The radiative transfer and atomic physics of kilonovae
6th September, 2023

Atomic calculations and radiative transfer simulations for modelling kilonova

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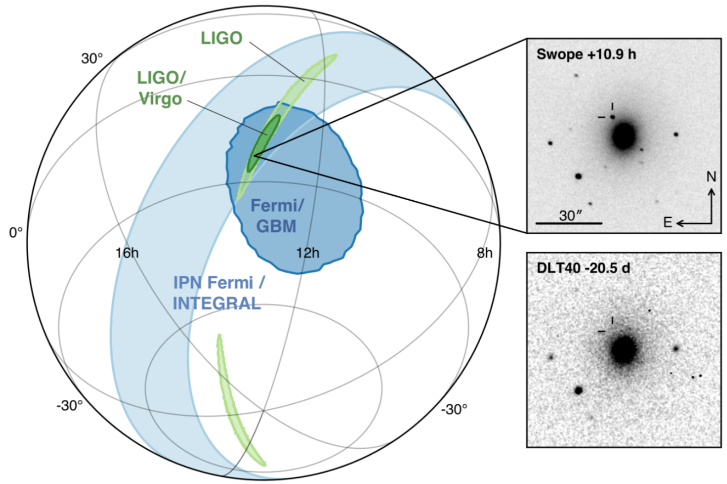
Kilonova observations

GW170817



e.g., Coulter et al 2017; Soares-Santos et al 2017; Arcavi et al 2017a; Troja et al 2017; Kilpatrick et al 2017; Smartt et al 2017; Drout et al 2017; Evans et al 2017; Abbott et al 2017d; Utsumi et al 2017; Covino et al 2017

GRB211211A

e.g., Rastinejad et al. 2022

GRB130603B

GRB230307A

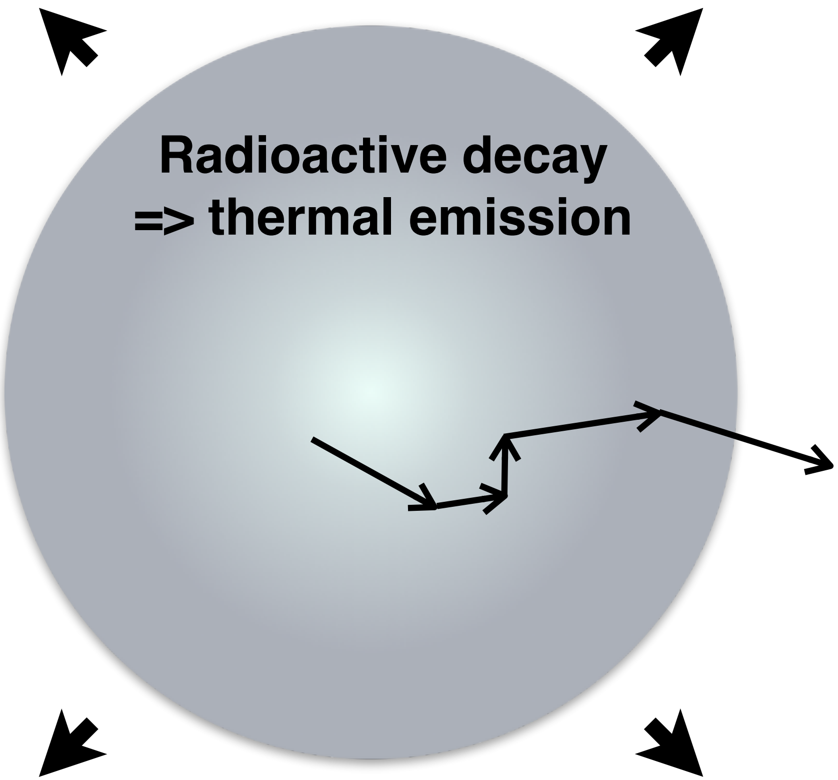
Li & Paczynski 1998

e.g., Levan et al. 2023, Gillanders et al. 2023

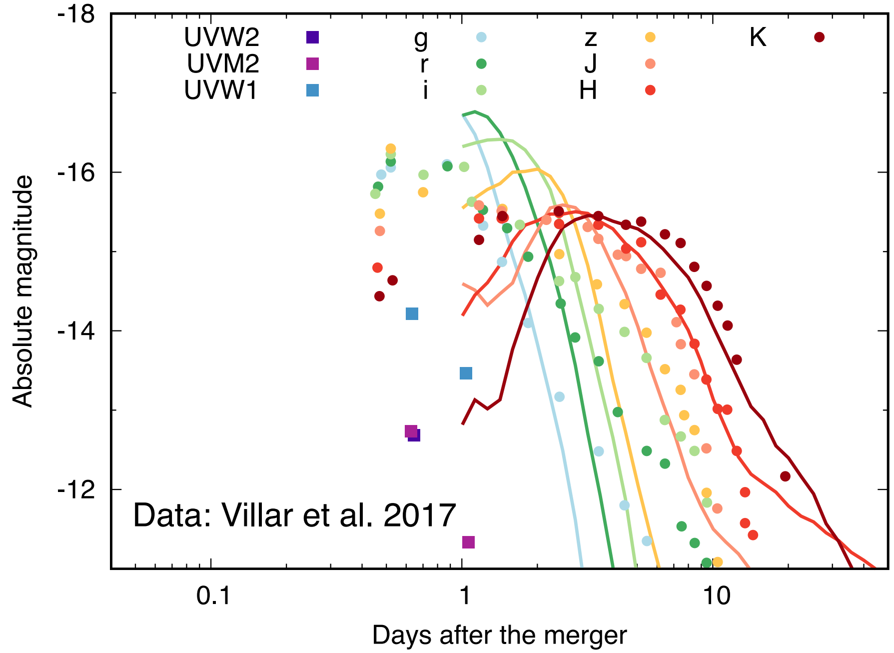
e.g., Tanvir et al. 2013, Berger et al. 2013

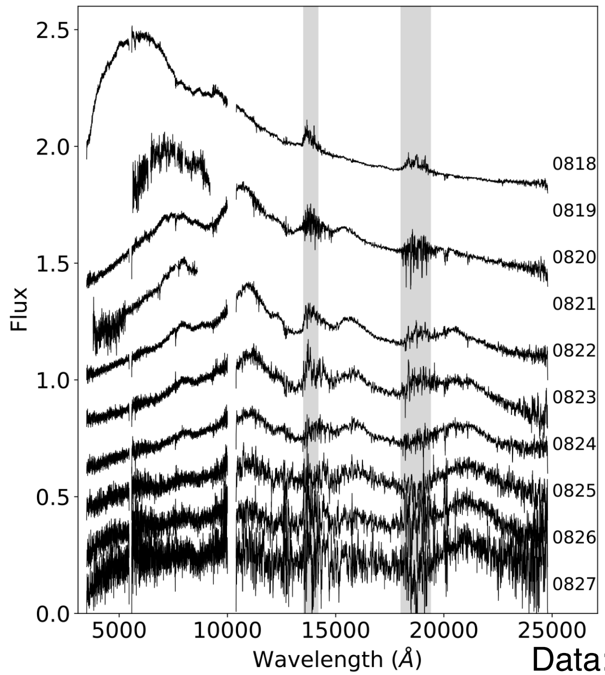
1998 2000 2010 2020 2030

Kilonova



Determined by microphysics: requires atomic cross-sections

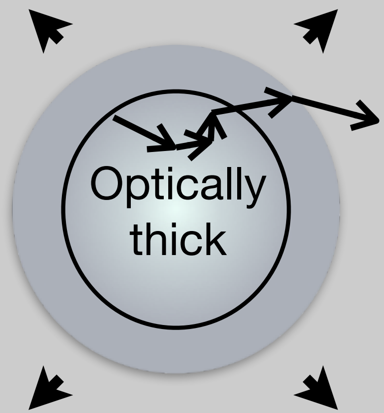




Data: Pian et al. 2017

What is needed?

Photospheric phase

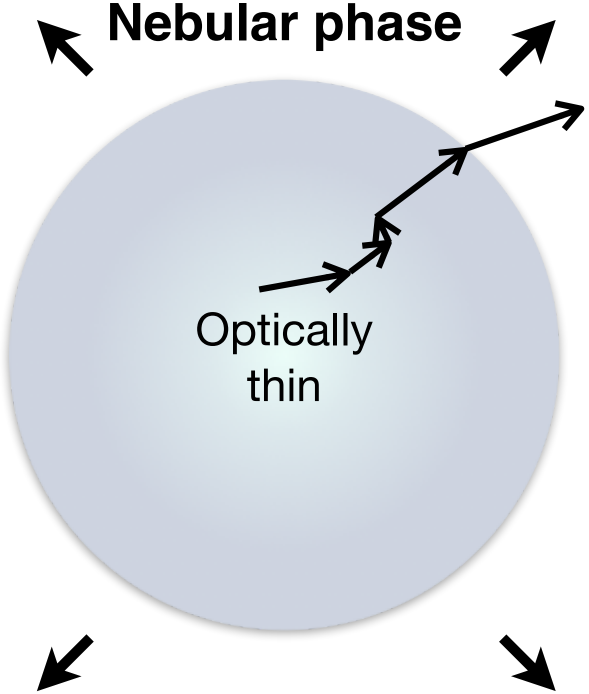


Early time (LTE):

Required atomic data:

- Energy levels
- E1 transitions

Nebular phase



Late time (Non-LTE):

Required atomic data:

- E1+ M1 transitions
- Collisional cross-sections
- Recombination coefficients
- Photo-ionization cross-sections…

