# Lanthanide and Actinide Opacity Computations for Kilonova Modeling

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ASOS-14, Paris, France

July 10, 2023

# Team

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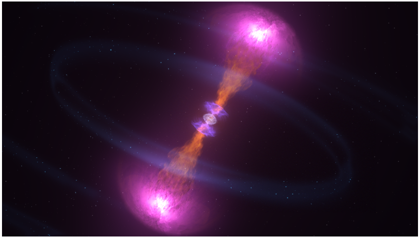
# Outline

1. Neutron star mergers and kilonovae
2. Theoretical method
    - Atomic structure computation: HFR
    - Expansion opacity
3. Existing works
4. Results
    - Opacity sensitivity to atomic properties
    - Lanthanide and actinide expansion opacities
    - Actinide VS lanthanide opacities
5. Conclusion

# Kilonovae

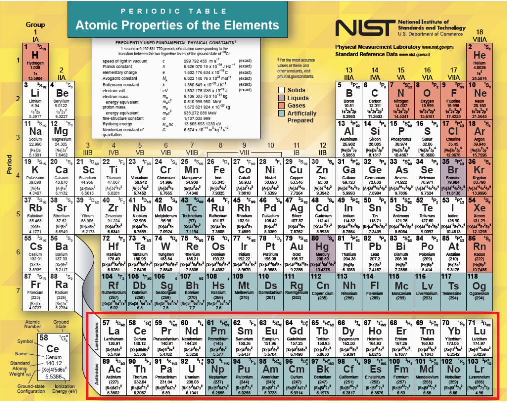
- Detection of gravitational waves from neutron star merger GW170817 for the first time on August 17, 2017
  (Abbott B.P. *et al.*, Phys. Rev. Lett. **119**, 161101, 2017)



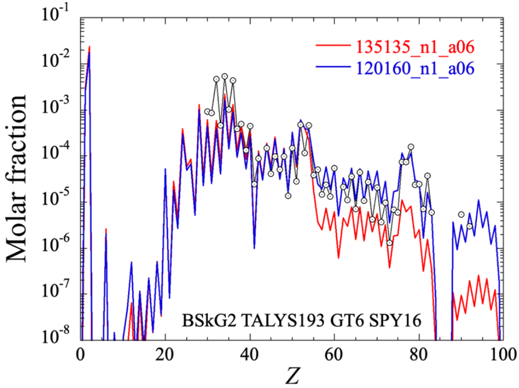
- NSMs also produce an electromagnetic signal powered by the ejection of hot and radioactive matter: **kilonova** (KN)
- GW170817 EM counterpart also detected: KN AT2017gfo
- KNe thought to be responsible for heavy element production

# Kilonova opacity

- KN light curve modeling strongly depends on atomic opacities
- KN opacity dominated by millions of lines from f-shell elements ($\rightarrow$ lanthanides + actinides) newly created by r-process



# Kilonova opacity



(S. Goriely, O. Just, private communication)

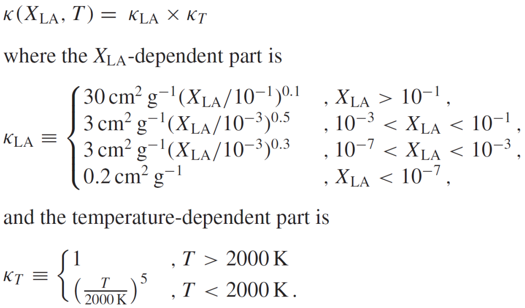
⇒ Lanthanide and actinide contributions to the opacity are of paramount importance due to their large spectral density and abondances

# Kilonova modeling

- Many studies are based on a simple but powerful one-zone approximation (*e.g.* Metzger 2019, Hotokezaka & Nakar 2020)
  → Ejecta = expanding homogeneous sphere with gray opacity
- Monte-Carlo approaches solve the radiative-transfer eqs very accurately using atomic-physics based opacities, but are computationally expensive and often assume analytic ejecta distributions (*e.g.* Kasen *et al.* 2017, Kawaguchi *et al.* 2019)
- Intermediary approach: truncated two-moment approximation (so-called M1 scheme), which assumes a local closure relation ("equation of state") for the radiation field (Just *et al.* 2022)
  → fills the gap between the two approaches above in terms of both accuracy and complexity

