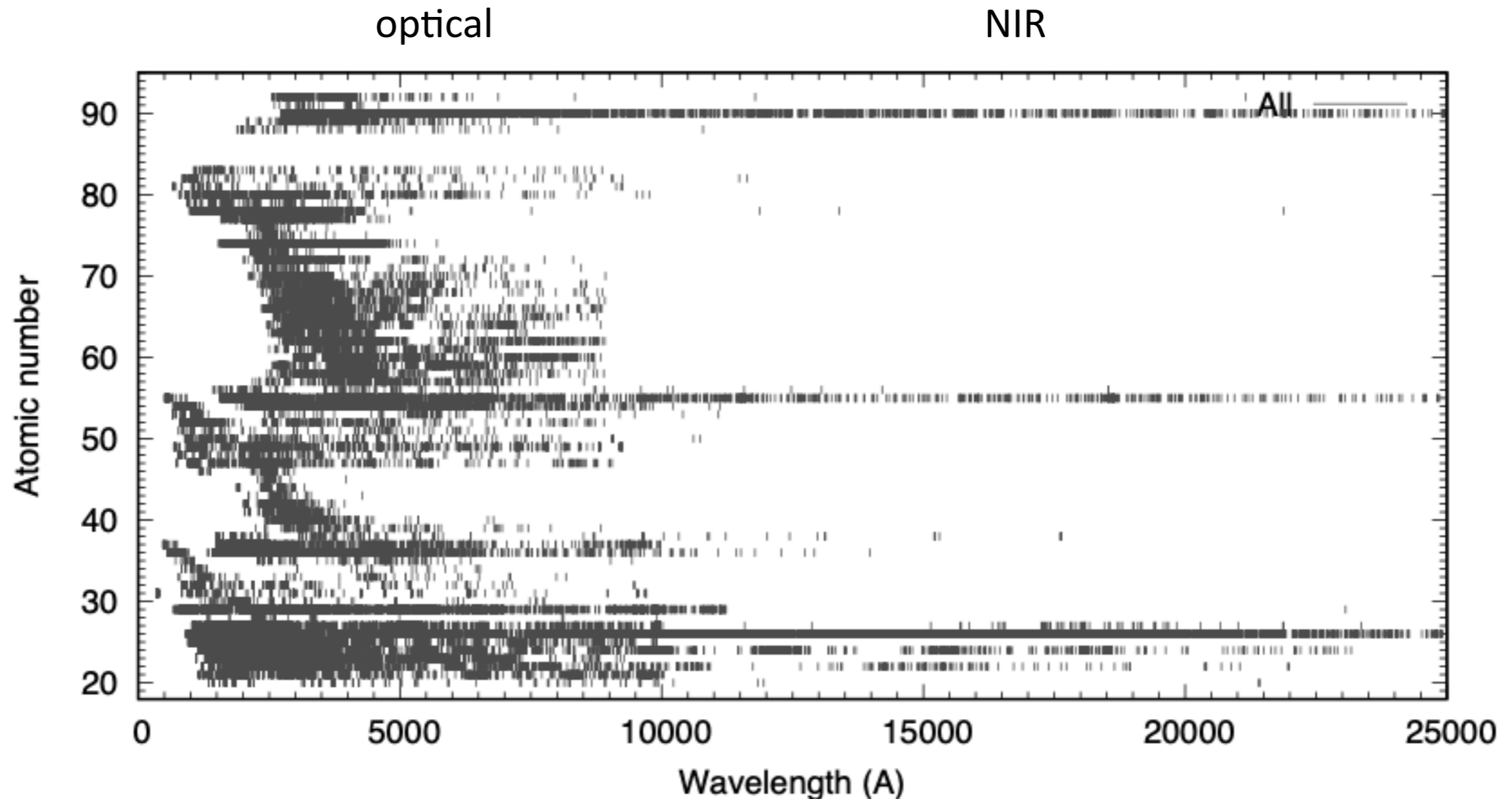
see also talks by N. Domoto, A. Snepken, N. Vieira, ...