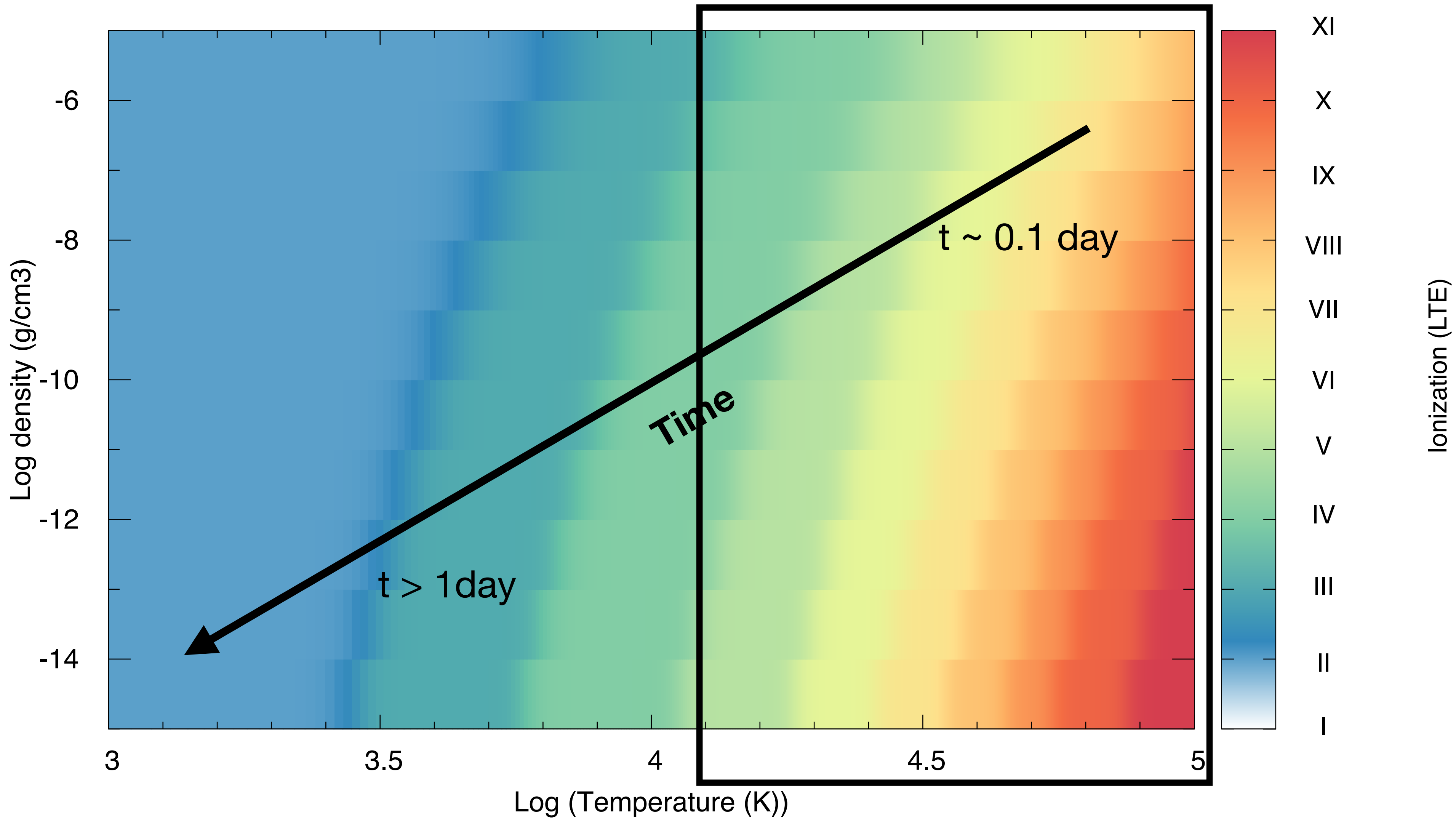
Time

$t \sim$ a few days

$t \geq$ week

Also see Q. Pognan's talk

Physical conditions



Ionized to I-IV:
Kasen et al. 2013; Tanaka & Hotokezaka 2013; Fontes et al. 2017, 2020, 2022; Wollaeger et al. 2017; Gaigalas et al. 2019; Tanaka et al. 2018, 2020; Rynkun et al. 2022a,b; Flors et al. 2023

See talks by M. Tanaka, D. Kasen, C. Fontes, R. Silva, A. Flors

Atomic calculation

- **Code: HULLAC (Hebrew University Lawrence Livermore Atomic Code)**

Bar-Shalom et al. 2001

We design a method to determine ground configuration of lanthanides

Obtain atomic orbitals for multiple central potential
=> systematically vary $4f^{N_1}\,5p^{N_2}, N_1 + N_2 = \text{constant}$

Banerjee et al. 2022, ApJ
Banerjee et al. 2023, submitted

Example : Gd V
Gd IV has ground configuration 4f7 5p6 (NIST ASD)

Gd V test configurations : 4f6 5p6 and 4f7 5p5
(Energy level calculated for both configurations in all cases)

Cases	Potential felt by last electron	Minimization	Ground configuration
A	$4f^6\,5p^5$	$4f^6\,5p^6$	$4f^6\,5p^6$
B	$4f^5\,5p^6$	$--'' --$	$4f^6\,5p^6$
C	$4f^7\,5p^4$	$4f^7\,5p^5$	$4f^6\,5p^6$
D	$4f^6\,5p^5$	$--'' --$	$4f^6\,5p^6$

Our finding:
=> Ground energy level always coming from one set of N_1, N_2

Ground states of Lanthanides

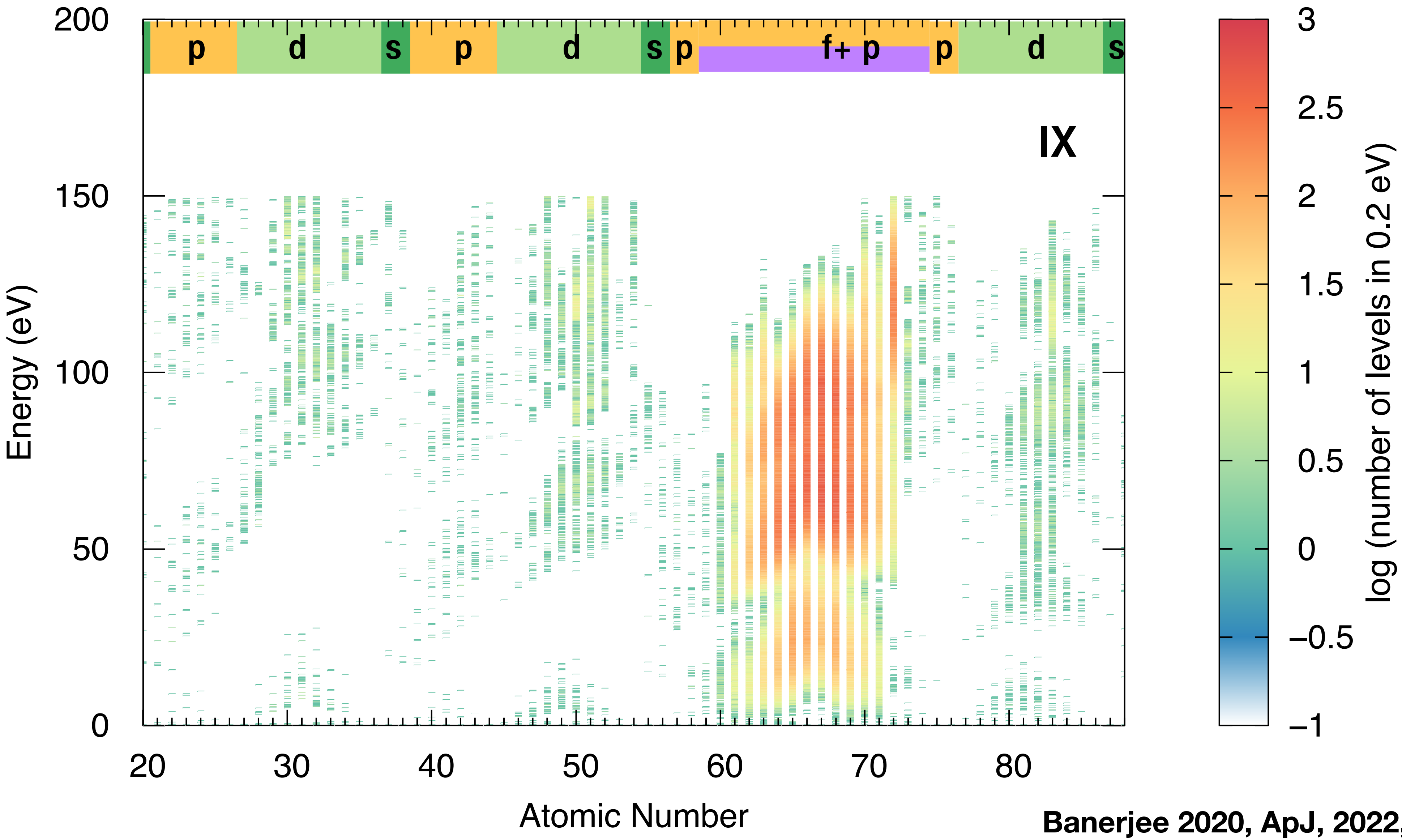
Our work => Systematic theoretical calculation for the highly ionized lanthanides