# Kilonova opacity

So far, the KN total opacity in Just *et al.* 2022's code is estimated using crude approx to atomic-physics based model, motivated by fits to bolometric KN light curves



$$\kappa(X_{\rm LA}, T) = \kappa_{\rm LA} \times \kappa_T$$

where the $X_{\rm LA}$-dependent part is

$$\kappa_{\rm LA} \equiv \begin{cases} 30\,{\rm cm}^2\,{\rm g}^{-1}(X_{\rm LA}/10^{-1})^{0.1} & , X_{\rm LA} > 10^{-1}\,, \\ 3\,{\rm cm}^2\,{\rm g}^{-1}(X_{\rm LA}/10^{-3})^{0.5} & , 10^{-3} < X_{\rm LA} < 10^{-1}\,, \\ 3\,{\rm cm}^2\,{\rm g}^{-1}(X_{\rm LA}/10^{-3})^{0.3} & , 10^{-7} < X_{\rm LA} < 10^{-3}\,, \\ 0.2\,{\rm cm}^2\,{\rm g}^{-1} & , X_{\rm LA} < 10^{-7}\,, \end{cases}$$

and the temperature-dependent part is

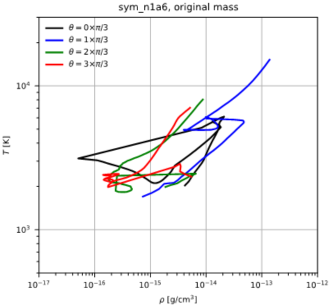
$$\kappa_T \equiv \begin{cases} 1 & , T > 2000\,{\rm K} \\ \left(\frac{T}{2000\,{\rm K}}\right)^5 & , T < 2000\,{\rm K}\,. \end{cases}$$

(Just, Kullman, Goriely *et al.*, MNRAS **510**, 2820, 2022)

$X_{\rm LA}$: average lanthanide + actinide mass fraction

→ Realistic KN opacity would require big amounts of reliable atomic data (structure + radiative data for all transitions) for both lanthanides and actinides

# Kilonova: physical conditions



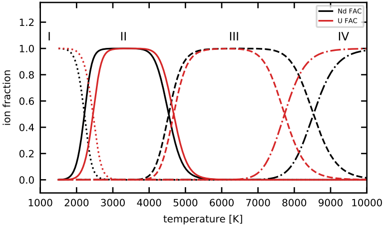
Temperature VS density of the KN photosphere

Just and Goriely, private communication

$$\Rightarrow 10^{-17}\ \mathrm{g/cm^3} < \rho < 10^{-13}\ \mathrm{g/cm^3}$$

and

$$1000\ \mathrm{K} < T < 10000\ \mathrm{K}$$



Flörs, Silva, Deprince *et al.* 2023 (accepted)

⇒ Only the first ionization stages (I – IV) of the elements are present in the KN ejecta

# Pseudo-relativistic Hartree-Fock Method

- Based on Schrödinger equation
- Orbitals obtained for each config. by solving the HF eqs ($\hookrightarrow$ variational principle to the config. average energy)
- Relativistic corrections added perturbatively

Advantages of HFR method:

- Calculation is relatively quick, even for a large number of configurations considered ($\rightarrow$ large number of transitions)
- States from all the configurations are optimized

$\Rightarrow$ Suitable to compute physical properties as opacity which requires to consider large numbers of transitions ($\rightarrow$ lanthanides and actinides) all fairly well described

# Expansion opacity

Expansion opacity:

$$\kappa^{\mathrm{bb}}_{\mathrm{exp}}(\lambda) = \frac{1}{\rho c t} \sum_{l} \frac{\lambda_l}{\Delta\lambda}(1 - \mathrm{e}^{-\tau_l})$$

with the Sobolev optical depth:

$$\tau_l = \frac{\pi e^2}{m_e c} t n_l \lambda_l f_l$$

⇒ Radiative wavelength $\lambda_l$ and oscillator strength $f_l$ are needed to compute the expansion opacity (+ level population $n_l$)

