Atomic Structure Calculations in Lanthanide and Actinide ions relevant to kilonovae

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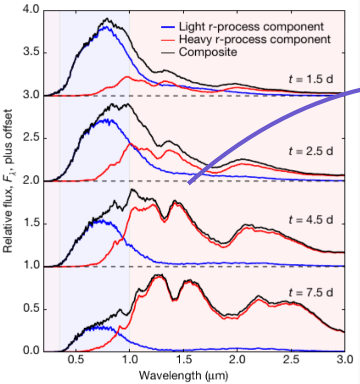
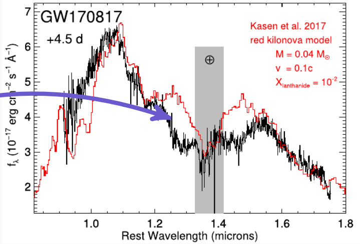




- Heavy r-process models match observations

Are kilonovae a site of heavy element production?

Kasen et al. Nature (2017)

$$k^{bb}_{\text{exp}}(\lambda) = \frac{1}{\rho c t}\sum_l \frac{\lambda_l}{\Delta\lambda_{bin}}\left(1 - e^{-\tau_l}\right) \qquad \tau_l = \frac{\pi e^2}{mc}\underbrace{f_l}_{\text{Oscillator Strenght}}\overbrace{n_l}^{\text{Lower level density}}\underbrace{\lambda_l}_{\text{Transition Wavelenght}}$$

LTE approach:

Boltzmann:

$$n_l = \frac{g_l}{g_0} n e^{-E_l/k_B T}$$

Saha equation:

$$\frac{n^i}{n^{i-1}} = \frac{U^i(T)U_e(T)}{\underbrace{U^{i-1}}_{\text{Partition function}}(T)n_e} e^{-(E^i - E^{i-1})/k_B T}$$

$$\tau_l = \frac{\pi e^2}{mc}\left(\frac{n\lambda_l t}{g_0}\right) g_l f_l e^{-E_l/kT}$$

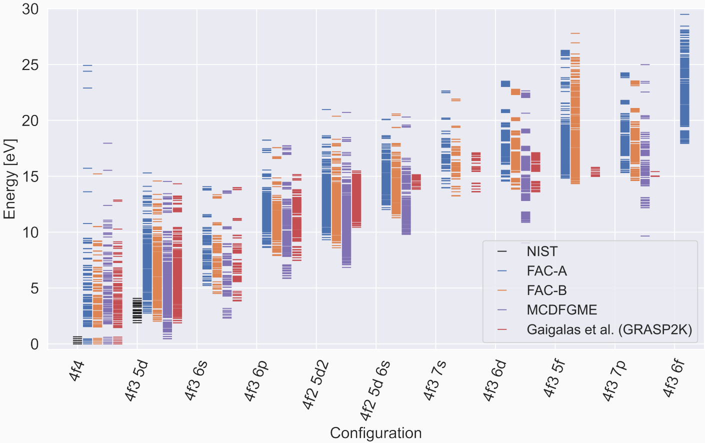
Nd III Calculations

Calculation of atomic parameters - Nd III

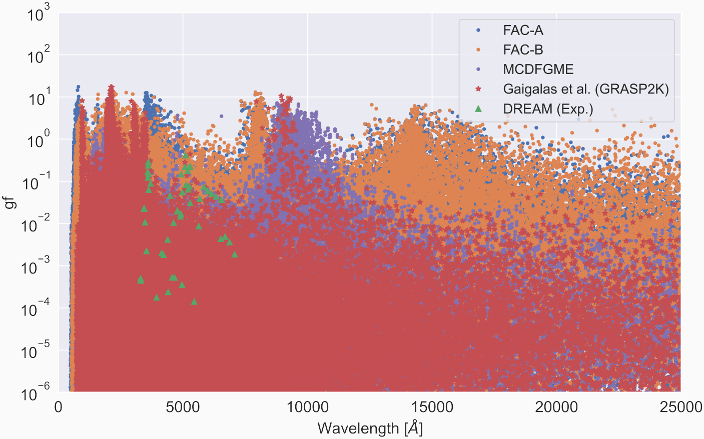
Label	Configs		All	
	Even	Odd	#Levels	#Lines
FAC (Calculation A)	$4f^4$, $4f^36p$, $4f^25d^2$ $4f^25d6s$, $4f^35f$ $4f^37p$, $4f^36f$	$4f^35d$, $4f^36s$, $4f^36d$, $4f^37s$	3206	708077
FAC (Calculation B)	$4f^4$, $4f^36p$, $4f^25d^2$ $4f^25d6s$, $4f^35f$ $4f^37p$	$4f^35d$, $4f^36s$, $4f^36d$, $4f^37s$	2702	579796
MCDFGME	$4f^4$, $4f^36p$, $4f^25d^2$ $4f^25d6s$	$4f^35d$, $4f^36s$,	2232	178778
GRAPS2K(Gaigalas et al)	$4f^4$, $4f^36p$, $4f^25d^2$ $4f^25d6s$, $4f^35f$ $4f^37p$	$4f^35d$, $4f^36s$, $4f^36d$, $4f^37s$	1453	148759
DREAM	$4f^4$	$4f^35d$	-	51
NIST	$4f^4$	$4f^35d$	29	-