# Available atomic data

Data from the NIST ASD

## Transitions with known wavelengths

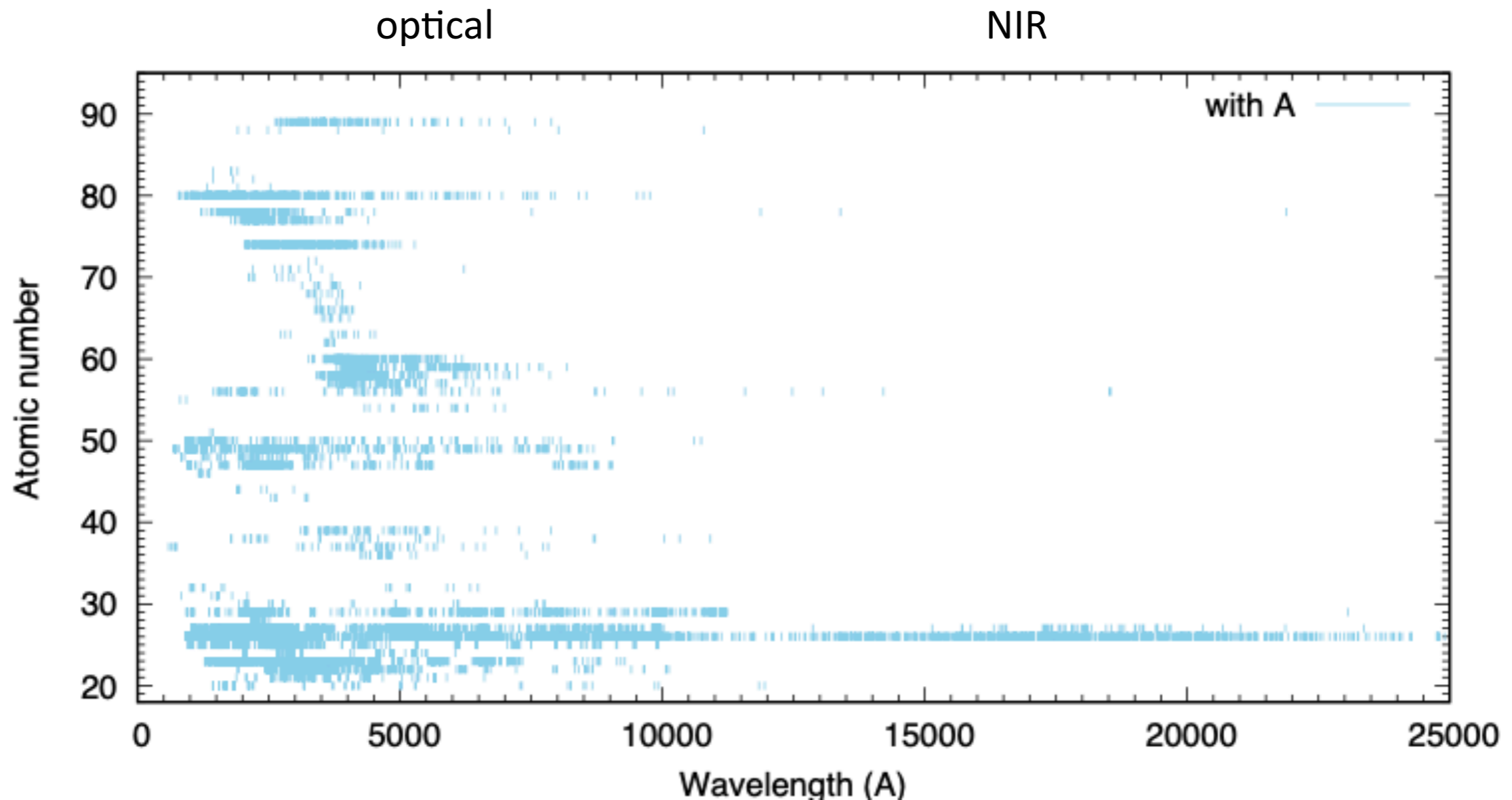




# Available atomic data

Data from the NIST ASD

## Transitions with known transition probability



Accurate transition data are highly incomplete (in particular NIR)



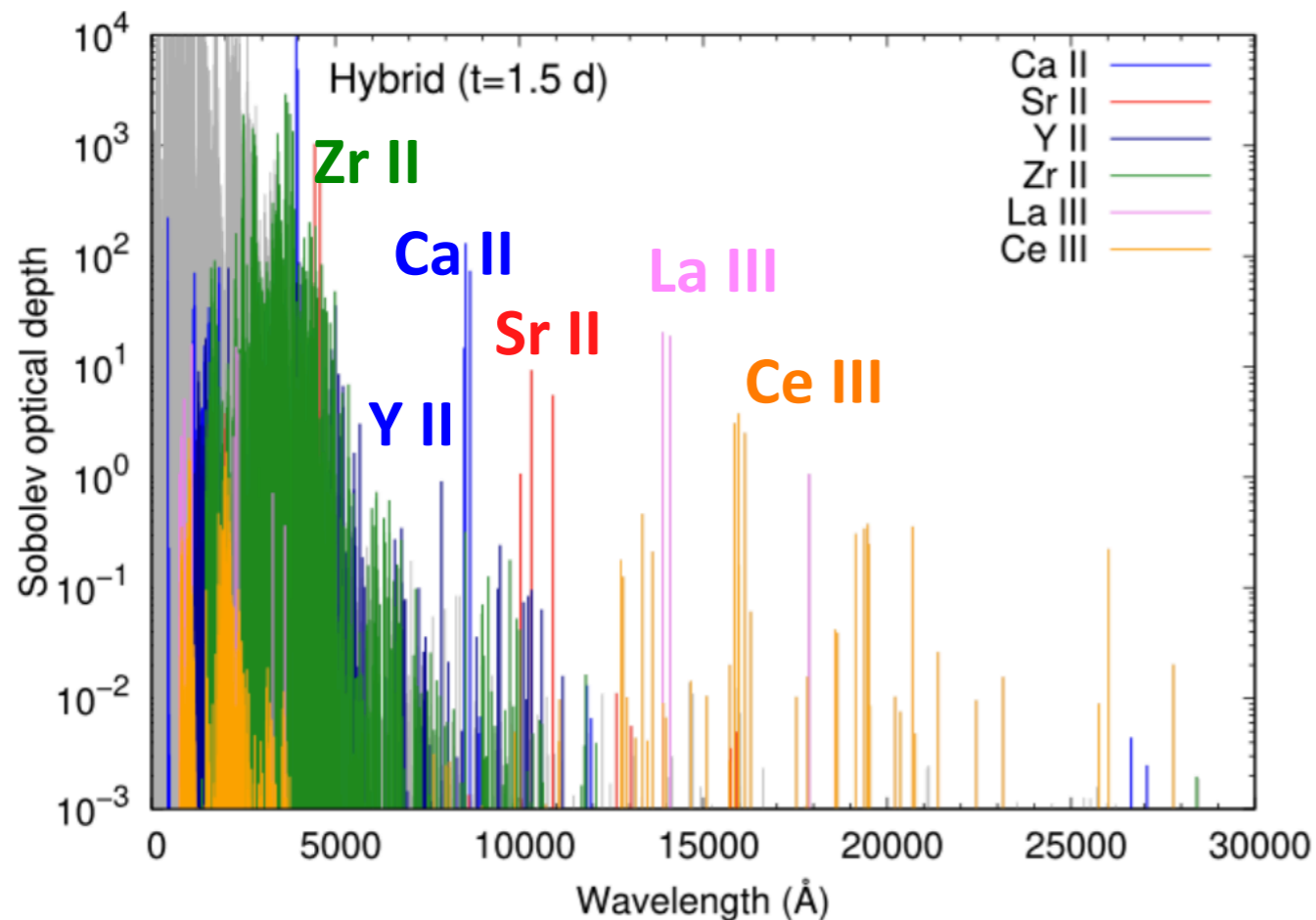
# Important elements for spectral features

see N. Domoto's talk

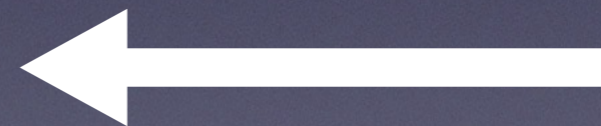
Constructed from **complete** data (MT+20)

Domoto+22

$$\tau_l = \frac{\pi e^2}{m_e c} n_{i,j} t \lambda_l f_l \frac{g_k}{g_0} e^{-\frac{E_k}{kT}}$$



1																	2
H																	He
3	4											5	6	7	8	9	10
Li	Be											B	C	N	O	F	Ne
11	12											13	14	15	16	17	18
Na	Mg											Al	Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
55	56	57~71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
87	88	89~103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
		57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
		89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	