Ion	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
V	$5p^{5}$	$5p^{6}$	$4f^{1}5p^{6}$	$4f^{2}5p^{6}$	$4f^{3}5p^{6}$	$4f^{4}5p^{6}$	$4f^{5}5p^{6}$	$4f^{6}5p^{6}$	$4f^{7}5p^{6}$	$4f^{8}5p^{6}$	$4f^{9}5p^{6}$	$4f^{10}5p^{6}$	$4f^{11}5p^{6}$	$4f^{12}5p^{6}$	$4f^{13}5p^{6}$
VI	$5p^{4}$	$5p^{5}$	$5p^{6}$	**$4f^{1}5p^{6}$**	**$4f^{2}5p^{6}$**	$4f^{3}5p^{6}$	**$4f^{4}5p^{6}$**	**$4f^{5}5p^{6}$**	**$4f^{6}5p^{6}$**	**$4f^{7}5p^{6}$**	**$4f^{8}5p^{6}$**	**$4f^{9}5p^{6}$**	**$4f^{10}5p^{6}$**	**$4f^{11}5p^{6}$**	$4f^{12}5p^{6}$
VII	$5p^{3}$	$5p^{4}$	**$5p^{5}$**	**$5p^{6}$**	**$4f^{2}5p^{5*}$**	**$4f^{3}5p^{5*}$**	**$4f^{4}5p^{5*}$**	**$4f^{5}5p^{5*}$**	**$4f^{6}5p^{5*}$**	**$4f^{7}5p^{5*}$**	**$4f^{7}5p^{6}$**	**$4f^{8}5p^{6}$**	**$4f^{9}5p^{6}$**	**$4f^{10}5p^{6}$**	**$4f^{11}5p^{6}$**
VIII	$5p^{2}$	$5p^{3}$	**$5p^{4}$**	**$4f^{1}5p^{4*}$**	**$4f^{2}5p^{4*}$**	**$4f^{3}5p^{4}$**	**$4f^{4}5p^{4}$**	**$4f^{5}5p^{4}$**	**$4f^{6}5p^{4}$**	**$4f^{7}5p^{4}$**	**$4f^{7}5p^{5}$**	**$4f^{7}5p^{6}$** **$4f^{8}5p^{5}$**	**$4f^{9}5p^{5*}$**	**$4f^{10}5p^{5*}$**	**$4f^{10}5p^{6}$** **$4f^{11}5p^{5}$**
IX	$5p^{1}$	$5p^{2}$	**$5p^{3}$**	**$4f^{1}5p^{3}$**	**$4f^{2}5p^{3}$**	**$4f^{3}5p^{3}$**	**$4f^{4}5p^{3}$**	**$4f^{5}5p^{3}$**	**$4f^{6}5p^{3}$**	**$4f^{7}5p^{3}$**	**$4f^{7}5p^{4}$**	**$4f^{8}5p^{4*}$**	**$4f^{9}5p^{4}$**	**$4f^{10}5p^{4}$**	**$4f^{11}5p^{4*}$**
X	$5s^{2}$	$5p^{1}$	**$5p^{2}$**	**$4f^{1}5p^{2}$**	**$4f^{2}5p^{2}$**	**$4f^{3}5p^{2}$**	**$4f^{4}5p^{2}$**	$4f^{5}5p^{2}$	$4f^{6}5p^{2}$	**$4f^{7}5p^{2}$**	**$4f^{7}5p^{3*}$**	**$4f^{8}5p^{3}$**	**$4f^{9}5p^{3}$**	**$4f^{10}5p^{3}$**	**$4f^{11}5p^{3}$**
XI	$5s^{1}$	$5s^{2}$	$5p^{1}$	**$4f^{1}5p^{1}$**	**$4f^{2}5p^{1}$**	**$4f^{3}5p^{1}$**	**$4f^{4}5p^{1}$**	$4f^{5}5p^{1}$	$4f^{6}5p^{1}$	**$4f^{7}5p^{1}$**	**$4f^{7}5p^{2}$**	**$4f^{8}5p^{2}$**	**$4f^{9}5p^{2}$**	**$4f^{10}5p^{2}$**	**$4f^{11}5p^{2}$**

Energy level

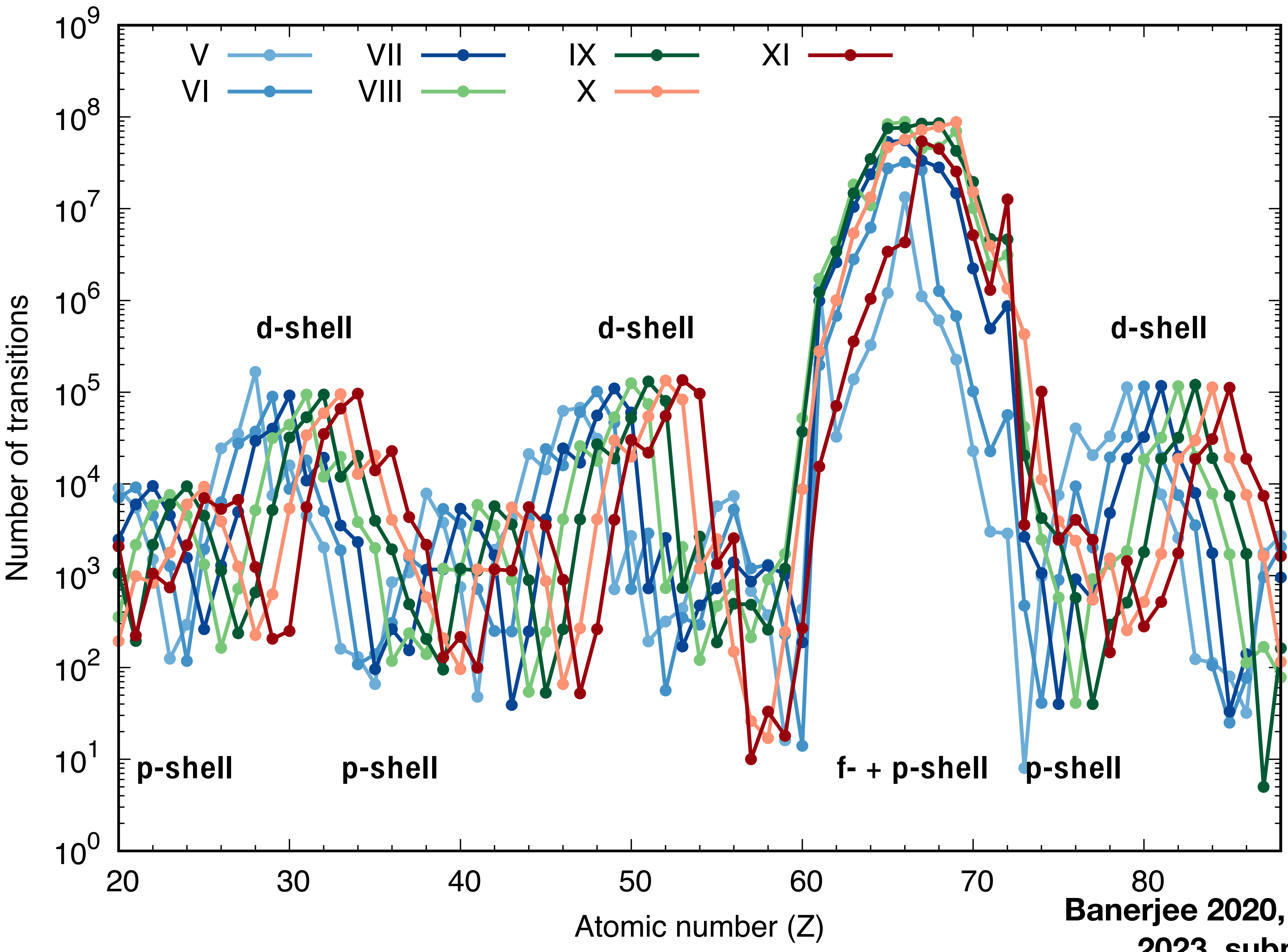
- **Atomic calculations: HULLAC (Hebrew University Lawrence Livermore Atomic Code)**

Bar-Shalom et al. 2001



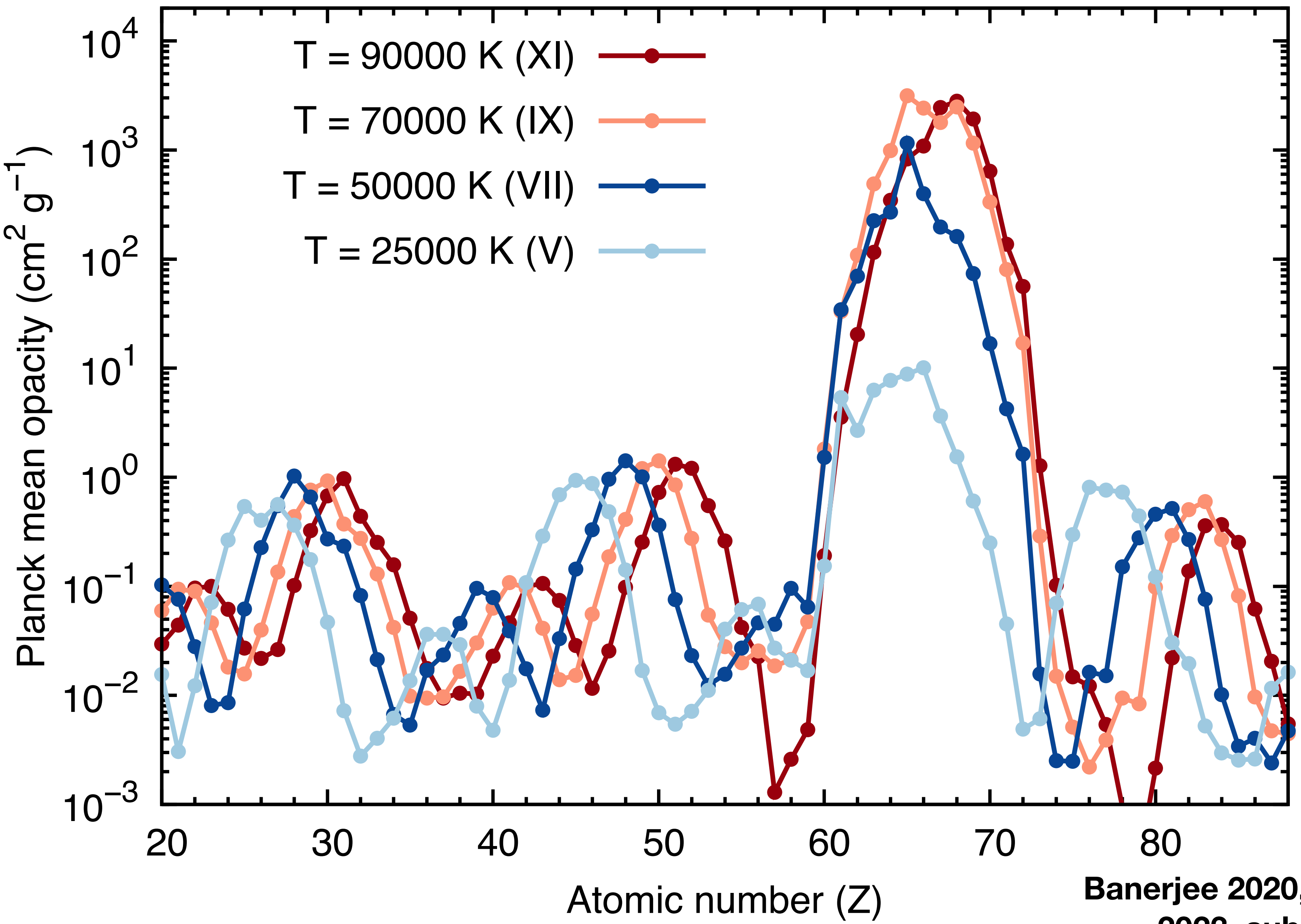
Banerjee 2020, ApJ, 2022, 2023, submitted