- MCDFGME and GRASP2K (MCDF codes): + better precision
  − computational expensive
- FAC (RCI codes): + shorter computing (and processing) times
  + able to calculate collision and ionization rates
  − typically less precision

Energy Levels Nd III

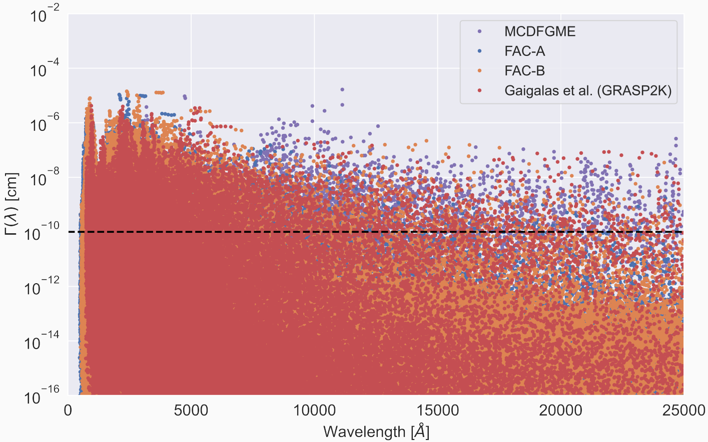


- Relevant differences for more energetic configurations
- Number of configurations included affects FAC calculation



Two main concern regions:

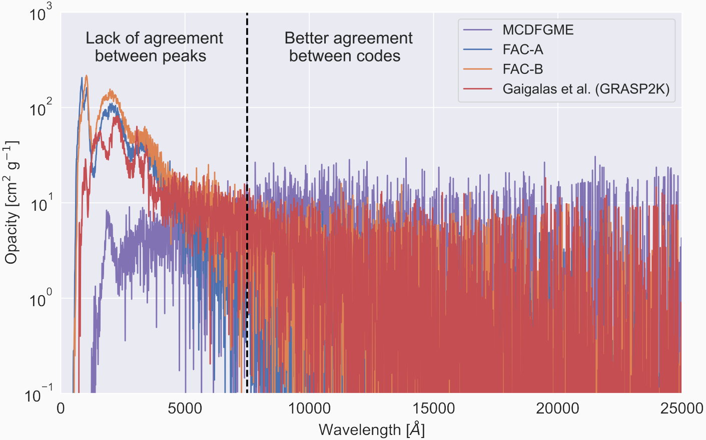
- < 5000 Å- lack of agreement on peak locations for multiple codes
- > 10000 Å- FAC calculates transitions with higher gf than MCDFGME and GRASPK2K



$T = 10000$K (∼0.86eV)

- $\tau_l \propto \Gamma(\lambda) \equiv \lambda gf \exp(-\overbrace{E_l}^{\text{Energy Lower Level}}/kT)$ - Transitions from lower levels have greater contributions $(1 - e^{-\tau} \approx 1)$
- Opacities will be more sensitive to more energetic transitions

Opacities Nd III



$\rho = 10^{-13}\mathrm{gcm}^{-3}$
$\mathrm{T} = 10000\mathrm{K}$ (∼0.86eV)
$\Delta\lambda = 10\text{Å}$