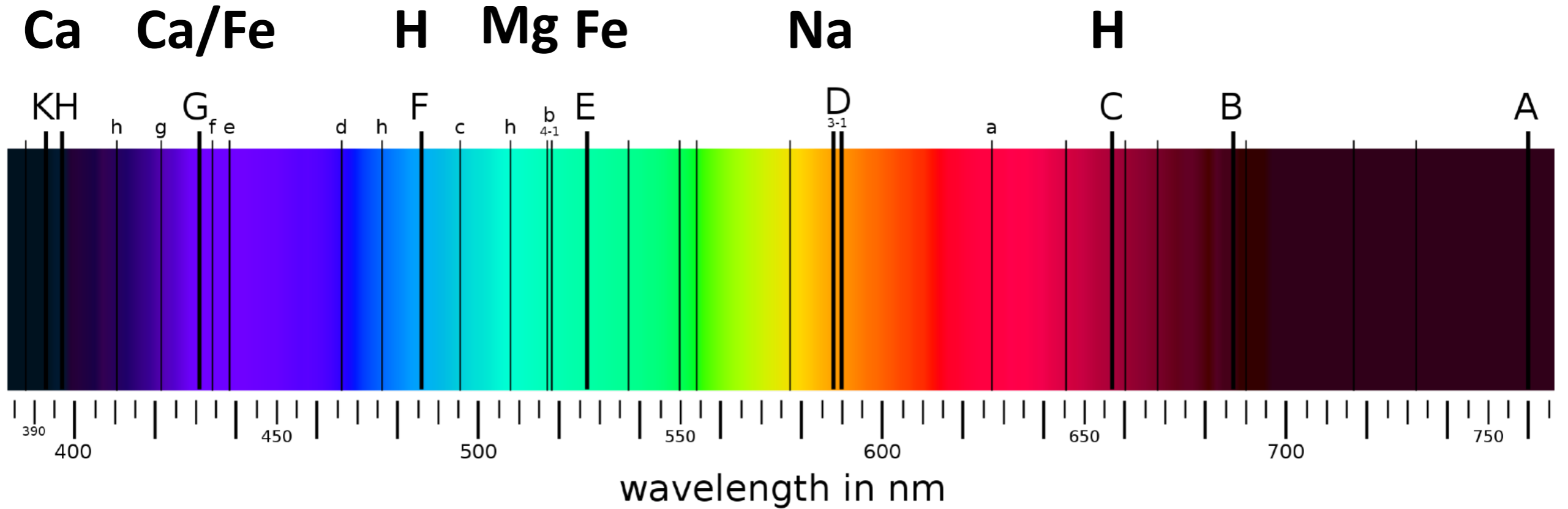
Elements with

- low-lying energy levels (higher population)
- relatively simple structure = small number of transitions = high transition probability (sum rule)



# Solar spectrum

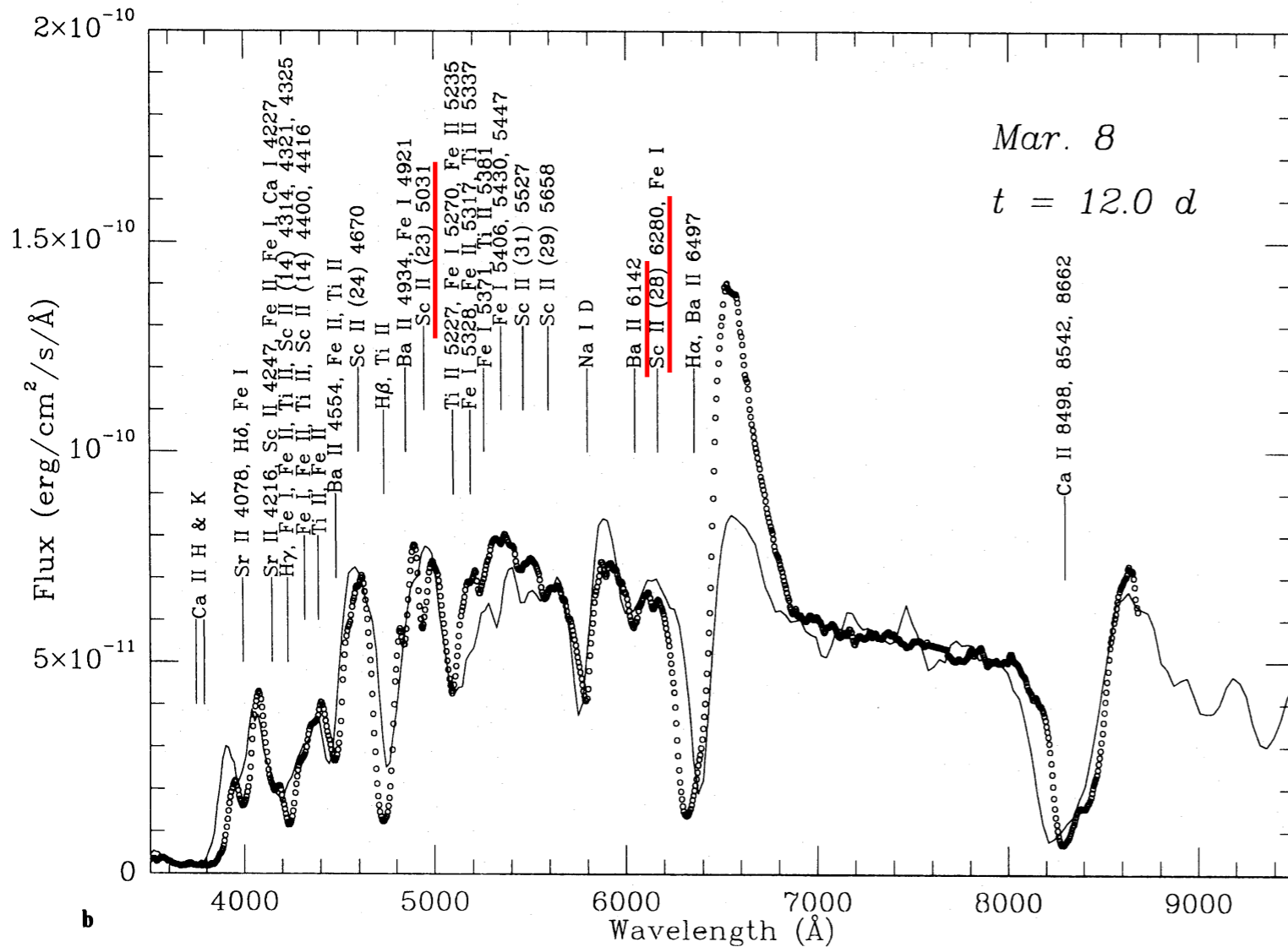
[https://en.wikipedia.org/wiki/Fraunhofer\\_lines](https://en.wikipedia.org/wiki/Fraunhofer_lines)



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	57~71 La-Lu	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	89~103 Ac-Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo																														
<table border="1"> <tbody> <tr> <td>57 La</td> <td>58 Ce</td> <td>59 Pr</td> <td>60 Nd</td> <td>61 Pm</td> <td>62 Sm</td> <td>63 Eu</td> <td>64 Gd</td> <td>65 Tb</td> <td>66 Dy</td> <td>67 Ho</td> <td>68 Er</td> <td>69 Tm</td> <td>70 Yb</td> <td>71 Lu</td> </tr> <tr> <td>89 Ac</td> <td>90 Th</td> <td>91 Pa</td> <td>92 U</td> <td>93 Np</td> <td>94 Pu</td> <td>95 Am</td> <td>96 Cm</td> <td>97 Bk</td> <td>98 Cf</td> <td>99 Es</td> <td>100 Fm</td> <td>101 Md</td> <td>102 No</td> <td>103 Lr</td> </tr> </tbody> </table>																		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
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																																	