($n_l$ is determined using Boltzmann and Saha equations)

# Works on lanthanide opacities

- Recent studies for weakly-charged lanthanide opacities, *e.g.*:
    - Kasen *et al.* (2013) → Nd I – IV, Ce II – III using AUTOS
    - Gaigalas *et al.* (2019) → Nd II – Nd IV using GRASP
    - Gaigalas *et al.* (2020) → Er III using GRASP
    - Radžiūtė *et al.* (2020) → Pr II – Gd II using GRASP
    - Tanaka *et al.* (2020) → All lanthanides using HULLAC
    - Fontes *et al.* (2020) → All lanthanides using Los Alamos codes
    - Carvajal Gallego *et al.* (2021) → Ce II – IV using GRASP
    - Rynkun *et al.* (2022) → Ce IV using GRASP and HULLAC
    - Gaigalas *et al.* (2022) → Pr IV using GRASP
    - Silva *et al.* (2022) → Nd III using FAC
    - Flörs, Silva, Deprince *et al.* (2023, accepted) ↪ Nd II – III using FAC and HFR (this work)
- \+ Several works on moderately-charged lanthanides (early-phase kilonovae) from Carvajal Gallego *et al.* and Banerjee *et al.*

# Works on actinide opacities

- Only very few works focused on actinide opacities, *e.g.*:
  - Silva *et al.* (2022) → (Nd III and) U III using FAC
  - Fontes *et al.* (2023) → All actinides using Los Alamos codes
  - Deprince, Carvajal Gallego, Godefroid *et al.* (2023)
    ↪ U II – IV using HFR (sensitivity studies, this work)
  - Flörs, Silva, Deprince *et al.* (2023, accepted)
    ↪ (Nd II – III) and U II – III using FAC and HFR (this work)

# Effect of the multiconfiguration model

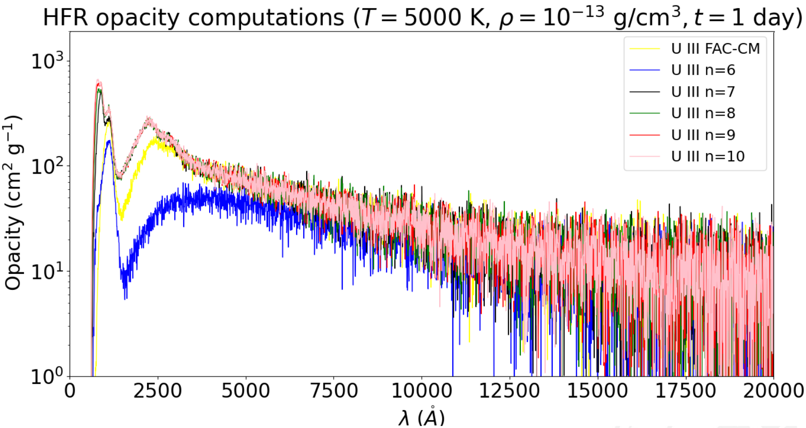
Models for U III

- Silva *et al.* 2022 (FAC):
  $5f^4 + 5f^3\{6d+6f\} + 5f^3\{7s+7p+7d\} + 5f^3\{8s+8p\}$
  $+ 5f^2\{6d^2+6d7s\}$
  (10 configurations)
- Our work (HFR):
  $5f^4 + 5f^3\{6d+6f+6g\} + 5f^3\{7s+7p+7d+7f+7g\}$
  $+ 5f^3\{8s+8p+8d+8f+8g\} + 5f^3\{9s+9p+9d+9f+9g\}$
  $+ 5f^2\{6d^2+6d7s+6d7p+6d7d+7s^2+7s7p+7s7d\}$
  (26 configurations)

How are the computed opacities affected by the multiconfiguration model (by the number of config.) ? Convergence of the models?

