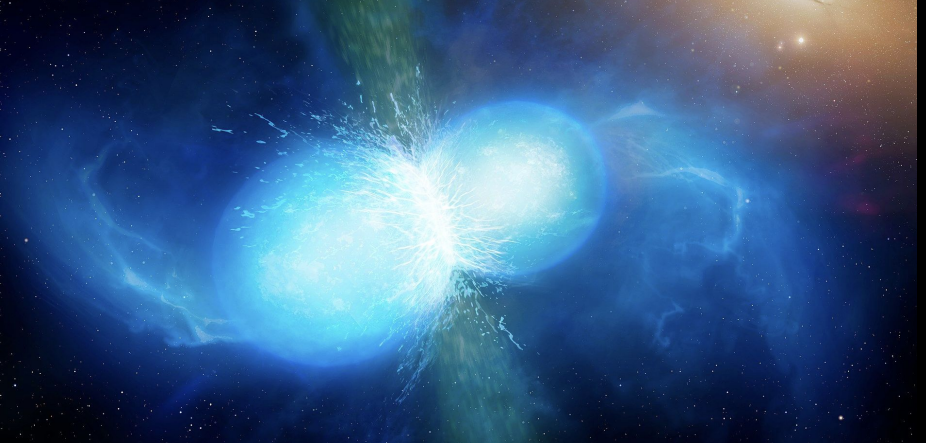
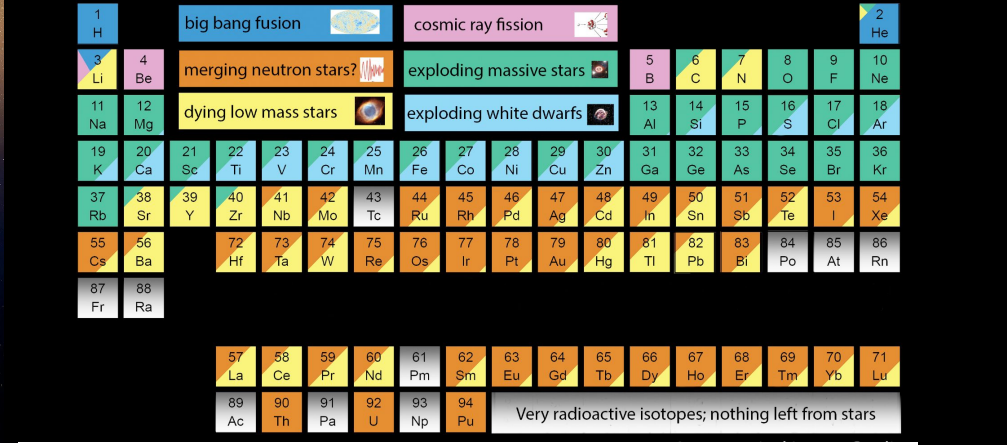




Towards a complete and calibrated set of lanthanide atomic data

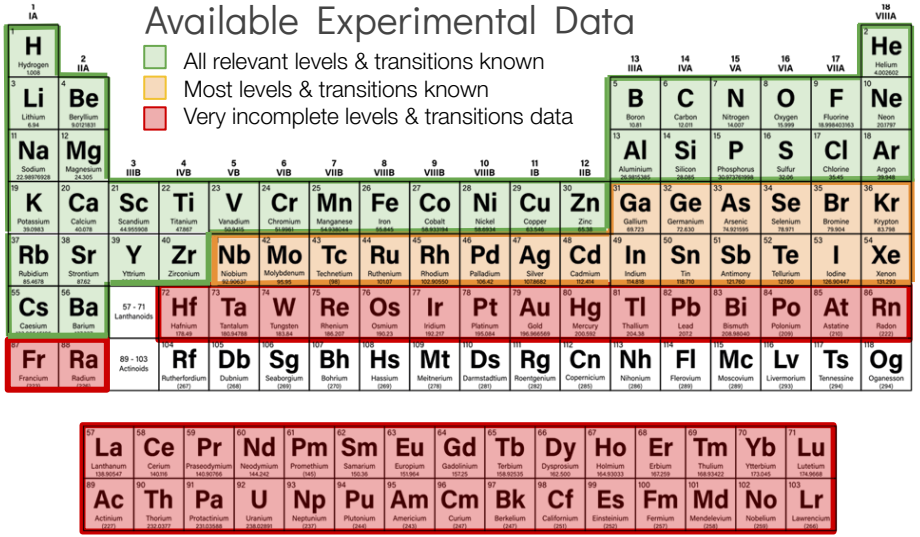
Andreas Flörs (GSI)

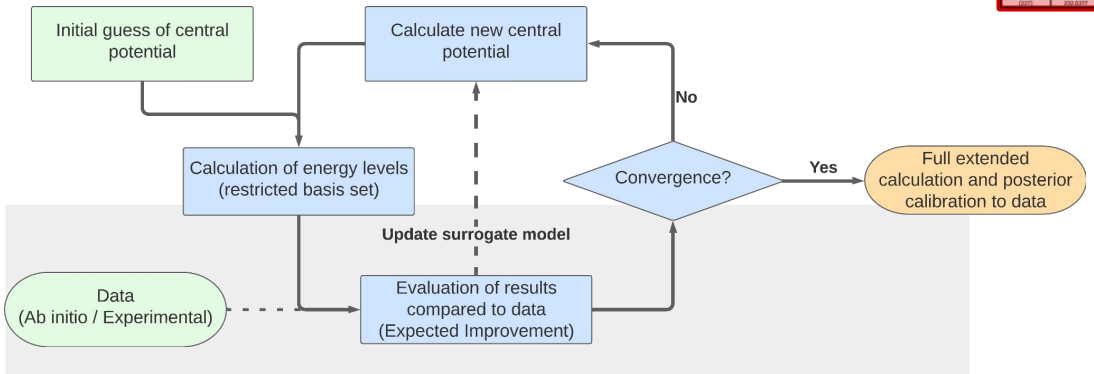
Ricardo Ferreira da Silva (LIP), Gabriel Martínez-Pinedo (GSI)

Atomic Opacities

LTE modelling (first few days, collisional rates ≫ radiative rates):
→ energy levels and E1 radiative transitions required:
Saha & Boltzmann equations
→ **bolometric light curves:** grey opacities from uncalibrated data good enough
→ **spectral models:** use of calibrated atomic data essential for line identification and obtaining the relevant spectral features