# Supernova spectrum (Type II)



1																	2
H																	He
3	4											5	6	7	8	9	10
Li	Be											B	C	N	O	F	Ne
11	12											13	14	15	16	17	18
Na	Mg											Al	Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
55	56	57~71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
87	88	89~103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71			
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103			
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Mazzali+92

see also Dessart et al. 08, 11



# Road to the line identification

“Candidate”

Wavelengths are consistent  
(w/ reasonable Doppler shift)  
**=> Need transition wavelengths**

Strong lines are expected  
(in terms of abundances, ionization, excitation, ...)  
**=> Need transition probabilities**

No other line can produce the feature  
**=> Need complete data for strong transitions**

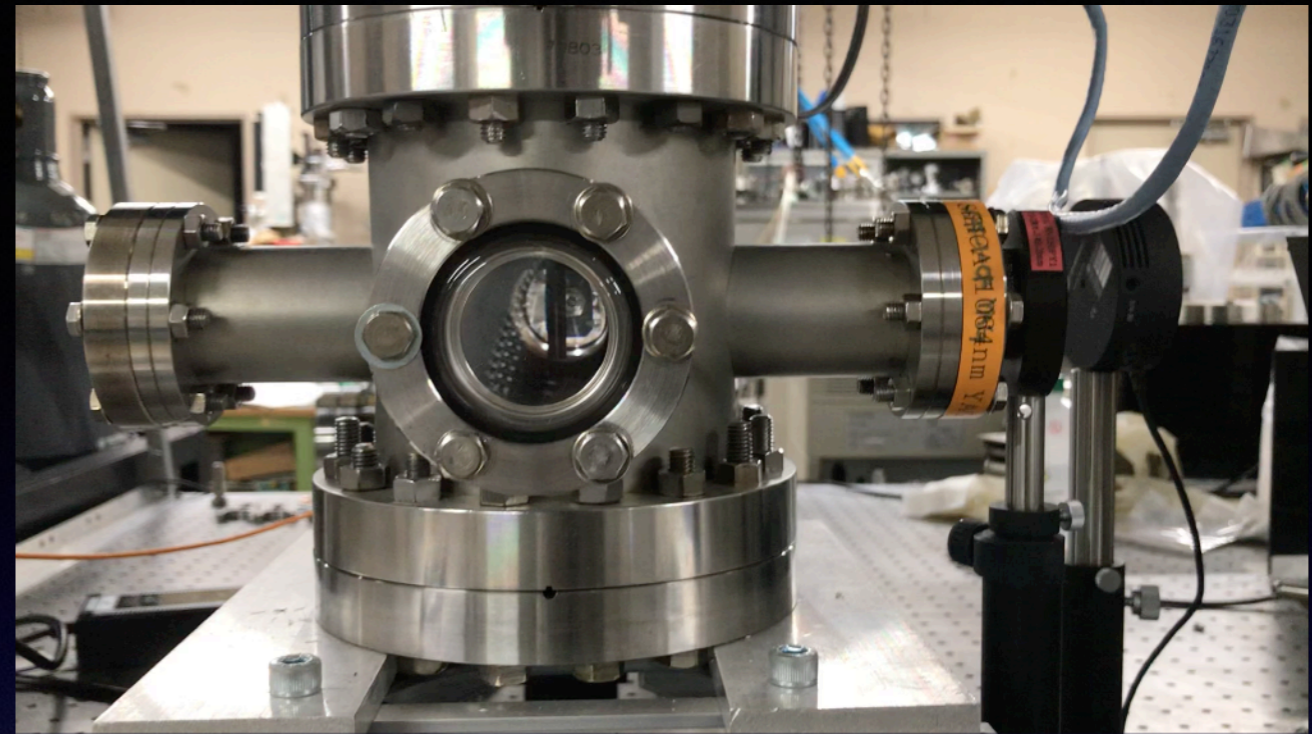
Line identification



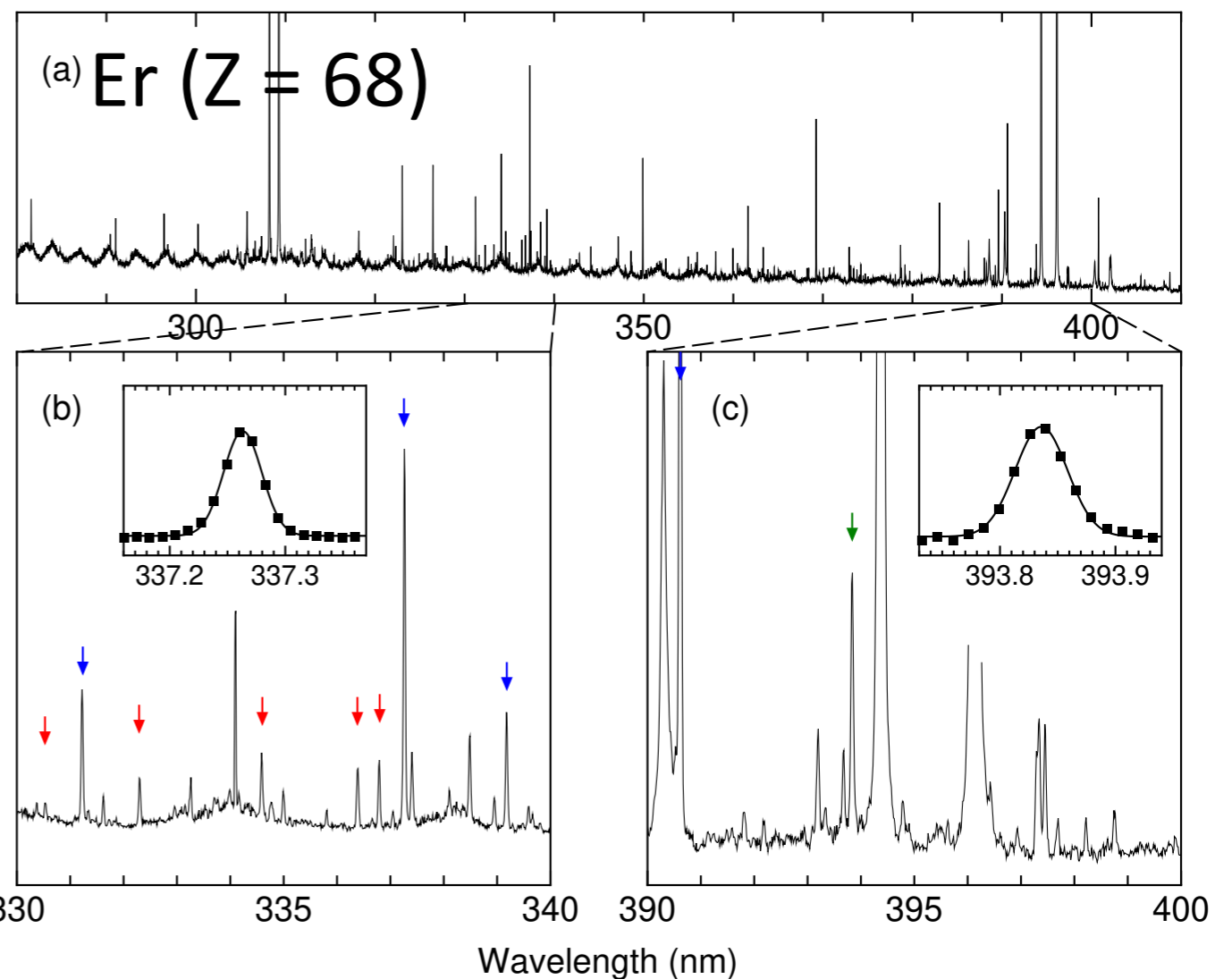
# Spectroscopic measurements for transition probabilities