# Model convergence for U III

Convergence of the opacity while considering growing models (more configurations added shell by shell)



# Calibration procedure

Calibration procedure used in HFR: adjustement of the configuration average energies to the ones deduces from available energy levels

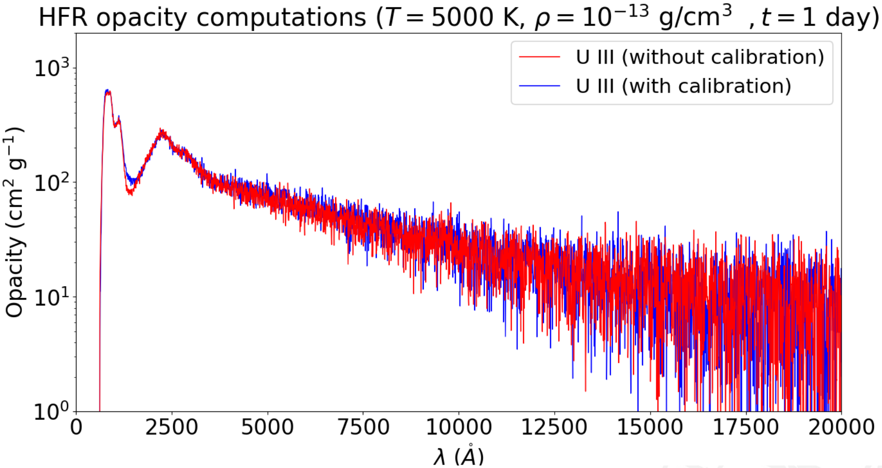
In both U II and U III, level inversion occurs in our computations between (namely) the ground state and one of the first excited states

→ Our calibration procedure solves this level inversion problem

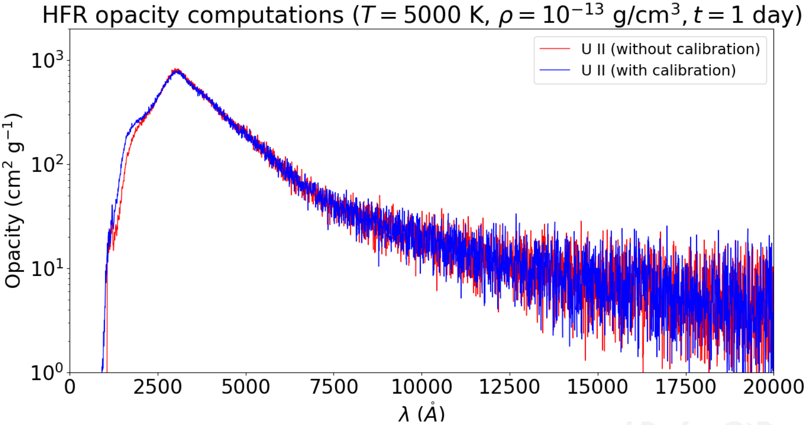
- Is such an adjustment procedure worth it in order to compute opacities (at least in a first step)?

(Deprince, Carvajal Gallego, Godefroid *et al.* 2023)