U III Calculations

Lack of atomic data available in the literature:

- Blaise *et al* (1992), Experimental data, *LAC Database & International Tables of Selected Constants* - 123 Levels
- Savukov et al (2015), CI-MBPT code, *Los Alamos* - 96 Levels
- Fontes *et al* (2020), ATOMIC code, *Los Alamos* - 1650 Levels / 233 822 Lines (Atomic data not available)
- NORAD-Atomic-Data, Superstructure code - Only data for highly ionized elements

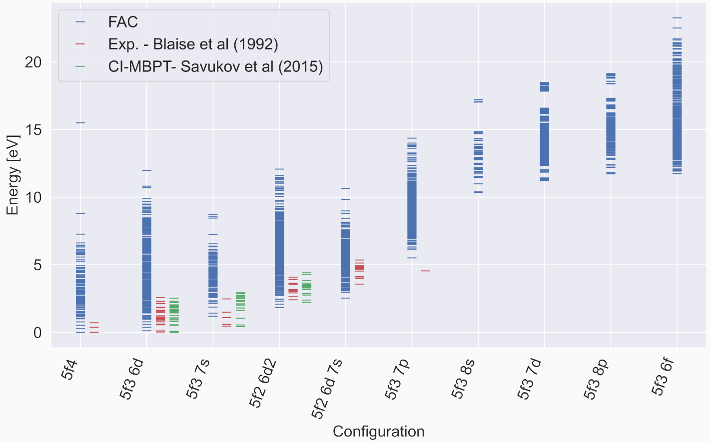
This work(FAC):

Nd III: [Xe] $4f^k\ 5d^m$ ...
U III: [Rn] $5f^k\ 6d^m$ ...

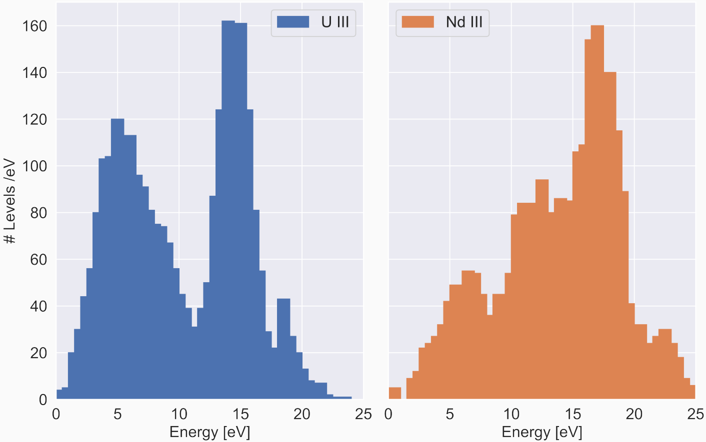
Even - $5f^4$, $5f^2 6d^2$, $5f^2 6d 7s$, $5f^3 7p$, $5f^3 8p$, $5f^3 6f$
Odd- $5f^3 6d$, $5f^3 7s$, $5f^3 8s$, $5f^3 7d$

2702 Levels & 579 796 Lines

Energy Levels U III

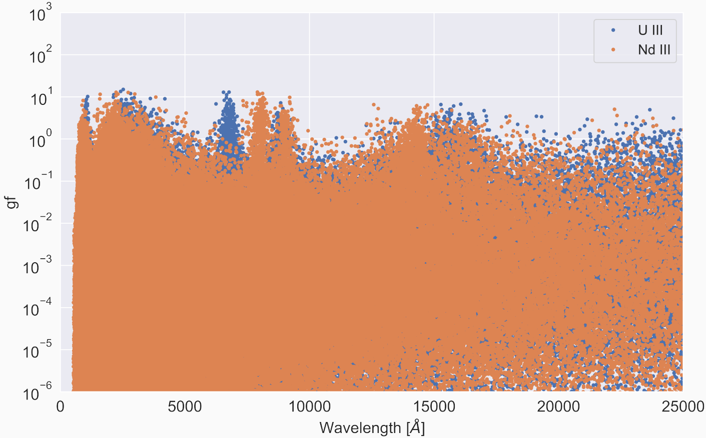


- Similar level distribution to Nd III
- Reasonable agreement for less energetic configurations (caveat at 7s orbital ⇒ possibility of improvement)