Laser induced breakdown spectroscopy (R ~ 10,000 in optical)

see P. Dunne's and H. Hartman's talk



Measurements of Ce and La in optical



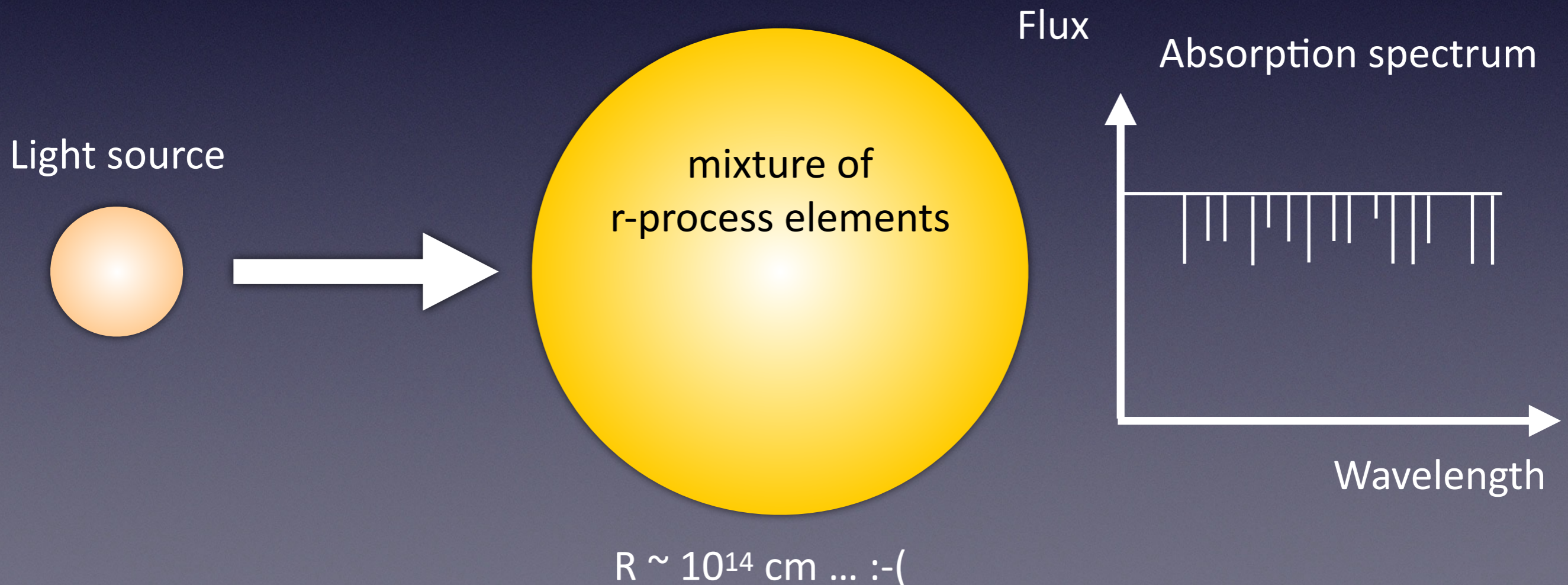


# How to assure the completeness of the strong transitions?

Domoto et al. 2022: use theoretical data for the completeness