NLTE modelling (after a few days, radiative rates ≫ collisional rates):
→ requires additional atomic data: electron-ion impact cross sections, photoionisation & recombination cross sections, forbidden (M1 and E2) transitions
→ due to lack of atomic data only possible using approximations





Systematic improvement of atomic data possible with the use of **experimental data** or *ab initio* calculations for few low lying levels

Kilonova atomic data

Many recent published calculations on singly / doubly ionised r-process elements:

Kasen+13, Kasen+17 AUTOSTRUCTURE - Lanthanides
Fontes+20, Fontes+22 Los Alamos Atomic Physics and Plasma Code - Lanthanides and Actinides (I-IV)
Tanaka+20 , Domoto+22, Banerjee+23 HULLAC - Multiple *r*-process elements (I - IX)
Gaigalas+19, Gaigalas+20, Radžiūtė+21 GRASP2K - Multiple lanthanides
Carvajal+22, Deprince+22 HFR - Multiple Lanthanides and Actinides,

F. Silva+22, Flörs+23, GSI + LIP FAC all lanthanides + Pt + Au (optimized potential where exp. data is available)

Team

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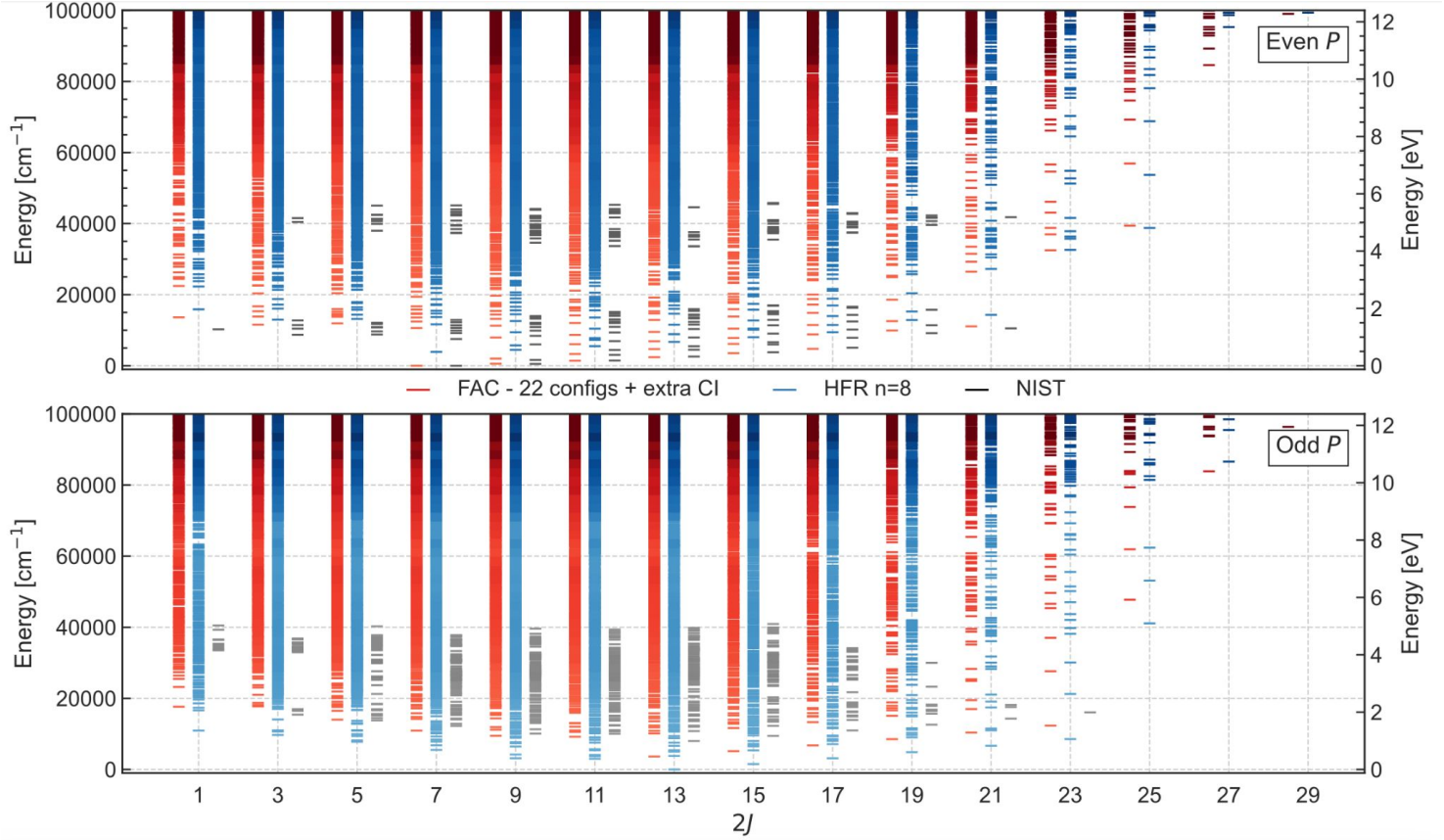
Luis Leitão
Jorge Miguel Sampaio
José Pires Marques
Pedro Amaro