- Higher density of low lying levels for U III

Oscillator Strengths U III



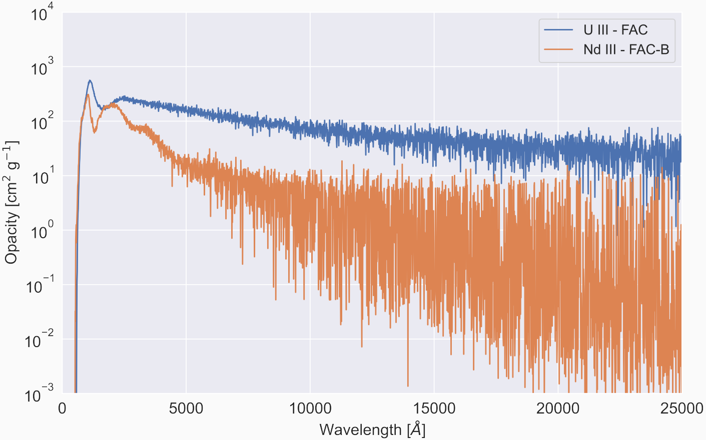
- Similar OS distribution to Nd III - expected from equivalent shell structure

Oscillator Strengths U III - contribution to the opacities

$T = 10000K$ $(\sim 0.86eV)$

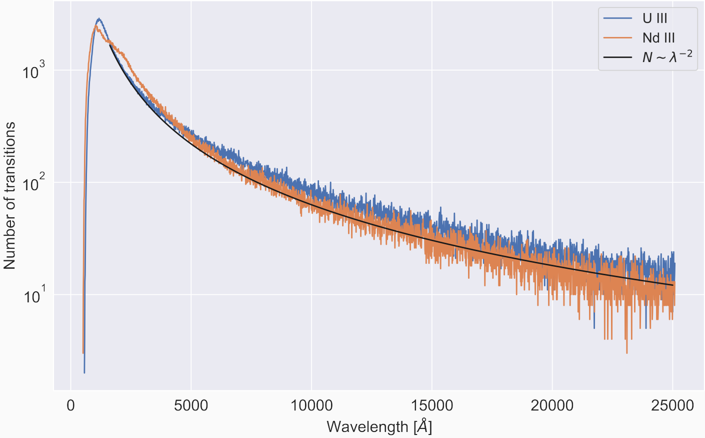
- Bigger contribution from U III due to less energetic levels

Opacities U III VS Nd III

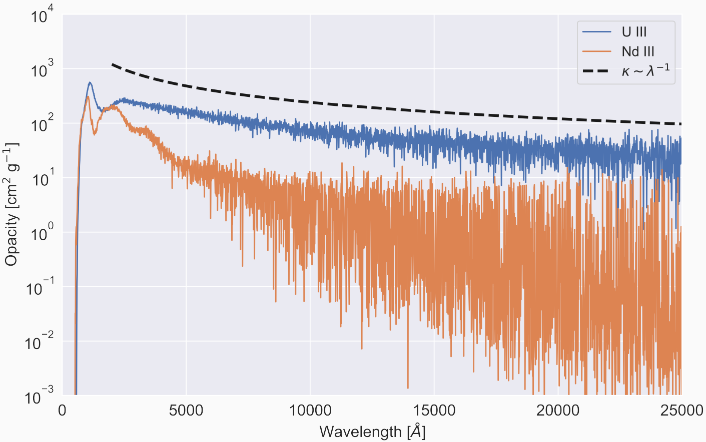


$\rho = 10^{-13}$gcm^{-3}
T $= 10000$K
(∼0.86eV)
$\Delta\lambda = 10$Å

Transition wavelength



- Similar distribution of the # transitions for corresponding Actinide and Lanthanide elements
- #Transitions follows a λ^{-2} power law



$\rho = 10^{-13}\text{gcm}^{-3}$
T $= 10000$K
(∼0.86eV)
$\Delta\lambda = 10$Å

$$\sum_l \frac{\lambda_l}{\Delta\lambda}(1 - e^{-\tau_l}) \approx \frac{N\lambda}{\Delta\lambda}(1 - e^{-\tau_l}) \sim \lambda^{-1} \quad \text{for } \tau \gg 1$$