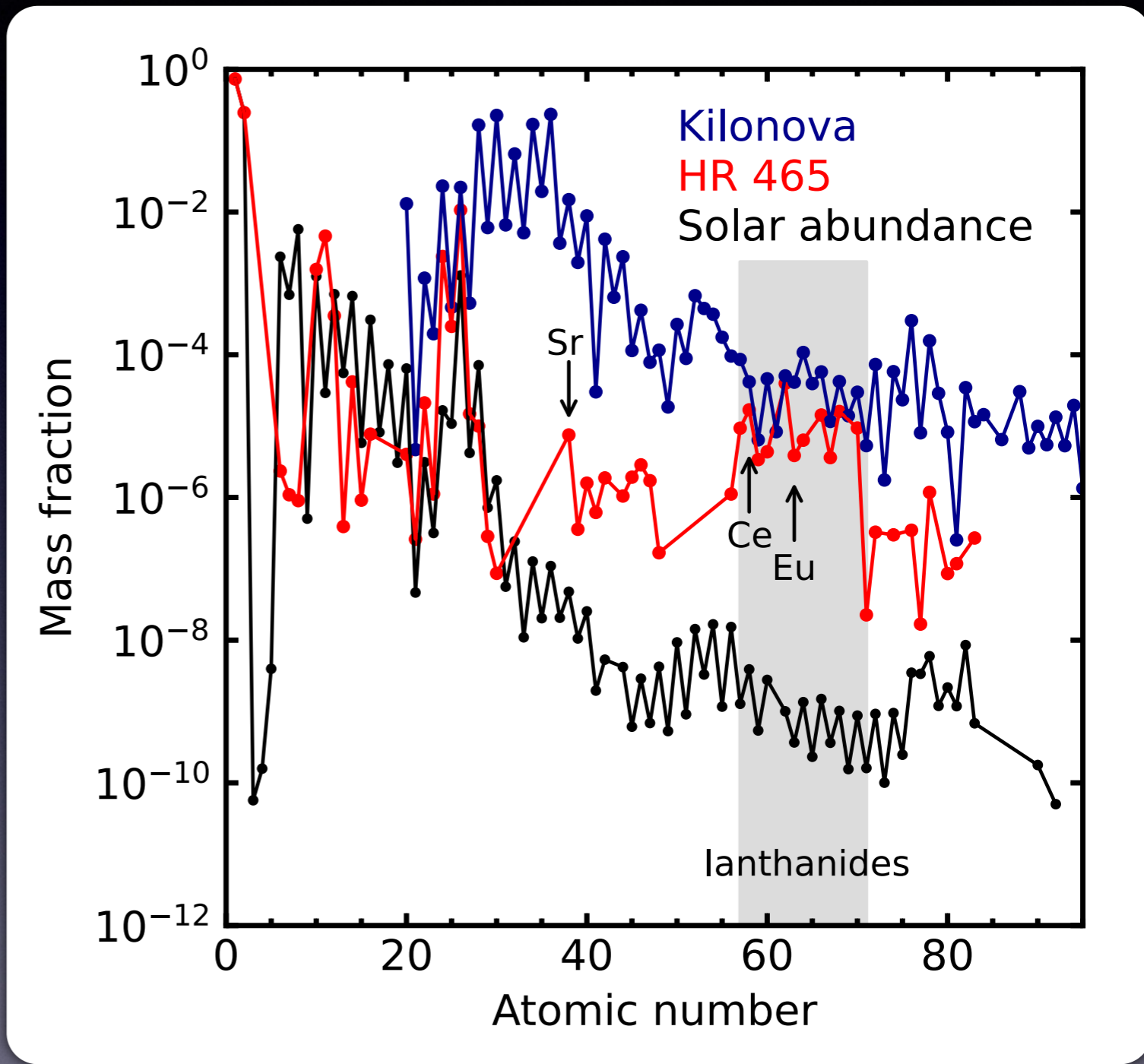
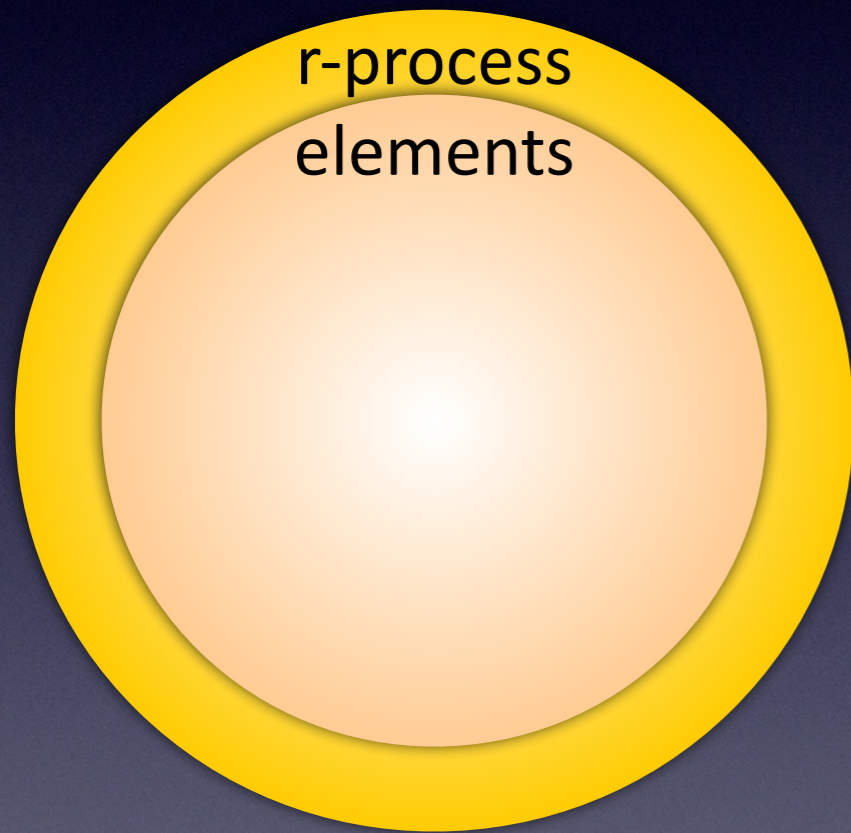
## The best spectroscopic experiment...

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





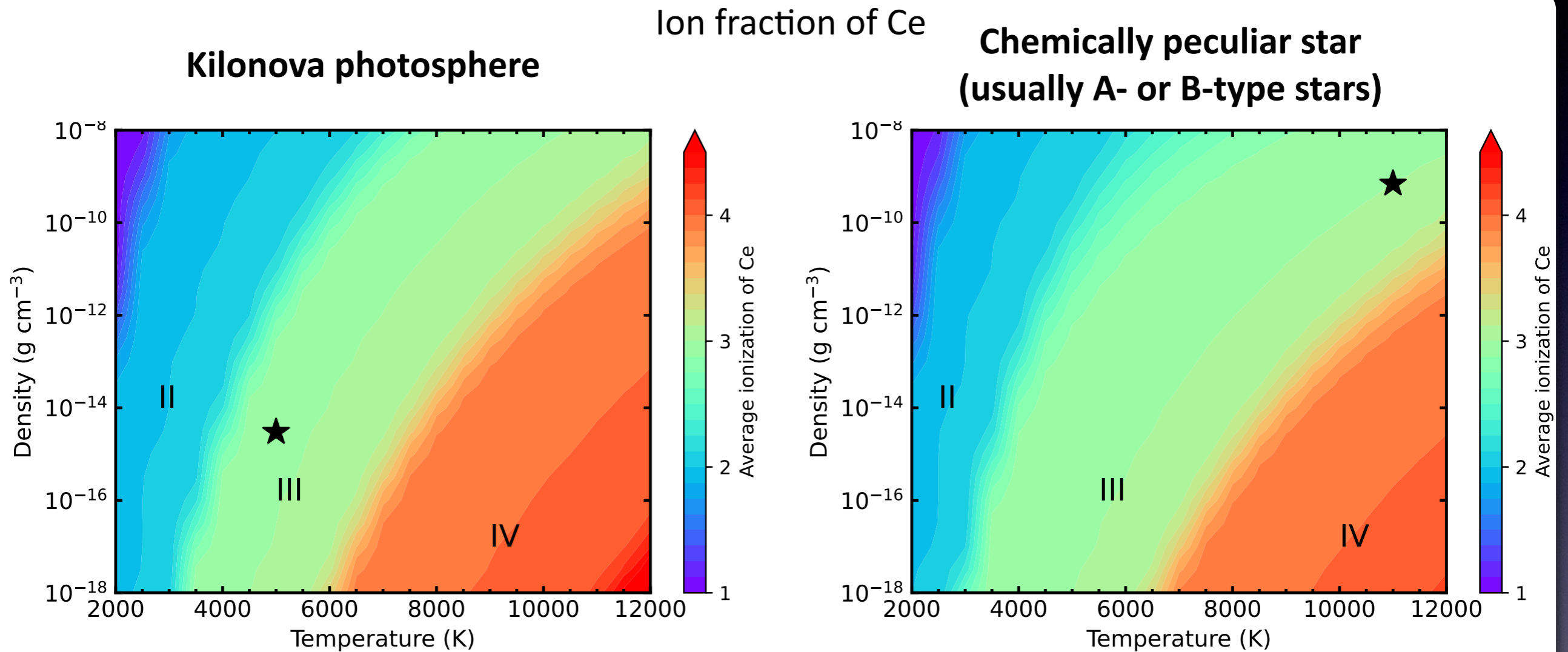
# How about using “chemically peculiar stars”?