# Calibration procedure (U III)



# Calibration procedure (U II)

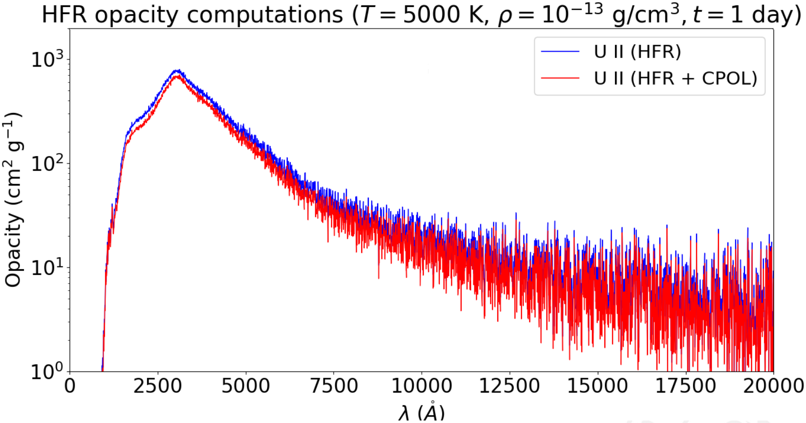


# Core-polarization effect

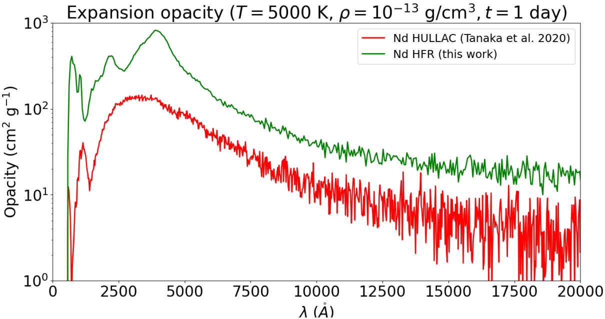
- HFR: not all the correlations are explicitly taken into account
  → Model = ionic core + config. involving valence electrons
- UMONS team (Atomic Physics and Astrophysics Unit) has modified Cowan's codes to include a core-polarization correction to the potential (Quinet *et al.*, MNRAS **307**, 934, 1999)
- Can be tricky to include for elements for which *n*f subshell is partially filled (ionic core not clearly defined)
- Is this effect worth being included in our opacity computations (in a first step)?

(Deprince, Carvajal Gallego, Godefroid *et al.* 2023)

# Core-polarization effect (U II)



# Importance of considering realistic partition functions (Nd opacity case)



Significant difference between our HFR opacity and the one computed by Tanaka *et al.* 2020 using HULLAC

- Atomic data → Importance of the multiconfiguration model! (7 and 8 configs included for Nd II and Nd III in Tanaka *et al.*)

# Importance of considering realistic partition functions (Nd opacity case)

- Expansion opacity computation itself

→ In Tanaka *et al.* (2020) (as well as in Gaigalas *et al.* 2019), the partition function $U(T)$ is approximated to $g_0$ in the evaluation of level populations $n_l$ ($\rightarrow \tau_l$):

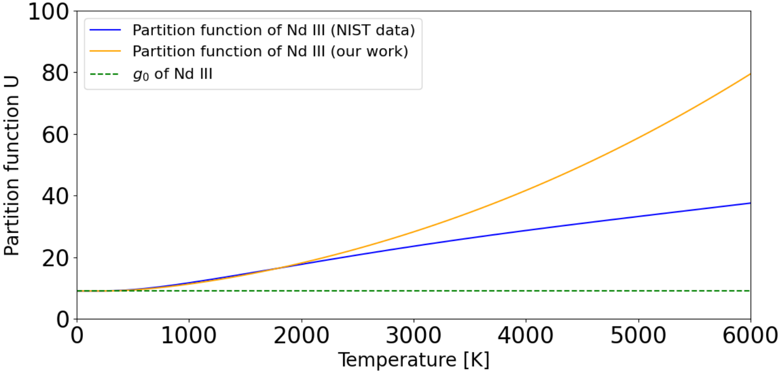
$$n_l = \frac{g_l n}{U(T)} \exp(-E_l/kT)$$

$$\tau_l = \frac{\pi e^2}{m_e c} t n_l \lambda_l f_l$$

$$U(T) = \sum_{i=0}^{\infty} g_i \exp\left(-\frac{E_i - E_0}{kT}\right), \qquad g_i = 2J_i + 1$$

# Partition Function of Nd III

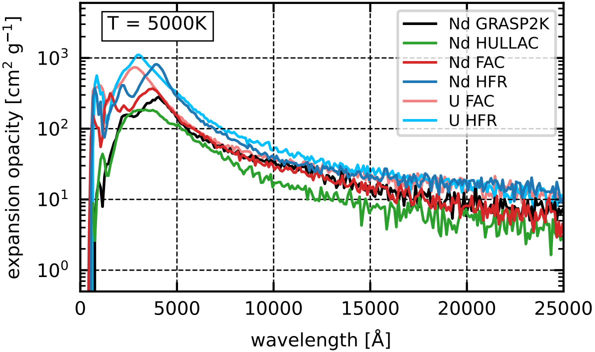
For Nd III, for $T = 5000$ K, $U$ is about 6 times greater than $g_0$!