Jérôme Deprince
Michel Godefroid
Stephane Goriely

Helena Carvajal
Patrick Palmeri
Pascal Quinet

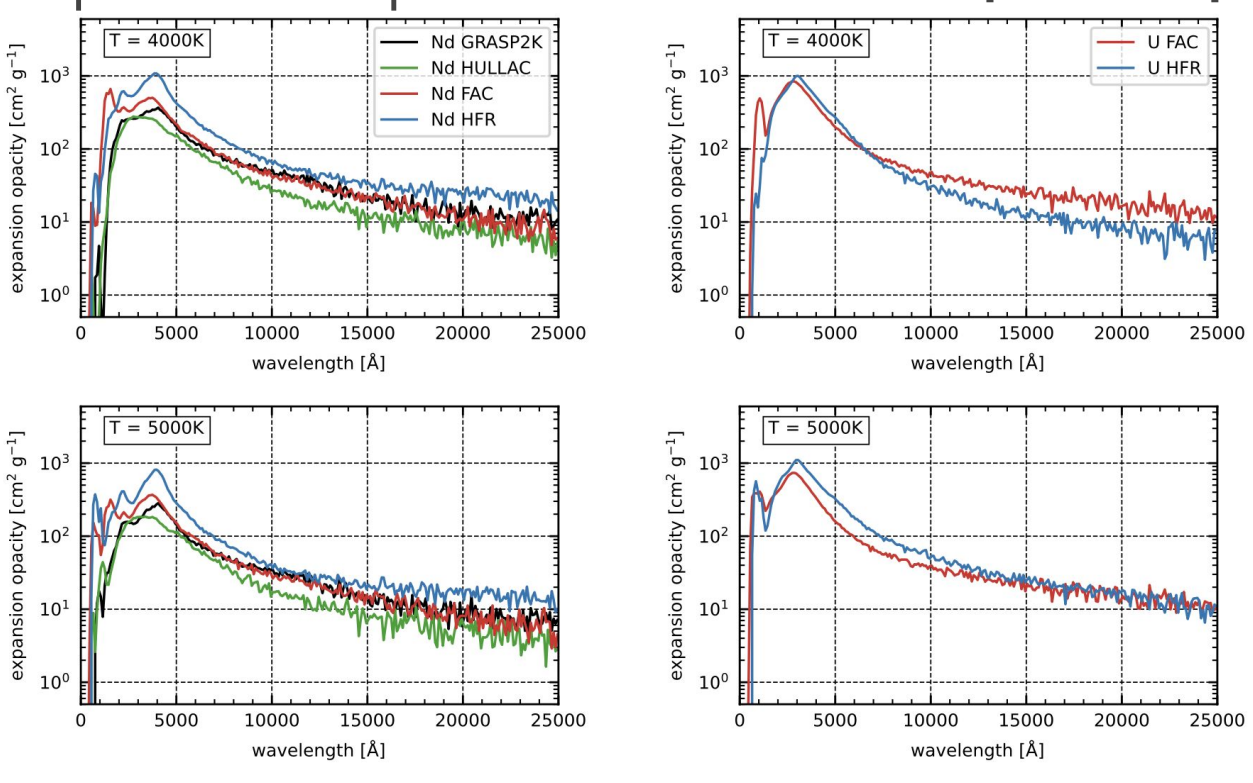
Nd II - Energy Levels

[A.Flörs+2023]



Nd & U - Expansion Opacities

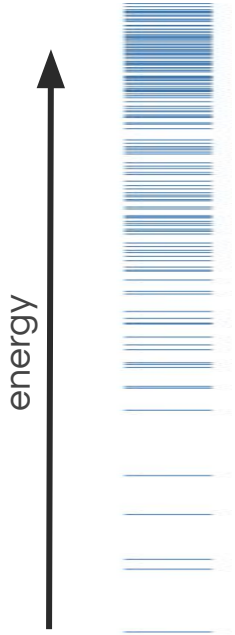
[A.Flörs+2023]

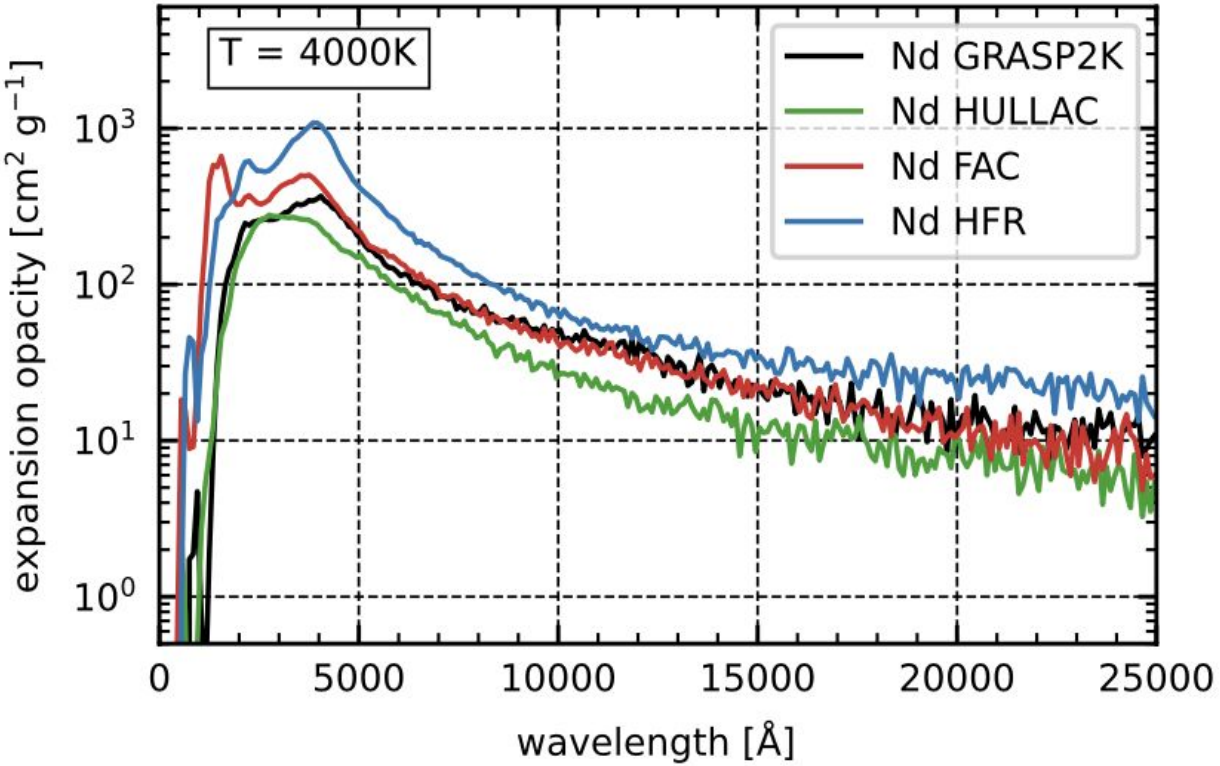


- Good general agreement with calculations using HULLAC & GRASP2K - differences at higher ionization stages (less experimental data available)