Transitions



Banerjee 2020, ApJ, 2022, 2023, submitted

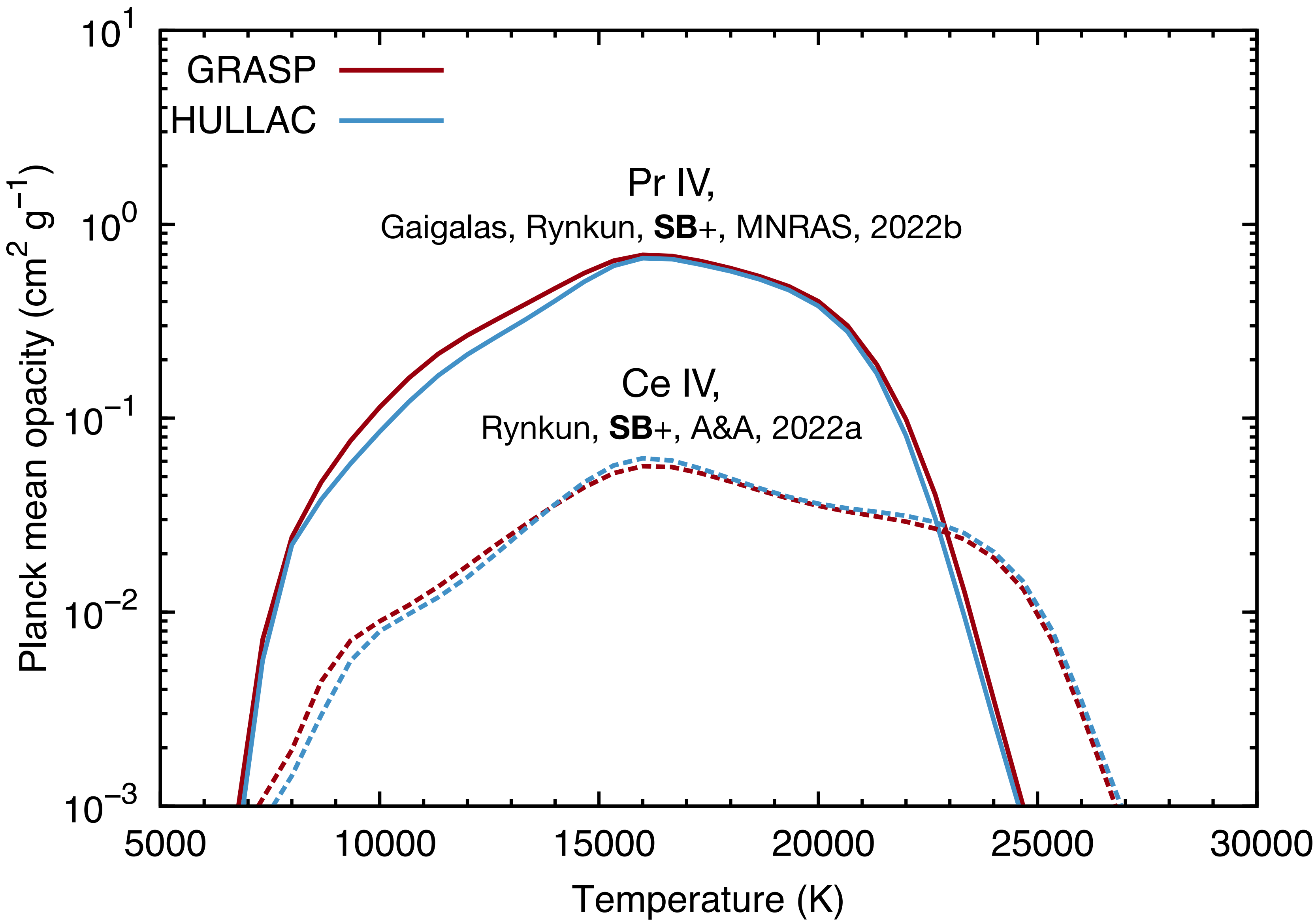
Opacity



Banerjee 2020, ApJ, 2022, 2023, submitted

Uncertainties

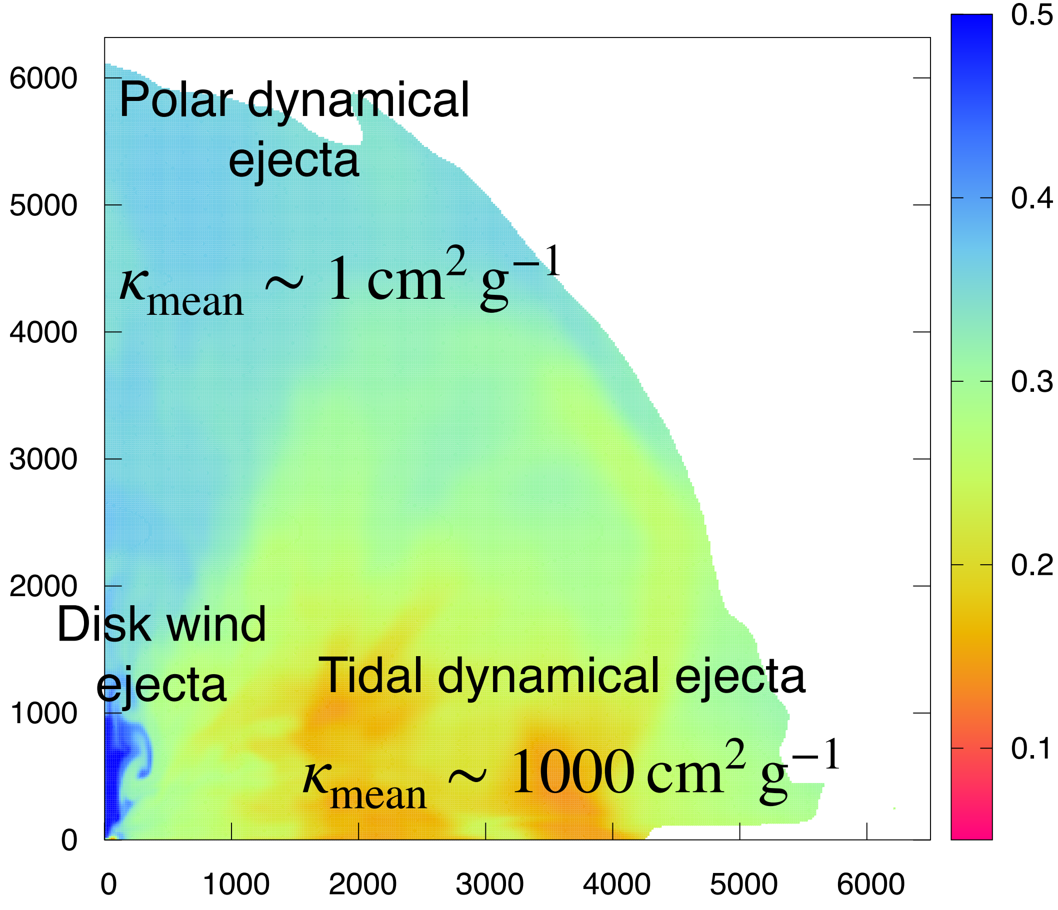
Calculations between different atomic calculations matches well