Similar lanthanide abundances



# What about ionization states?



**Ionization degrees are also similar**

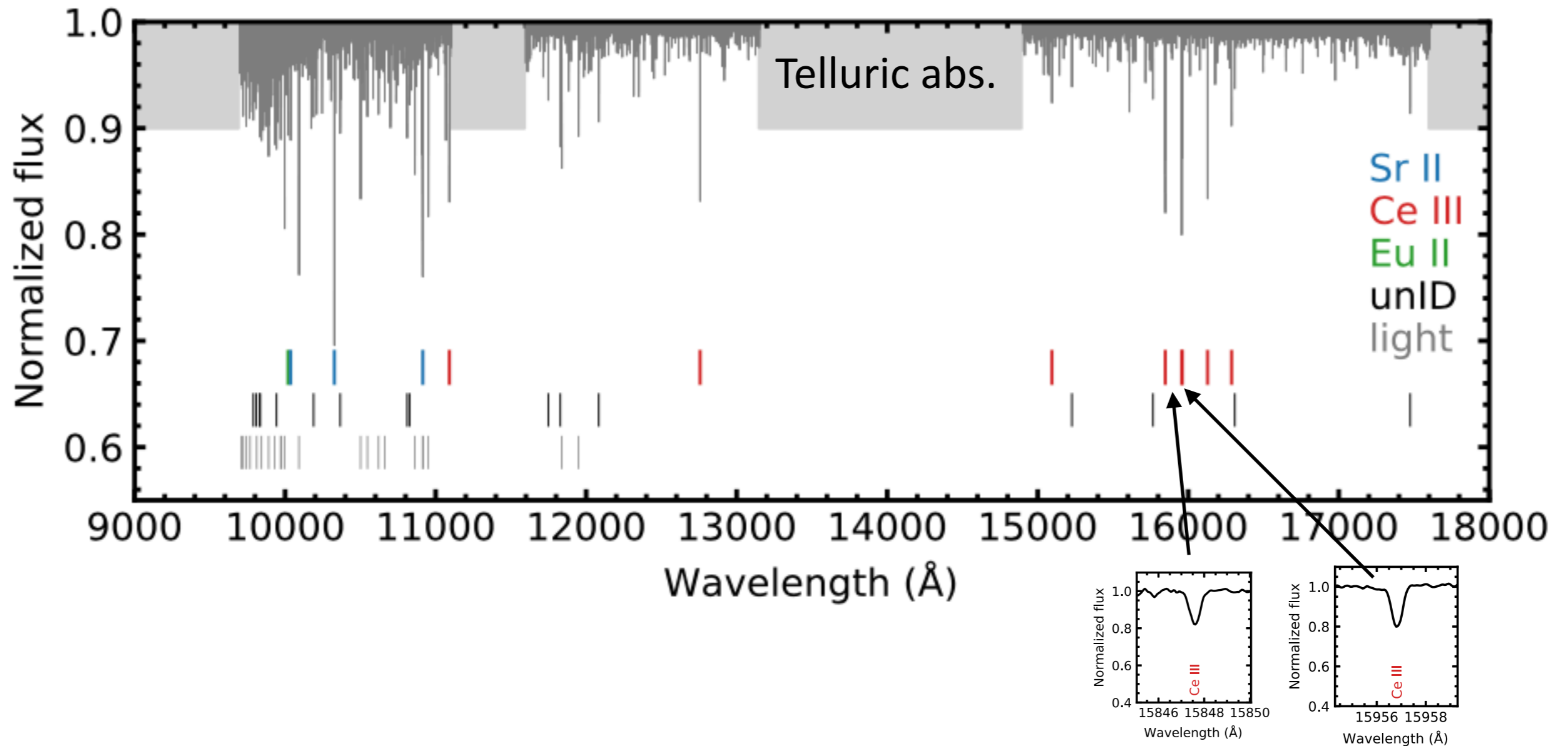
\* Excitation is higher in stellar atmosphere (higher T)



# NIR spectrum of a chemically peculiar star

Tanaka, Domoto, Aoki et al. 2023

Subaru/IRD (R ~ 70,000)