Carvajal Gallego, Deprince, Godefroid *et al.* 2023

+ *cf.* Carvajal Gallego *et al.*'s poster (moderately-charged lanthanides)

# Comparison with other works



GRASP: Gaigalas, Kato, Rynkun *et al.* (2019)

HULLAC: Tanaka, Kato, Gaigalas *et al.* (2020)

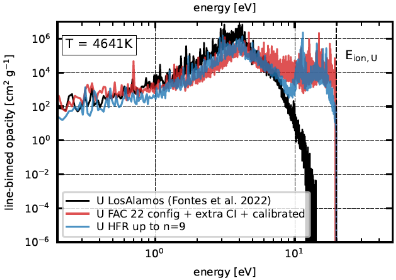
(Opacities recomputed using their atomic data → $U(T)$ NOT approximated to $g_0$)

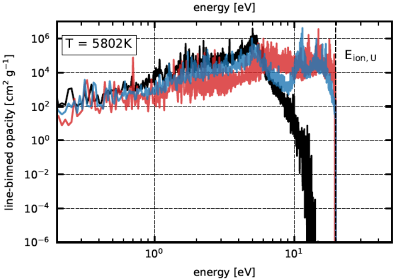
FAC + HFR (This work): Flörs, Silva, Deprince *et al.* (2023)

# Comparison with other works

$$\kappa^{b-b}_{g,n} = \frac{1}{\rho_n c t_n}\frac{1}{\Delta\lambda_g}\sum_{i\in\Delta\lambda_g}\begin{cases}\lambda_i\tau_i, & \text{for binned,}\\ \lambda_i(1-e^{-\tau_i}), & \text{for expansion}\end{cases}$$

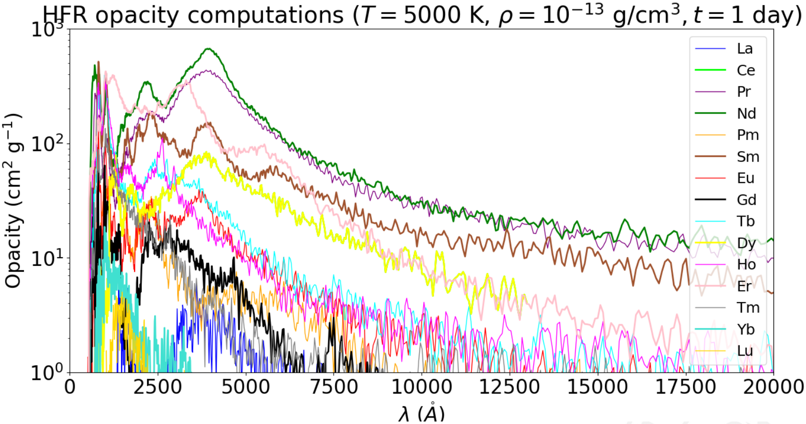
Fontes *et al.* (2020)
↪ Line-binned opacities
(instead of expansion)



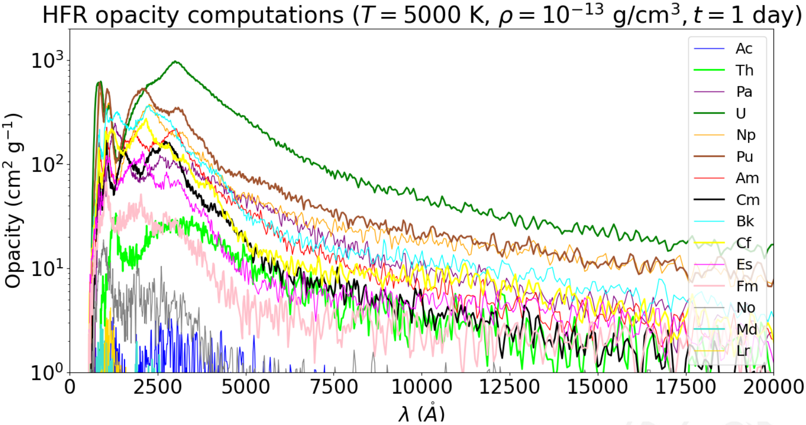


Flörs, Silva, Deprince *et al.* (2023)