Modelling light curves

$$Y_e = \frac{n_e}{n_n + n_e}$$

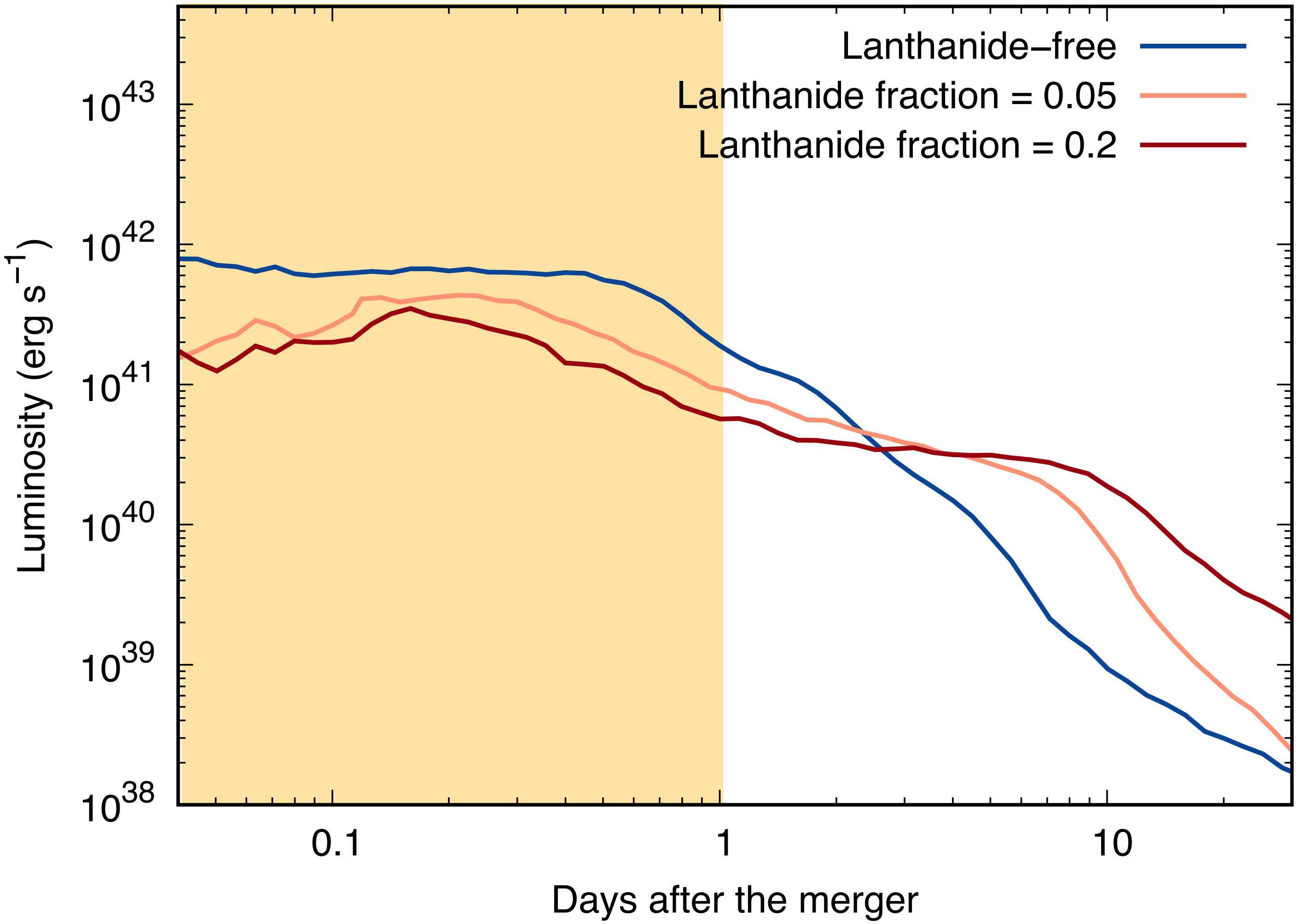
= 1- neutron fraction

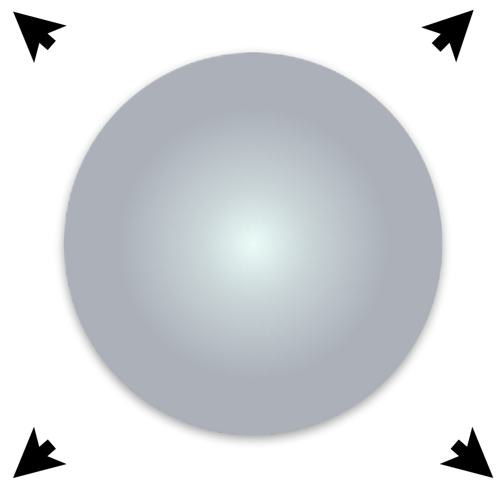


- Opacity vastly different across different components
- Angle dependence in light curves expected