- Higher Opacity from U III when compared to Nd III - possibly extended to all Actinides
- UV region more sensitive to atomic calculations
- Good agreement between opacity calculations from different codes in IR region

Next Challenges:

- Systematic calculation with FAC for multiple Lanthanide and Actanide Ions
- Energy threshold - Autoionization rates
- Collisional and photoionization rates
  $\Rightarrow$ Non-LTE approach

Kilonova Colaboration

LIP/Faculdade Ciências Universidade de Lisboa:

- Jorge Sampaio
- José Pires Marques

LIBPhys/Universidade Nova de Lisboa:

- Pedro Amaro

GSI/Technische Universität Darmstadt:

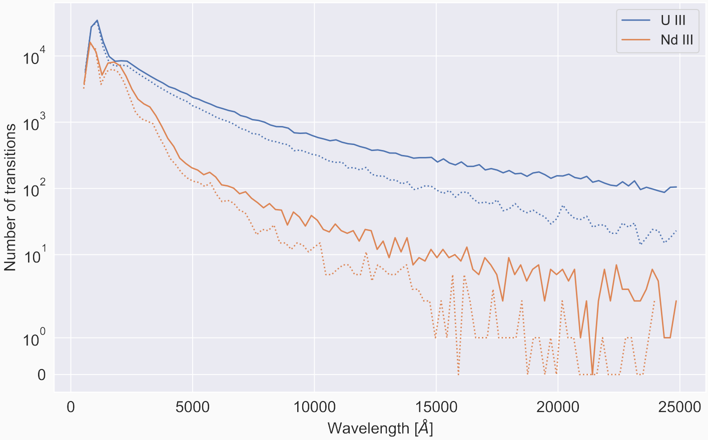
- Gabriel Martínez-Pinedo
- Andreas Flörs

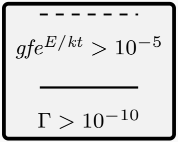
Queen’s University Belfast:

- Luke Shingles
- Stuart Sim

Thank you for your attention!

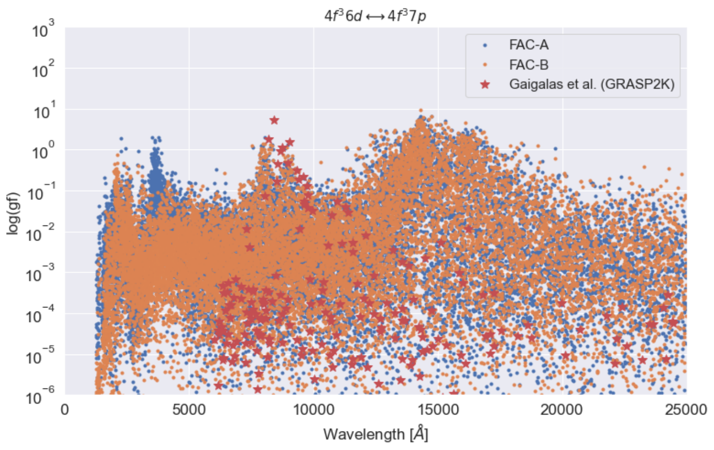
Number of significant lines U III





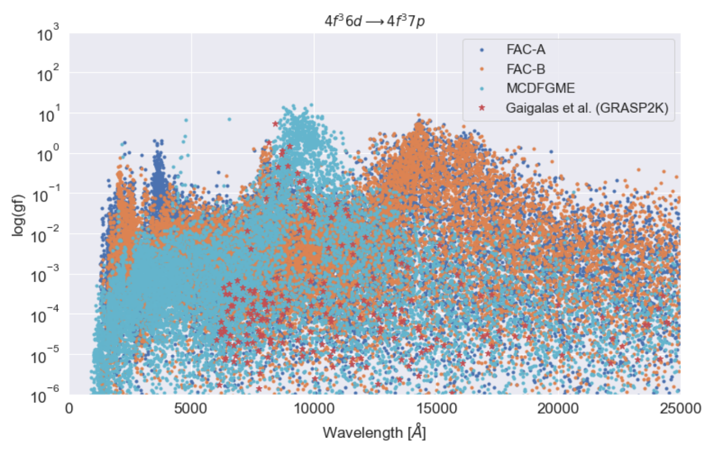
- Bigger contribution from U III due to less energetic levels