Nd & U - Expansion Opacities

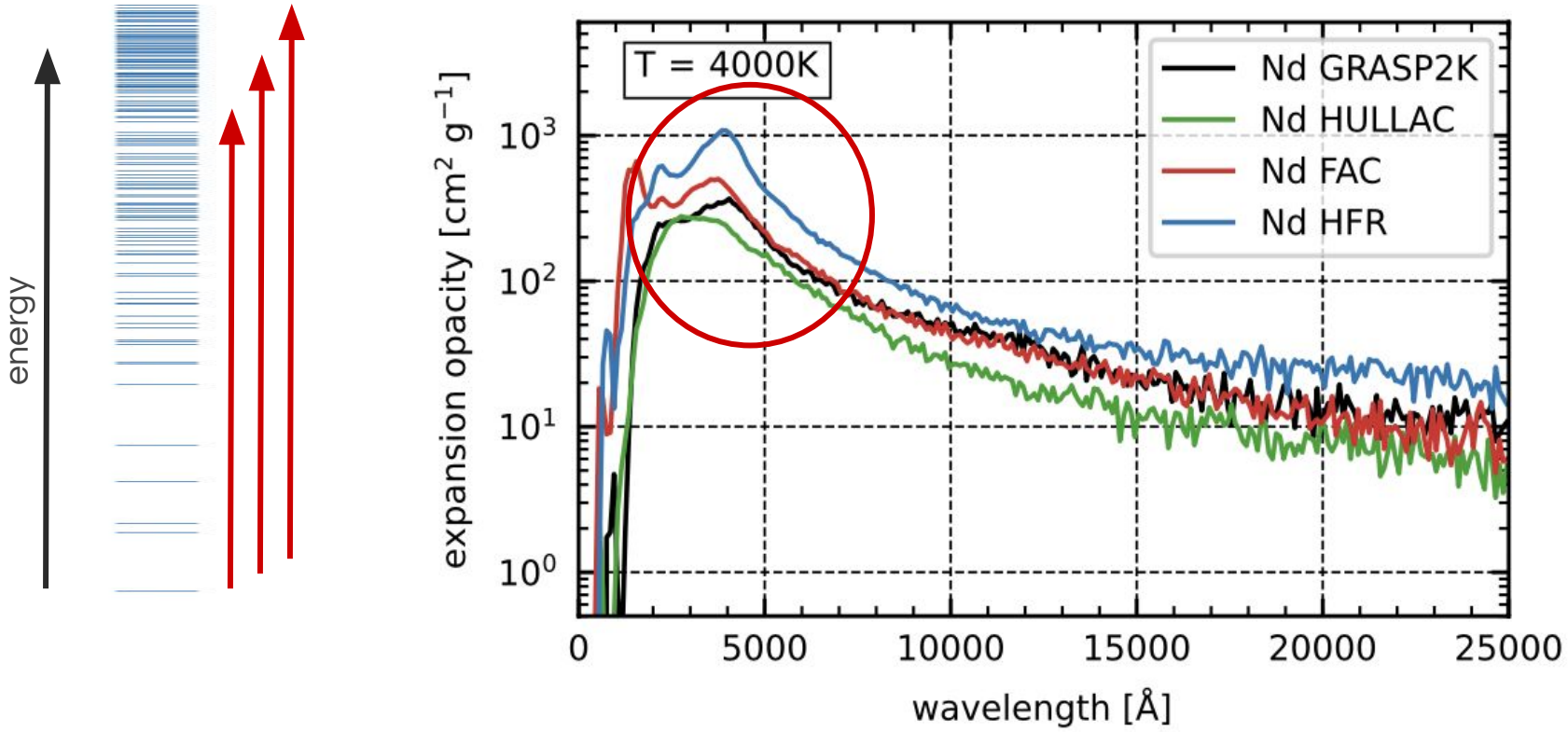
[A.Flörs+2023]





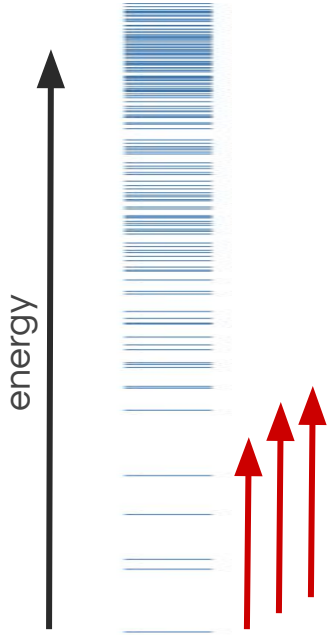
Nd & U - Expansion Opacities

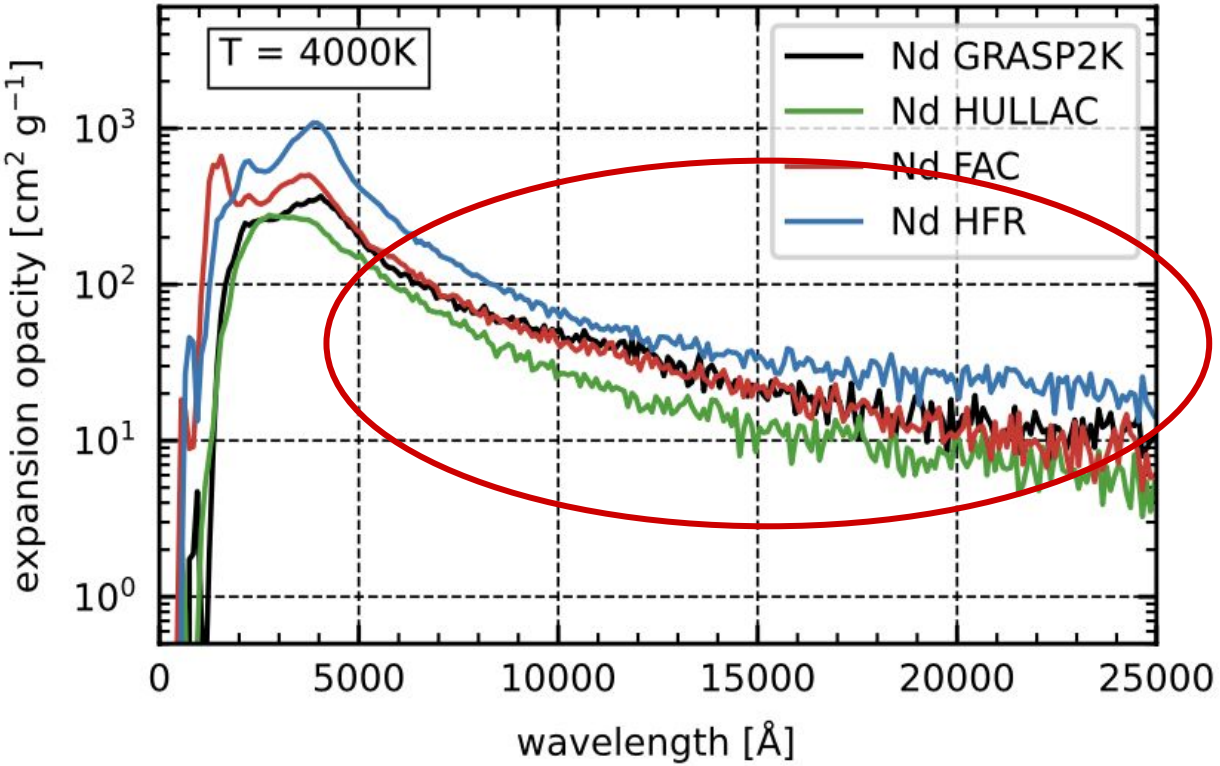
[A.Flörs+2023]