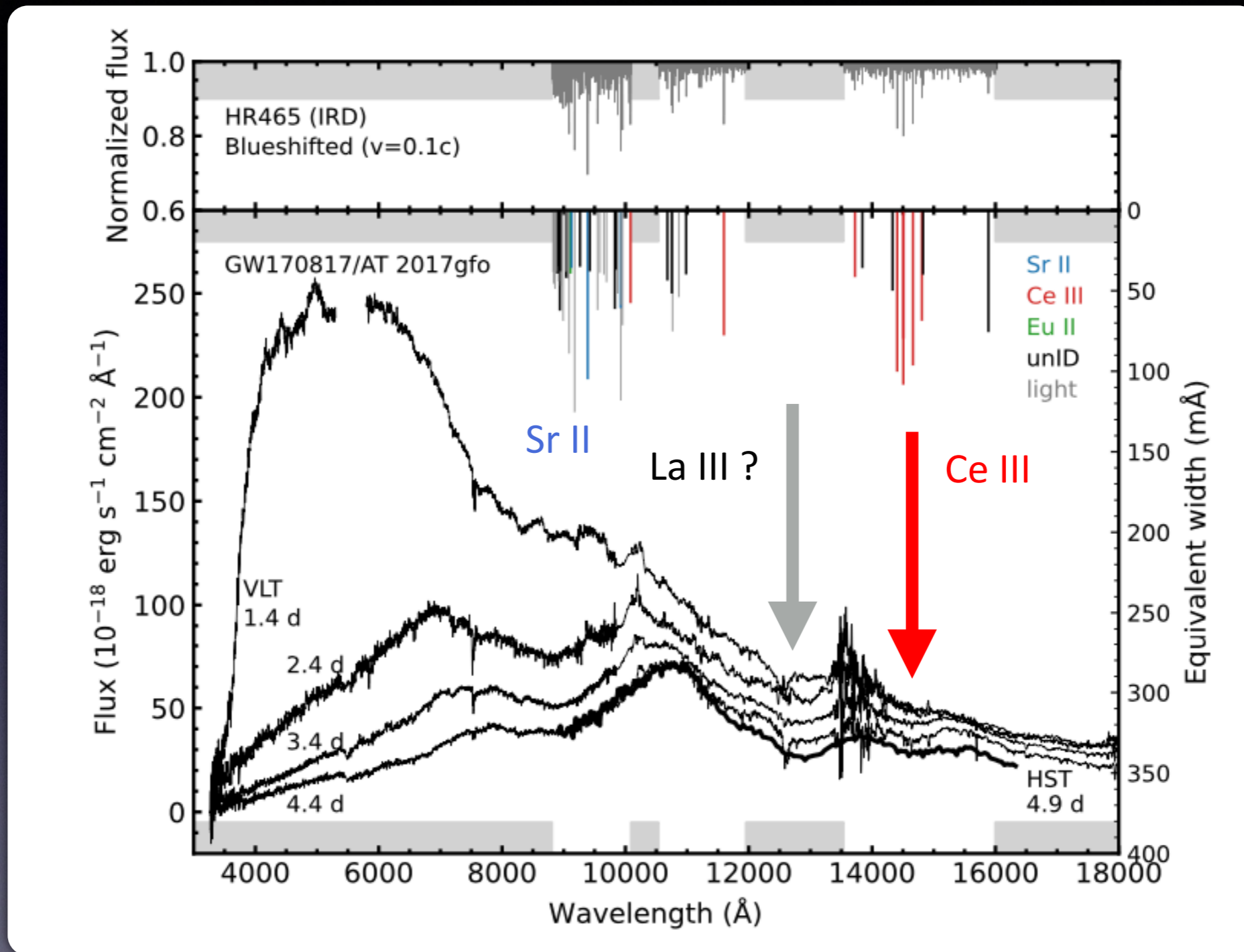
Strongest lines = Ce III, Sr II

No other comparably strong lines = completeness



# Chemically peculiar stars vs kilonovae

Tanaka, Domoto, Aoki et al. 2023



**The most dominant feature around 14,500  $\text{\AA}$  is Ce III ( $\leq$  Domoto et al. 2022)**

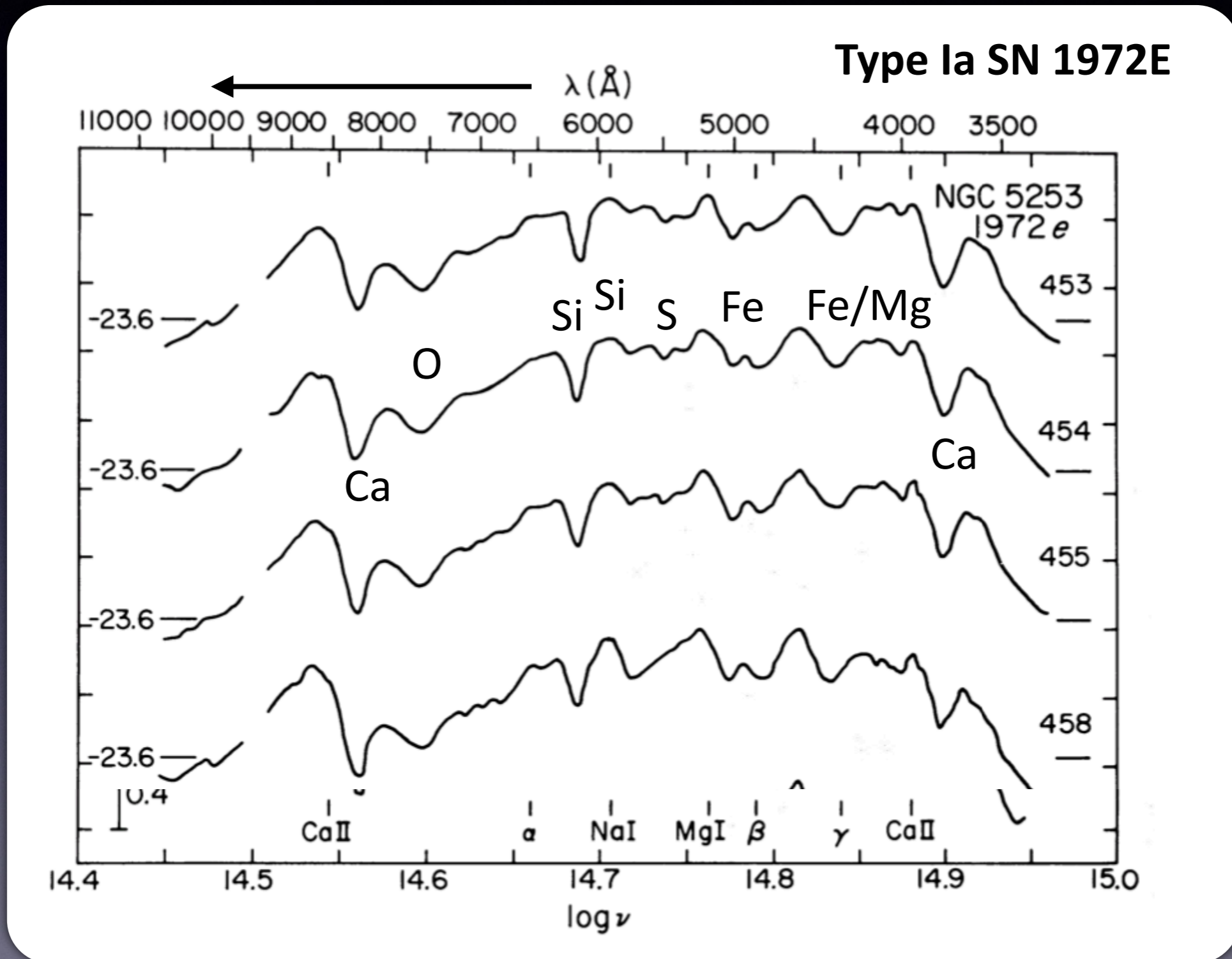
Another broad feature at 13,000  $\text{\AA}$  (La III) is in the gap of the atmospheric windows...



# Anders: "what we have learned from 50yr of SN studies?"

## Supernova spectra in 1970s

Kirshner+73





# Summary: kilonova light curves and spectra

- **Atomic data for light curves**
  - Systematic atomic data for LTE are available
  - Need more evaluation of the accuracy (in progress)
- **Atomic data for spectra**
  - Accurate data for selected ions (w/ strong lines) are available
  - From “candidate” to “identification”
    - Need experimental transition probabilities (in progress)
    - Completeness for strong lines is also important (use of stellar spectrum is a possible way)