Oscillator Strengths Nd III



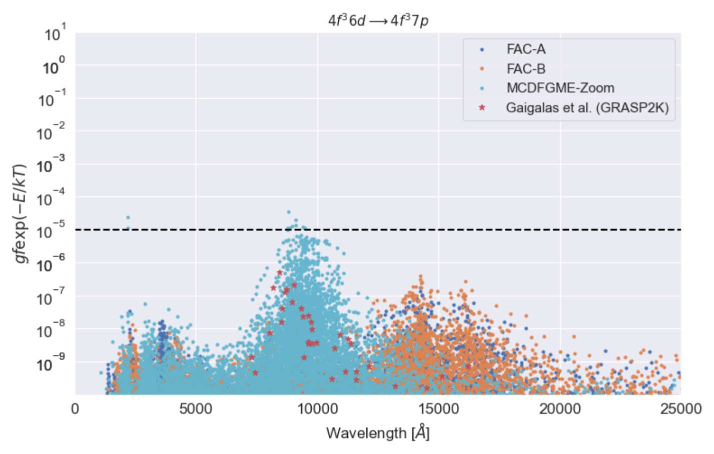
- Zooming in we see that a major part of the transitions in the $> 10000\text{Å}$ region are from transitions from $4f^3 6s \longrightarrow 4f^3 7p$

Oscillator Strengths Nd III



- We performed a specific MCDF calculation (MCDFGME-Zoom) for these two levels - better agreement with GRASP2K, doesn't reproduce the high OS at around 15000Å in FAC

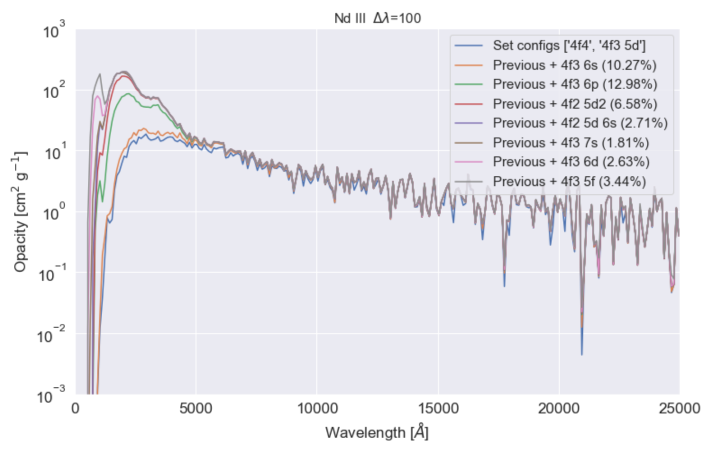
Oscillator Strengths Nd III - contribution to the opacities



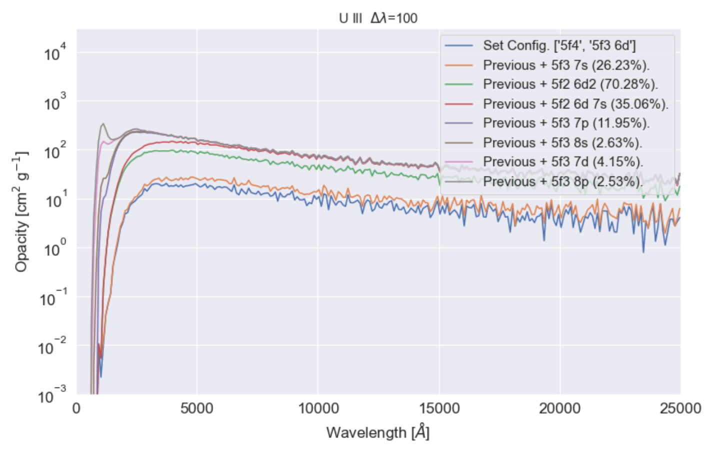
T = 10000 K

- Discrepancy on the OS less relevant at longer wavelengths ($1 - e^{-\tau} \sim 0 \Rightarrow$ small opacity contributions)
- Values for MCDFGME likely to be overestimated