Nd & U - Expansion Opacities

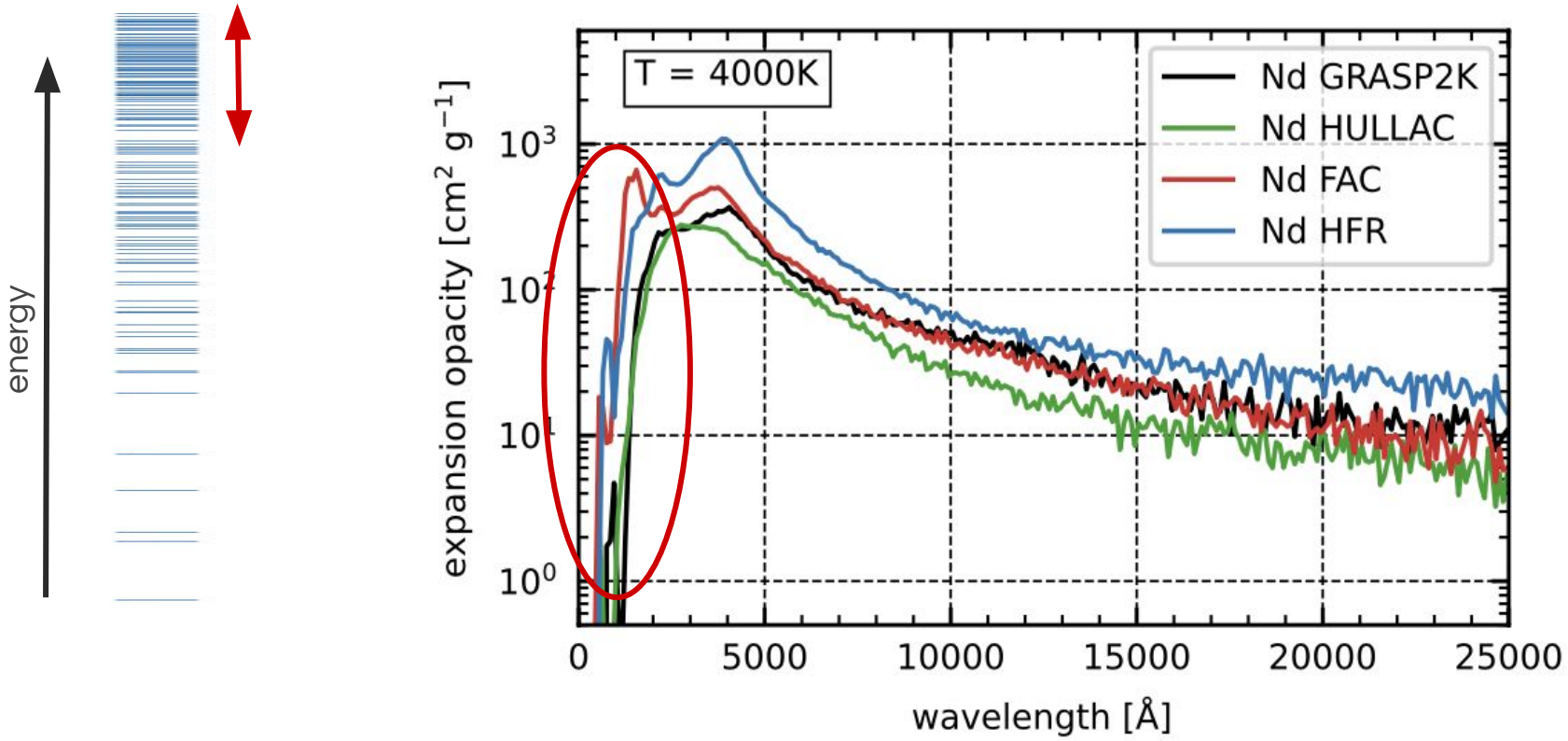
[A.Flörs+2023]





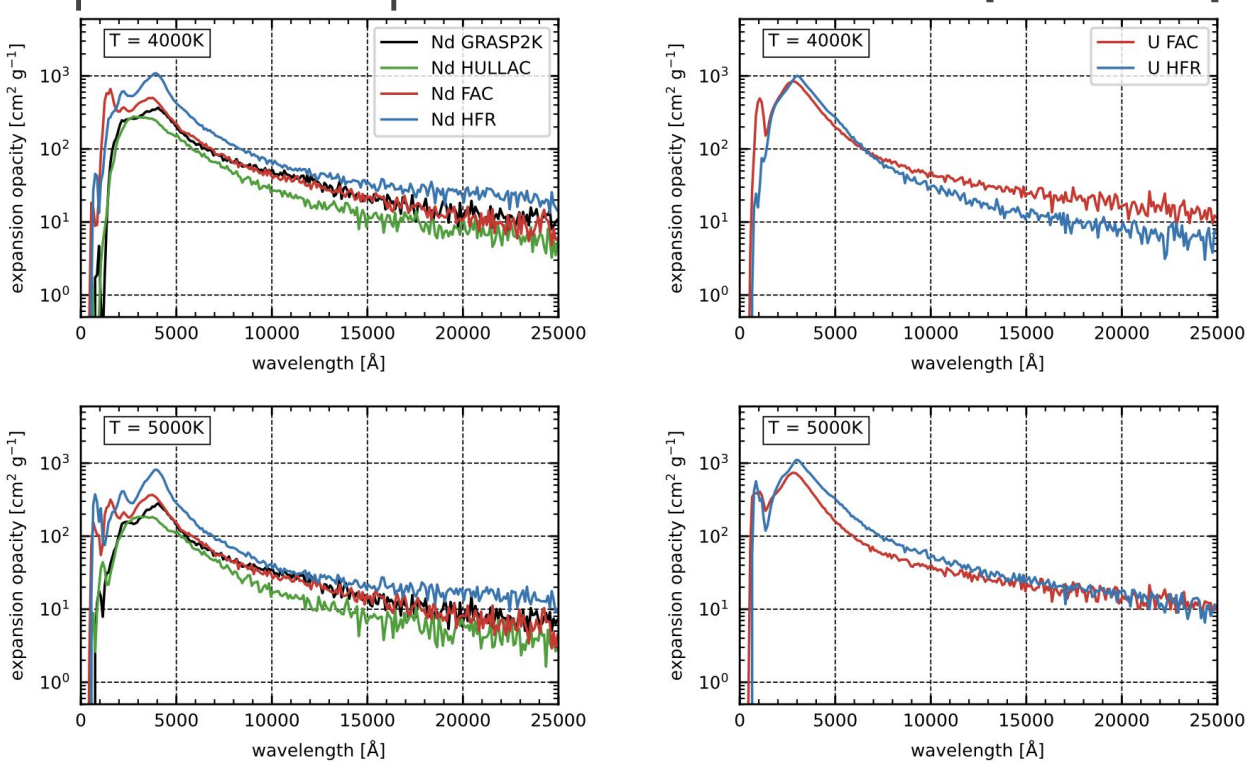
Nd & U - Expansion Opacities

[A.Flörs+2023]