Data : Fujibayashi et al. 2022

Bolometric light curve

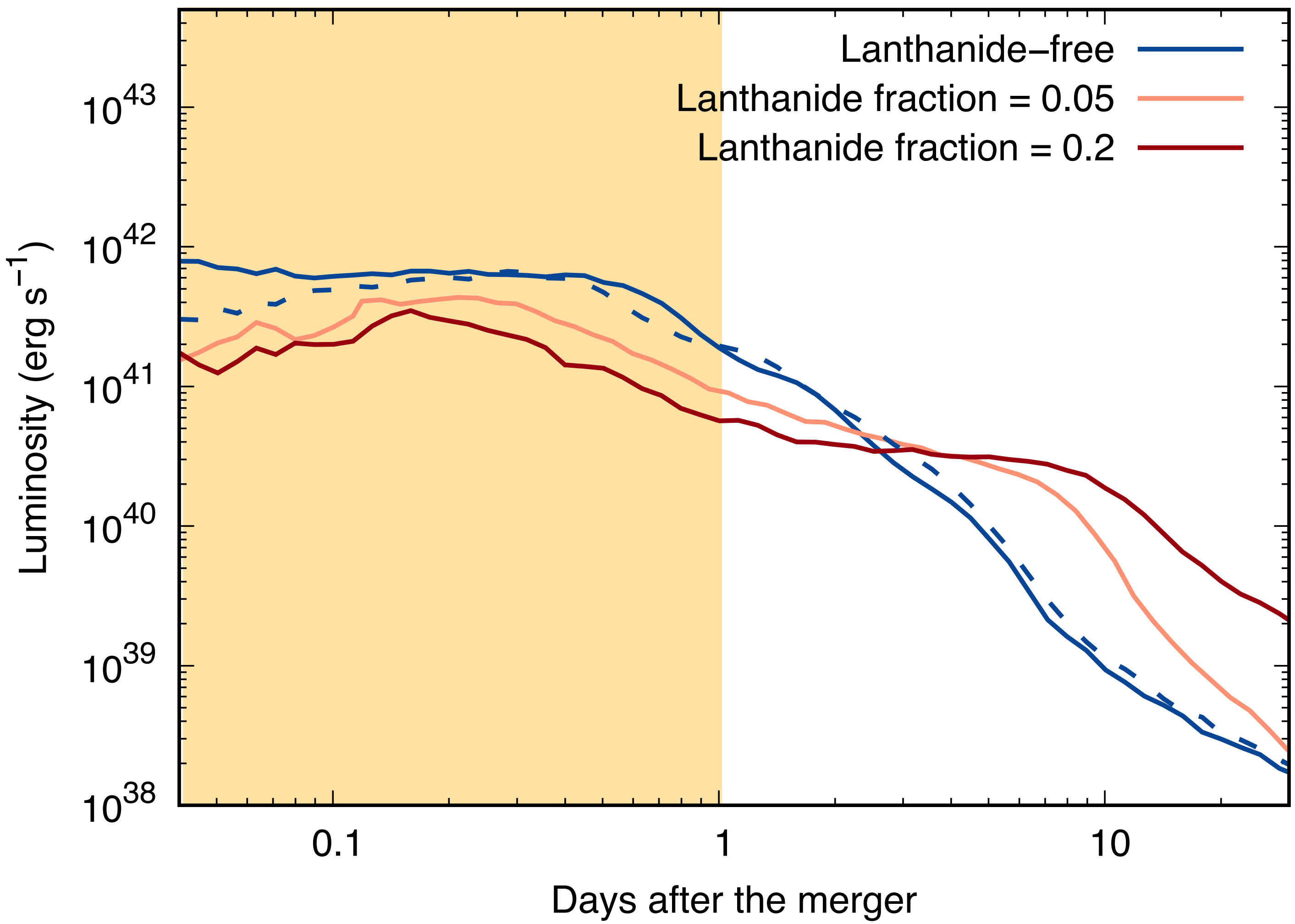


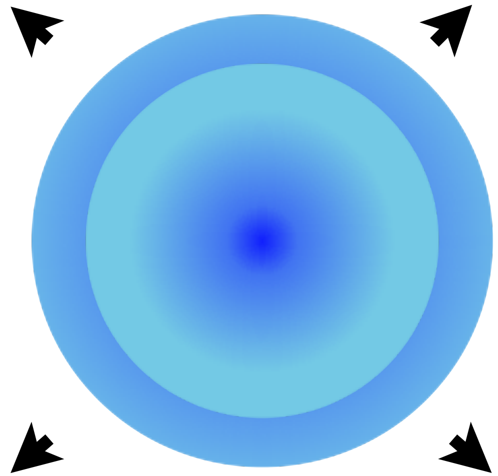


Banerjee+ 2020, 2022, 2023, submitted

Presence of lanthanides
=> Unique signature in kilonova at first few (~ 4) hours

Bolometric light curve

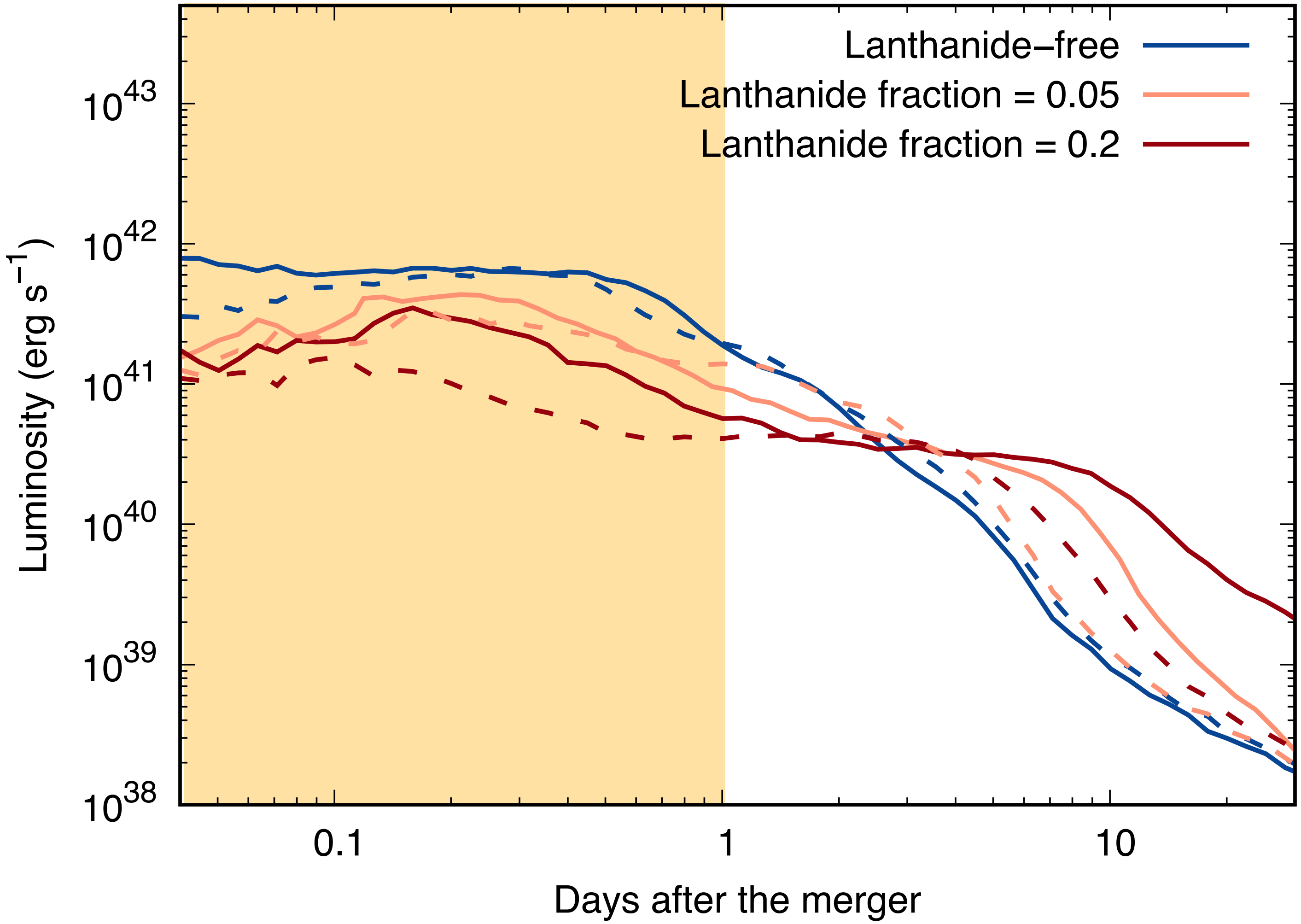


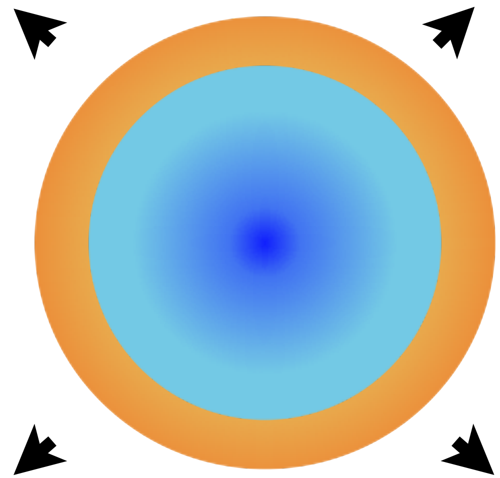


Banerjee+ 2020

Detectable ejecta structure signature in kilonova at first few (~ 4) hours

Bolometric light curve

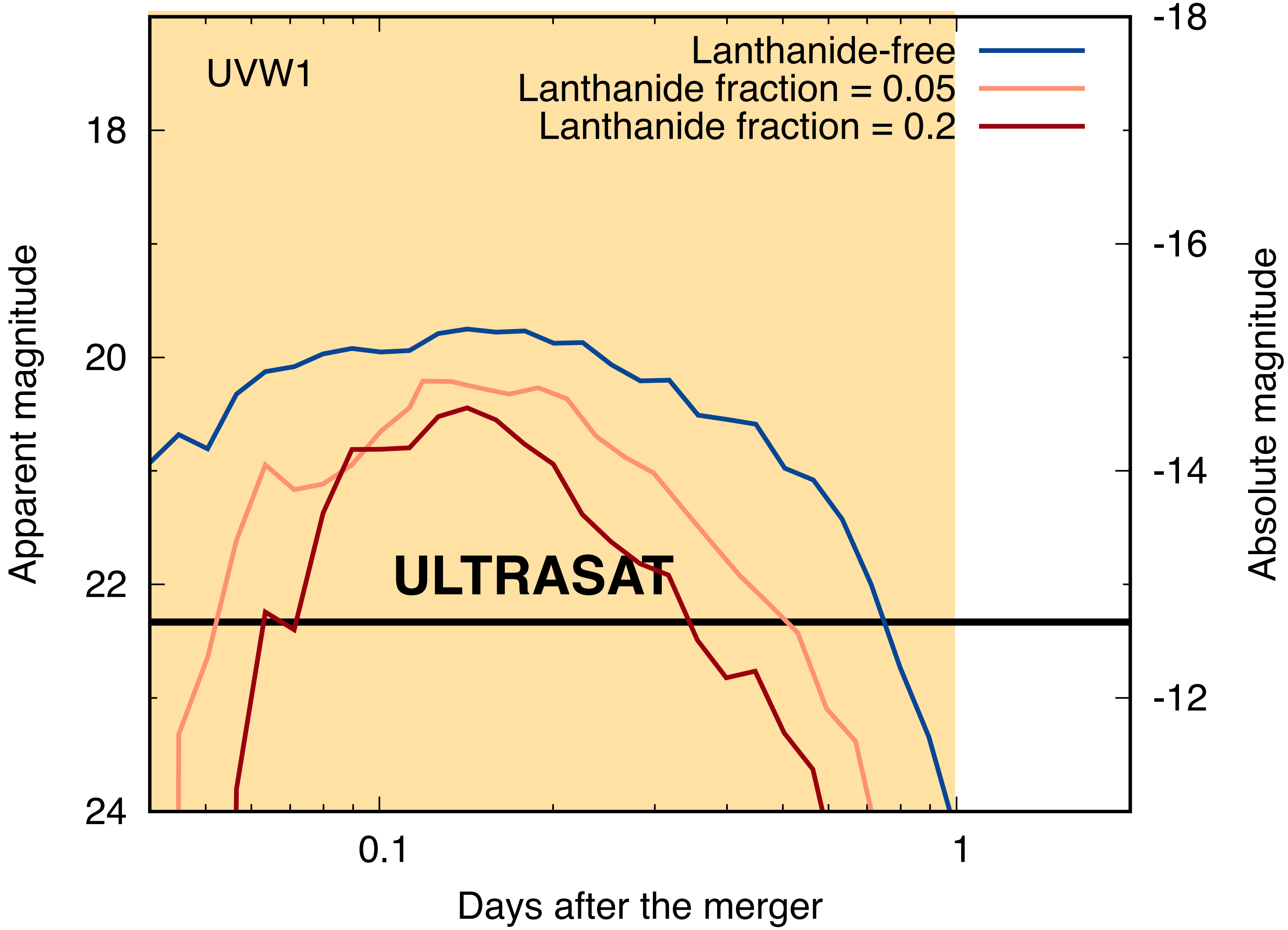




Banerjee+ 2023, submitted

Detectable ejecta structure signature in kilonova at first few (~ 4) hours

Future prospects (UV)



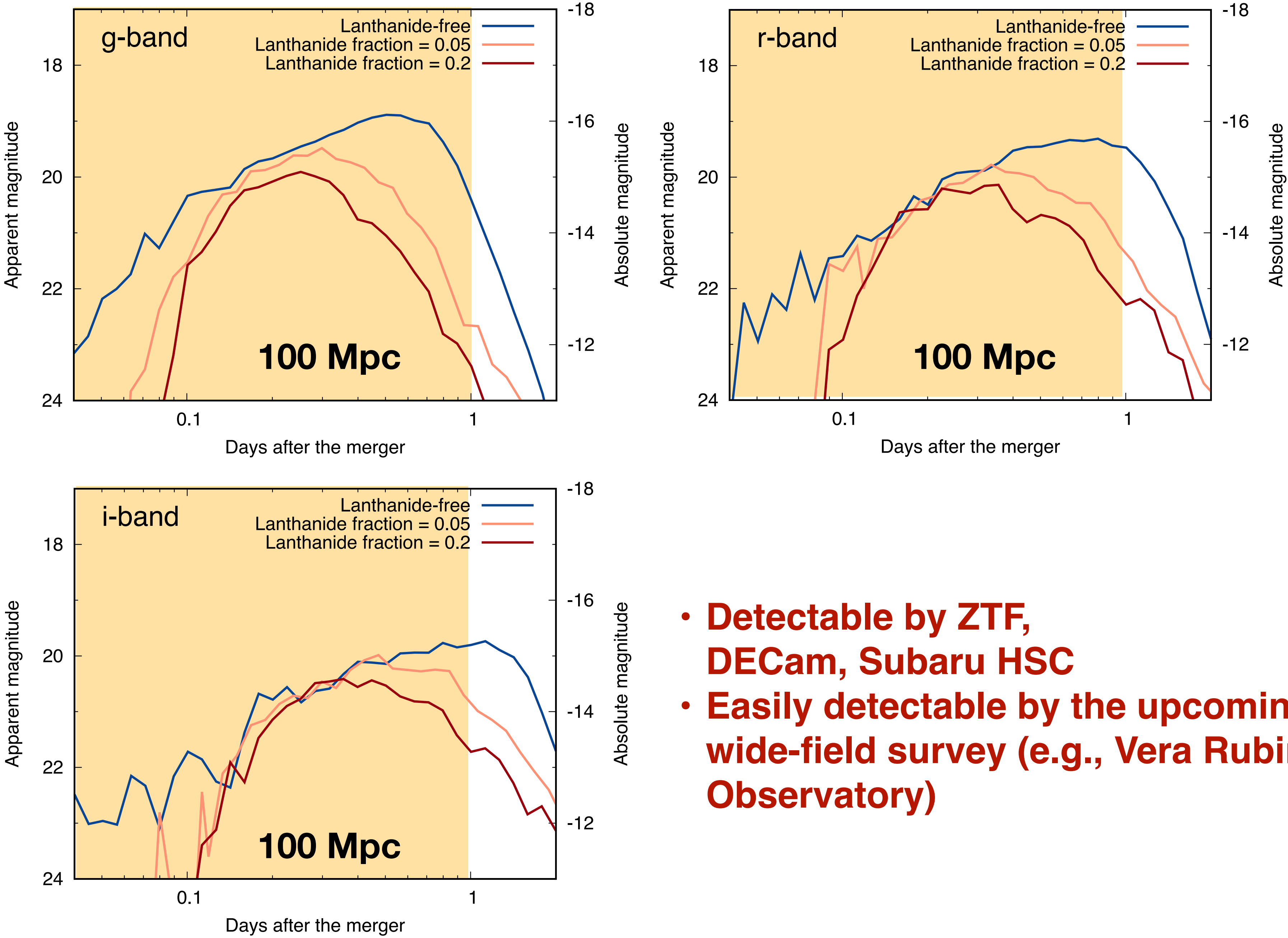
Mission	5σ (AB)
Dorado	20.5 (10 min. exp.)
ULTRASAT	22.3 (15 min. exp.)
UVEX	25 (15 min. exp.)