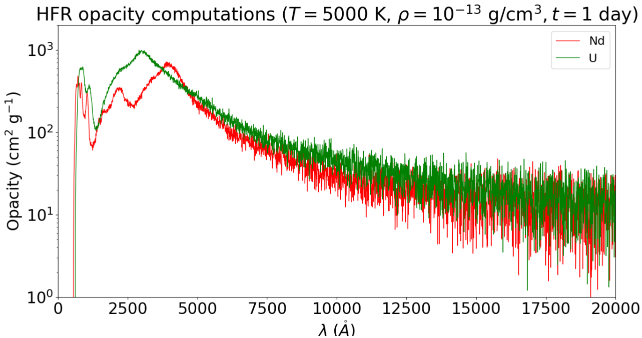
# Opacity of weakly-charged lanthanides



# Opacity of weakly-charged actinides

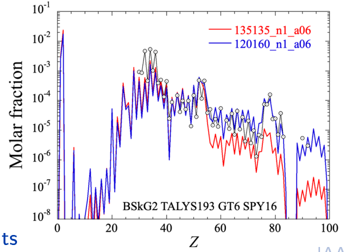


# U VS Nd opacities

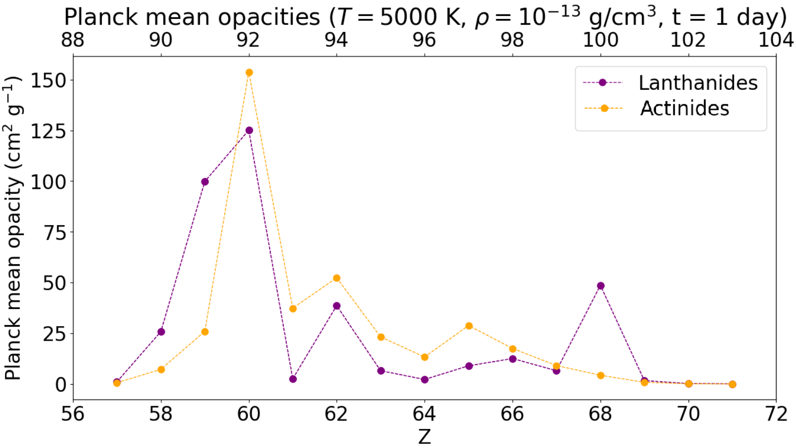


$\Rightarrow$ U opacity at least as large as Nd opacity

$\Rightarrow$ Importance of the actinide opacities as well



# Lanthanide and actinide Planck mean opacities



# Conclusion

- Opacity computations needed to model kilonova light curves

  ↪ Reliable atomic data for as many transitions as possible

  Especially for lanthanides and actinides which are expected to dominate the KN opacity

- Lanthanides: several works exist but can be improved
- Actinides: very few works

  → Multiconfiguration model choice is of crucial importance

  → Partition functions fully-computed (not approximated to $g_0$)

- HFR expansion opacities computed for all weakly-charged lanthanides and actinides for a grid of $T$, $\rho$ and time
- Opacity for U as large as for Nd or even greater

  ⇒ Actinides can be as important as lanthanides concerning their contributions to the KN opacity

# Prospects

- Average the computed opacities with the expected elemental abundances for several NSM cases (nucleosynthesis simulations from S. Goriely, ULB) to infer the KN total opacity
- Implement the new atomic opacity data in kilonova light curve model (O. Just's code, Just *et al.* 2022)
- Try to improve atomic data (especially for the most contributing species)
  $\Rightarrow$ Investigate impact on the computed opacities
- Exhaustive comparison with the opacities computed by other groups using other methods (GSI/Lisbon University, NIST-Los Alamos Lanthanide Opacity Database, Japan-Lithuania Opacity Database for Kilonova)