Nd & U - Expansion Opacities

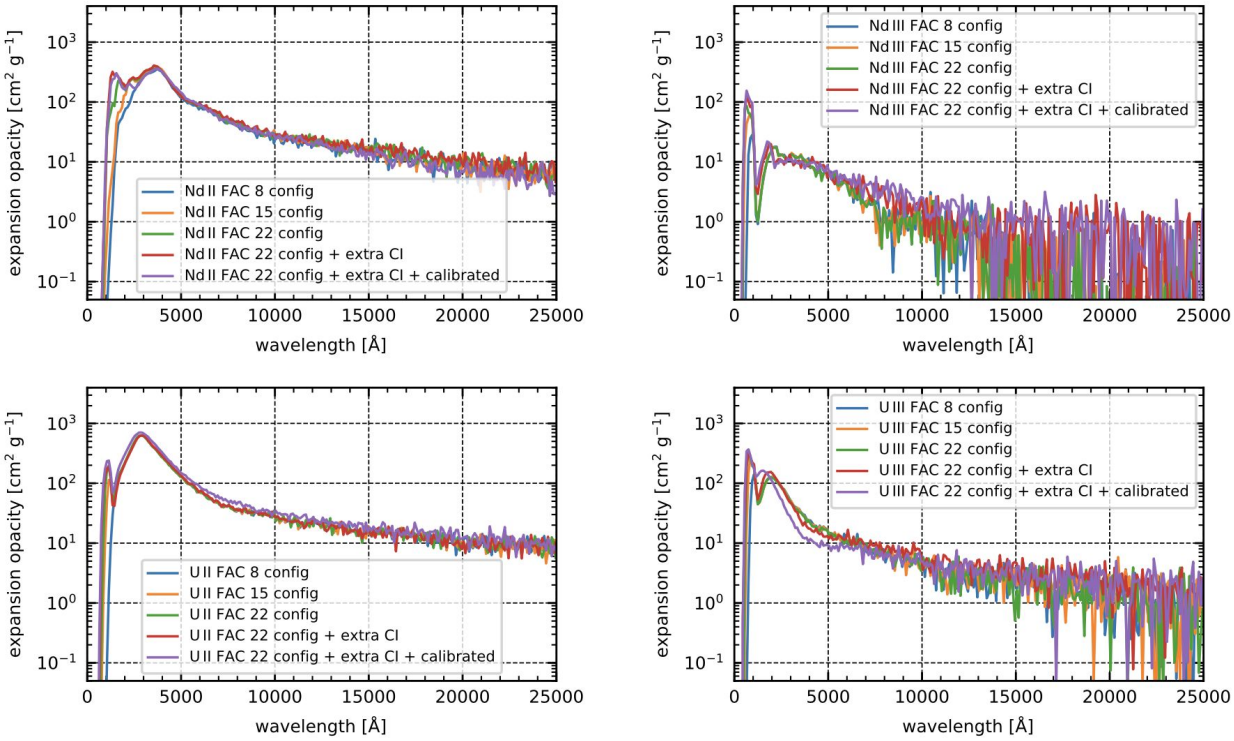
[A.Flörs+2023]



- Good general agreement with calculations using HULLAC & GRASP2K - differences at higher ionization stages (less experimental data available)

Results - Opacities

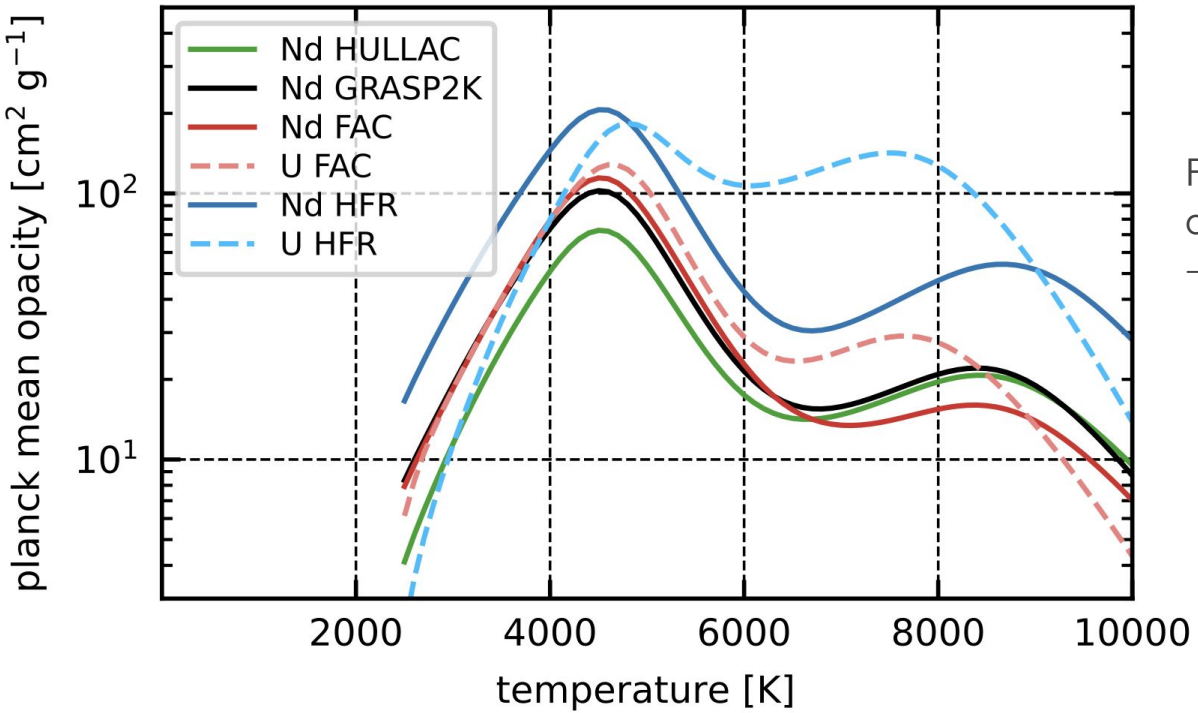
[A.Flörs+2023]