Dorsman et al. 2022

Multiple upcoming UV missions: ULTRASAT, Dorado, UVEX

Our model predicts detectable early bright UV emission

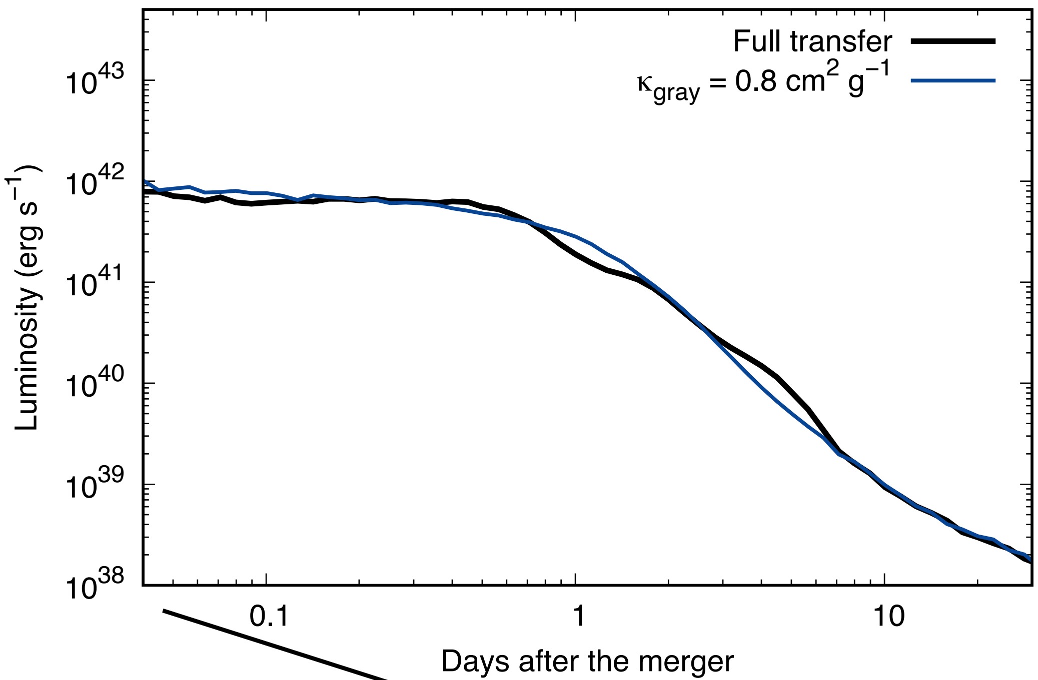
Lanthanide-rich kilonova (optical)



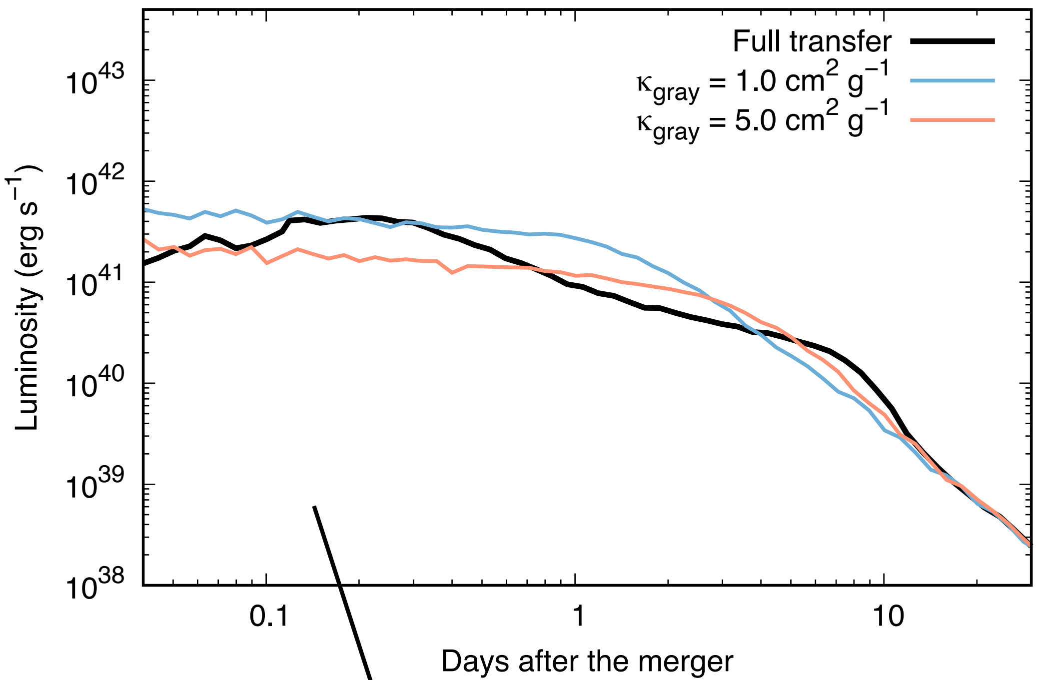
- **Detectable by ZTF, DECam, Subaru HSC**
- **Easily detectable by the upcoming wide-field survey (e.g., Vera Rubin Observatory)**