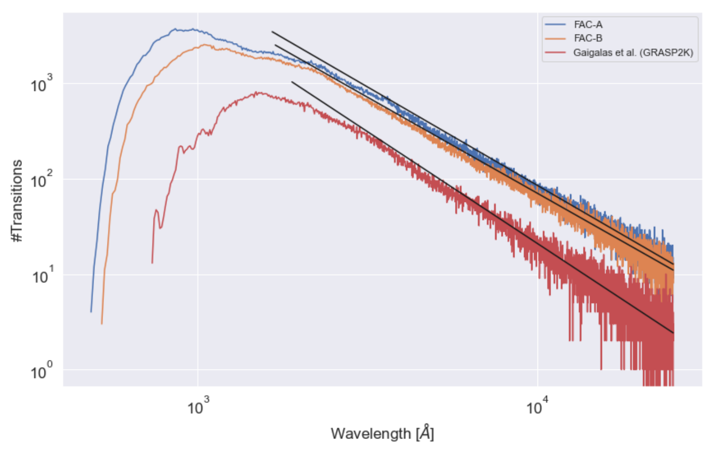
Convergence of opacity calculations



Convergence of opacity calculations



Transition wavelength



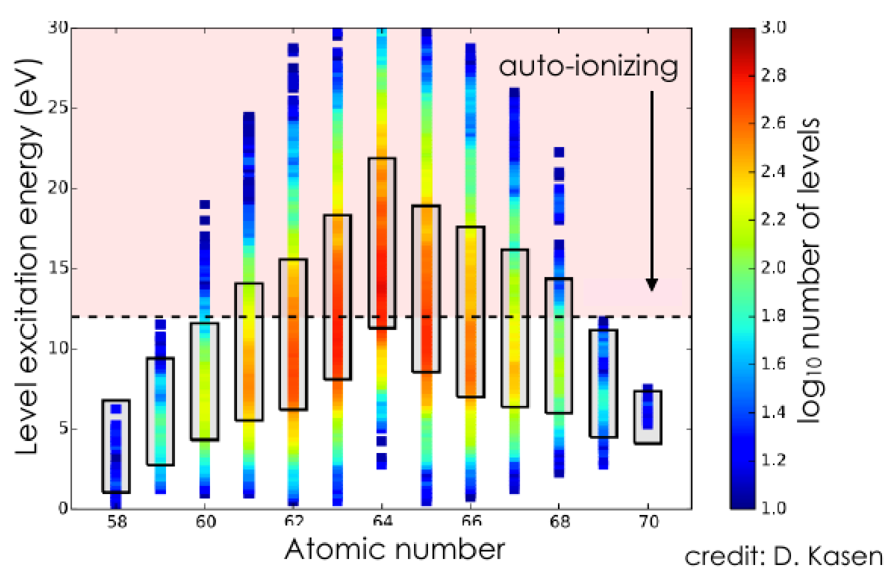
Slopes:

FAC-A = -2.01

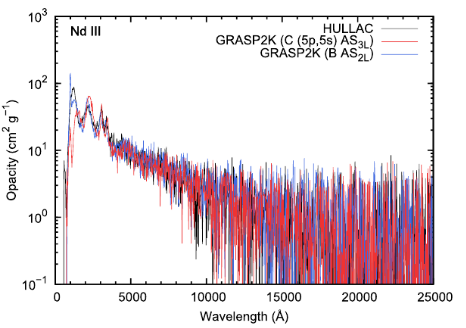
FAC-B=-2.06

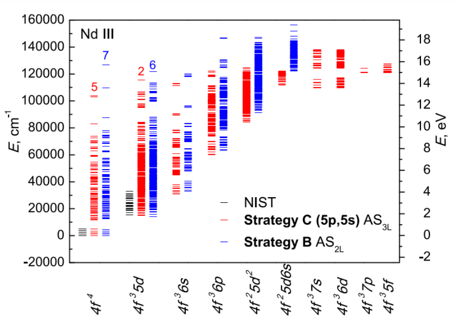
Gaigalas=-2.34

Autoionization



$$\rho = 1 \times 10^{-13}\mathrm{g/cm}^3 \quad T = 10000\mathrm{K}(0.86\mathrm{eV}) \quad \Delta\lambda = 10\text{Å}$$





- Transitions between energetic configurations and low energetic ones have larger contributions at low wavelengths

Gaigalas, G. *et al*(2019). Extended calculations of energy levels and transition rates of Nd II-IV ions for application to neutron star mergers