- convergence requires ~20 configurations for typical lanthanide ions

Nd & U - Opacities

[A.Flörs+2023]



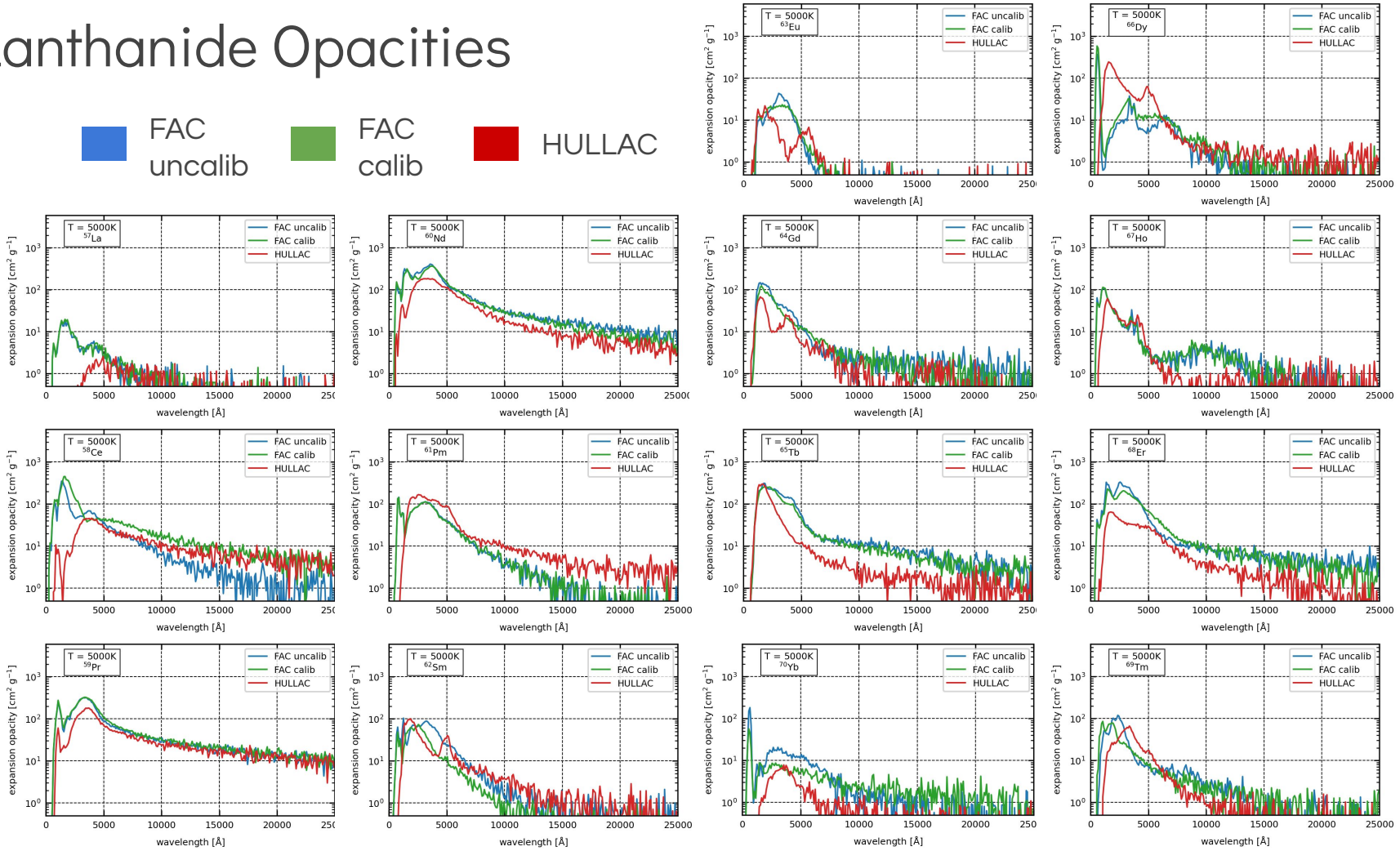
FAC results (levels / opacities) extremely close to GRASP2K
→ use this method on the remaining lanthanides