Suggested gray opacities

Lanthanide-free



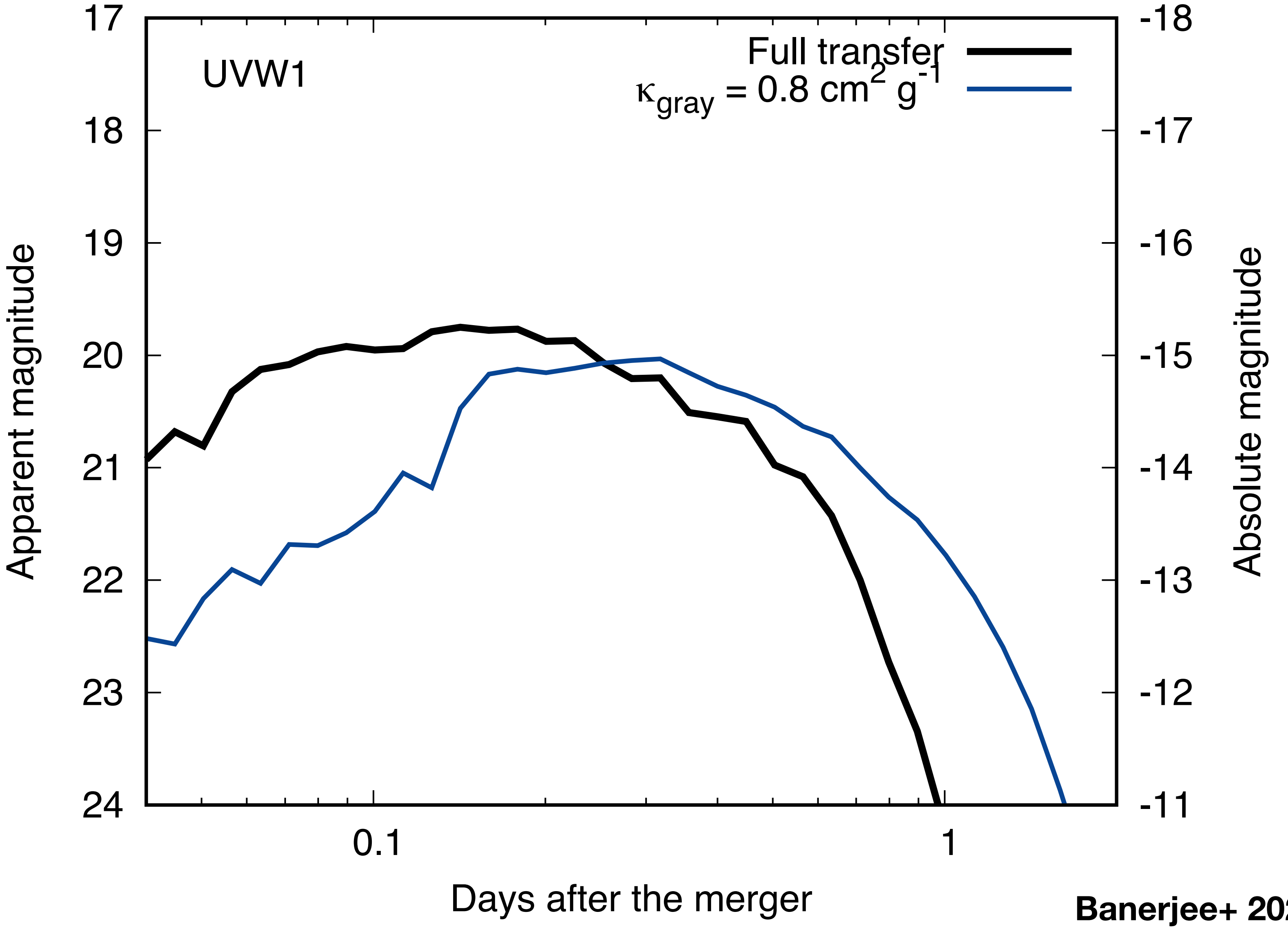
Lanthanide fraction = 0.05



Banerjee+ 2023, submitted

Models	Electron fraction		Suggested gray opacities ($cm^2\,g^{-1}$)
	$Y_{e,in}$ ($v = 0.05c - 0.2c$, $M_{ej,in} = 0.01 M_\odot$)	$Y_{e,out}$ ($v = 0.2c - 0.33c$, $M_{ej,out} = 0.001 M_\odot$)	
Model 1	0.10 – 0.20	–	2.0 – 10.0
Model 2	0.20 – 0.30	–	1.0 – 5.0
Model 3	0.30 – 0.40	–	0.8
Model 4	0.30 – 0.40	0.10 – 0.20	5.0 – 20.0
Model 5	0.30 – 0.40	0.20 – 0.30	3.0 – 10.0
Model 6	0.30 – 0.40	0.30 – 0.40	0.8 – 1.0

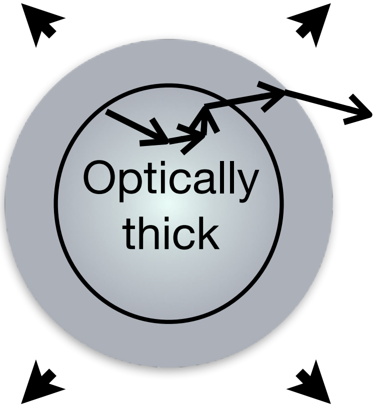
Suggested gray opacities

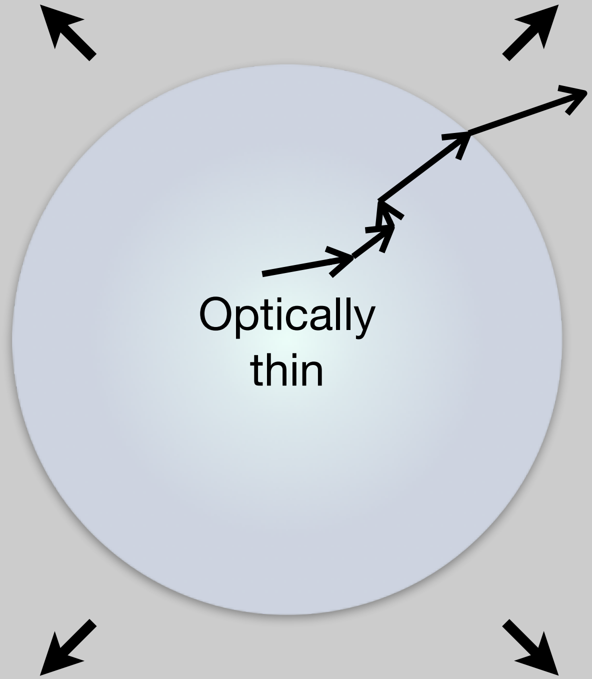


Banerjee+ 2023, submitted

Multi-color light curves cannot be reproduced

Ongoing works





Early time (LTE):
Required atomic data:
- Energy levels
- E1 transitions

All elements Ca - Ra: Tanaka+2020 (I -IV), Banerjee+ 2020, 2022, 2023, submitted (V -XI)

Late time (Non-LTE):
Required atomic data:
- E1+ M1 transitions
- Collisional cross-sections
- Recombination coefficients
- Photo-ionization cross-sections…

e.g., Hotokezaka et al. 2021, Pognan et al. 2022a,b

Time

$t \sim$ a few days

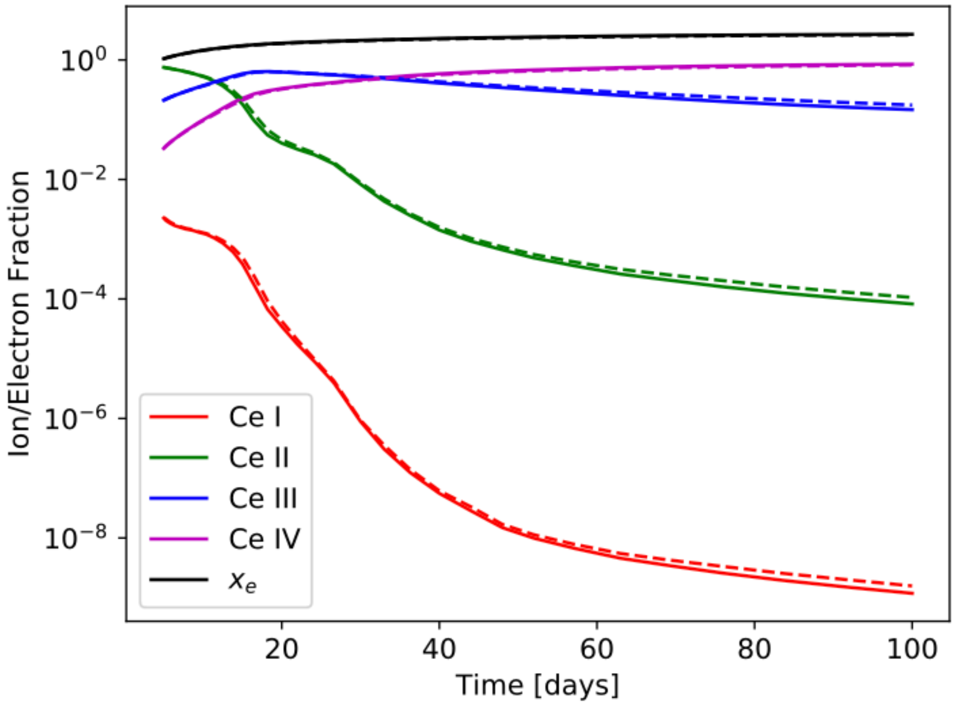
$t \geq$ week

See Q. Pognan's talk

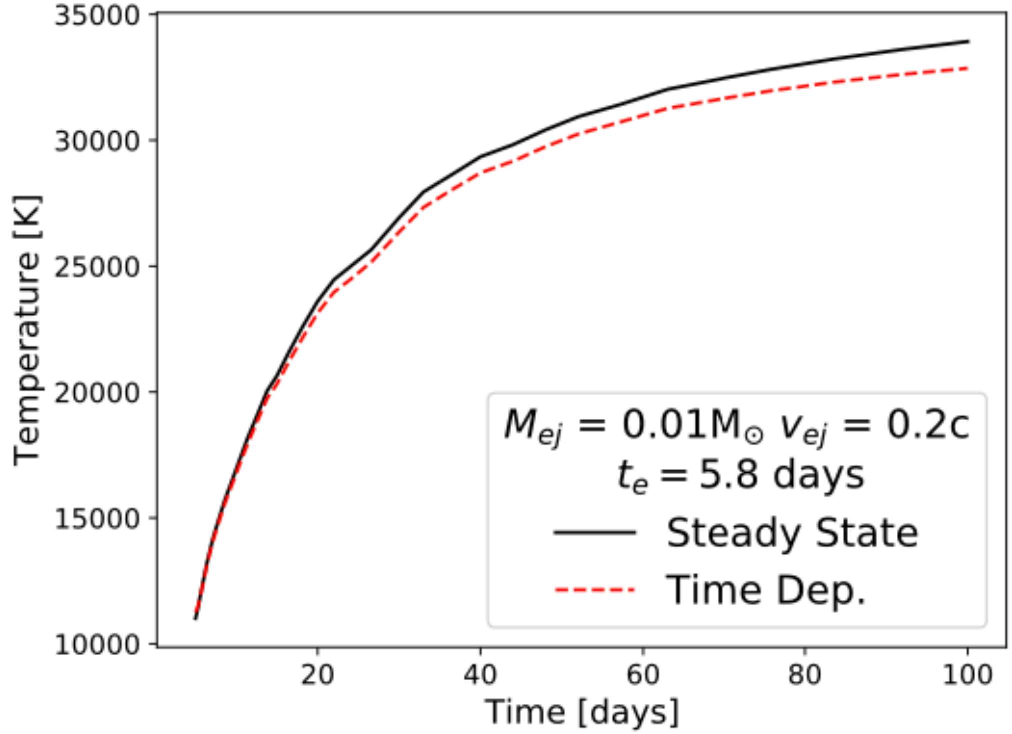
Physical conditions

For a AT2017gfo-like kilonova

By solving rate equation



By balancing radioactive heating + cooling



Pognan et al. 2022a

Spectra <= Ionization and temperature
<= Recombination rate

Conclusion

- Towards more observations <= More detailed physics calculations required
- Atomic data for heavy elements required for modelling all phases
- Huge efforts to understand photospheric phase ongoing
- Nebular phase is relatively unexplored..
  slowly but surely has started now!