Lanthanide Opacities

FAC uncalib

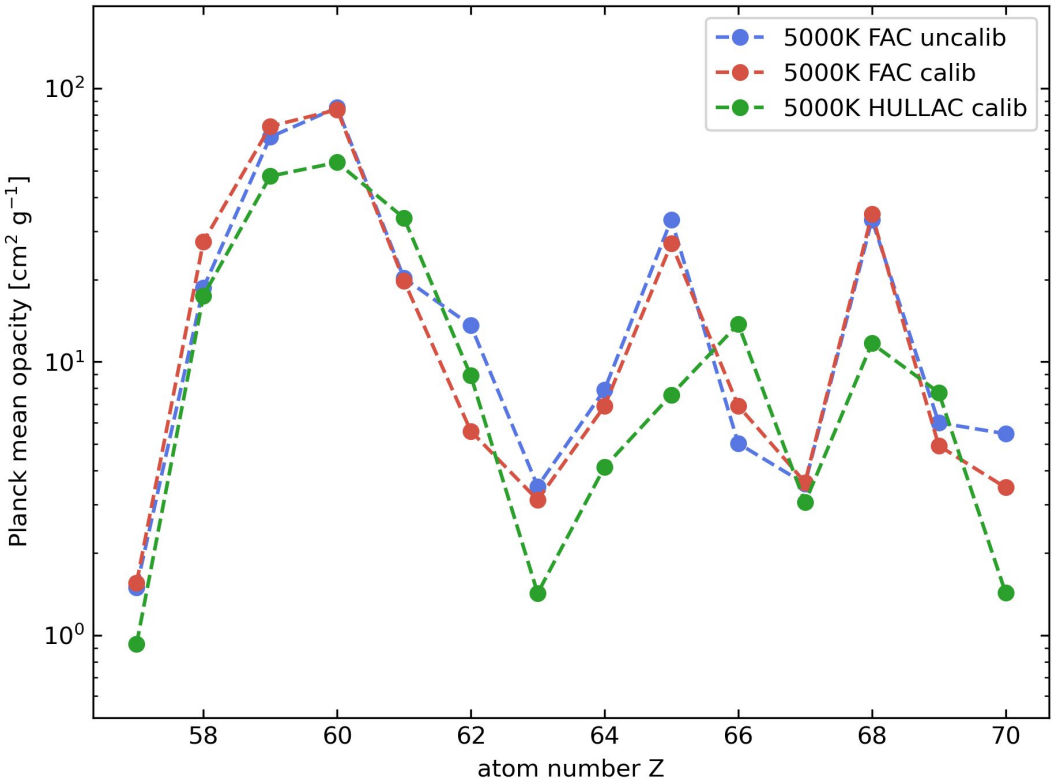
FAC calib

HULLAC

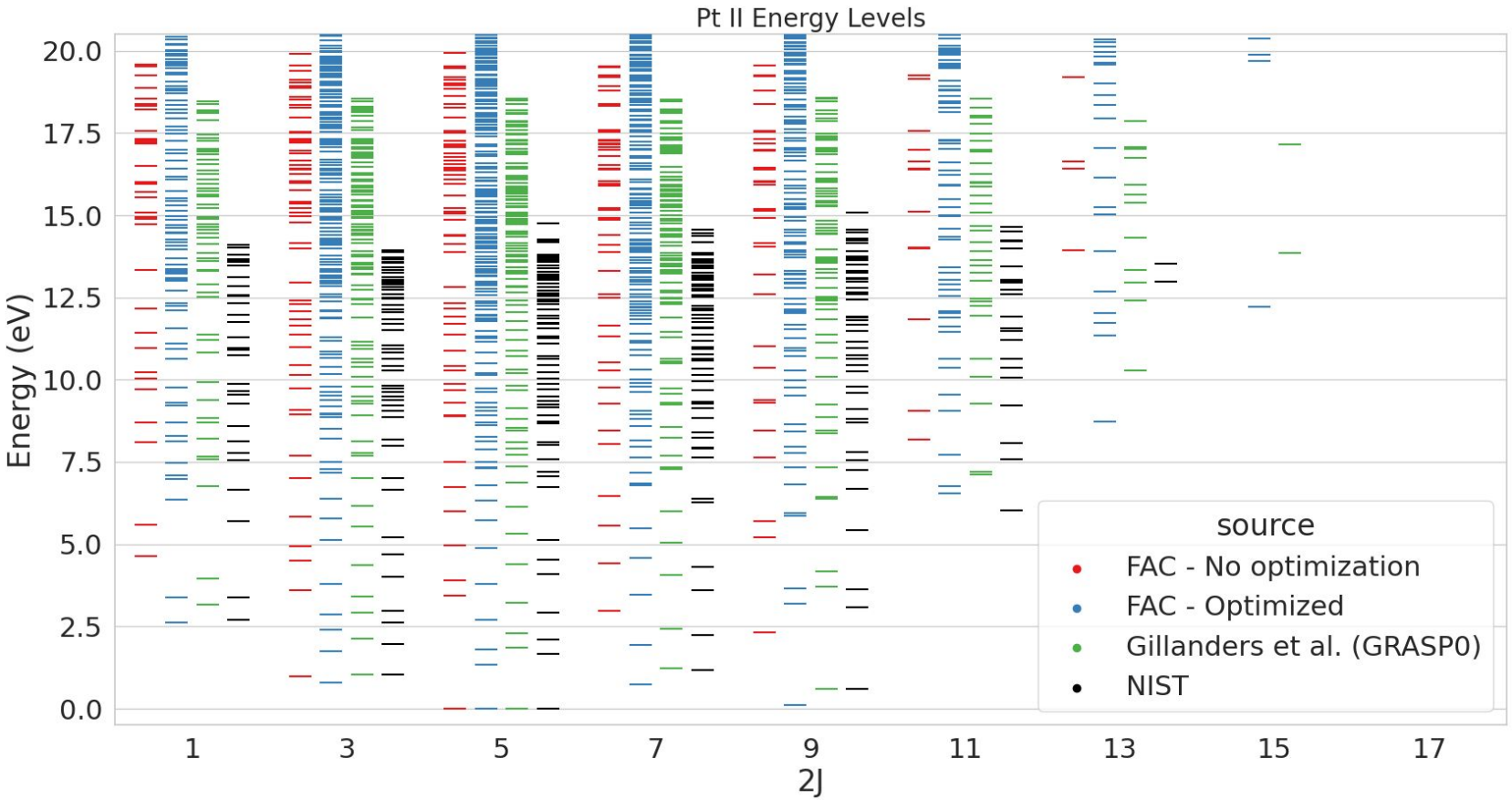


Planck Mean Opacities

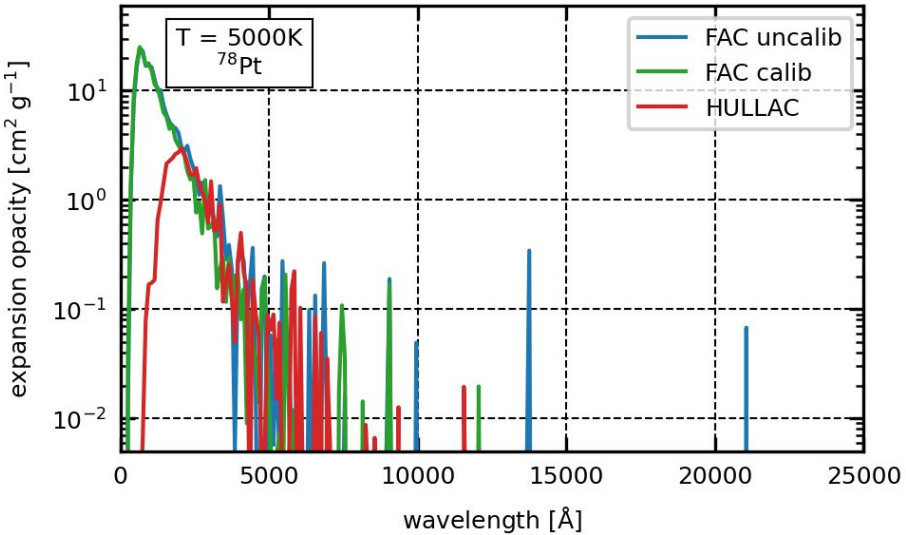
- Similar shape of HULLAC and FAC Planck mean opacities
- FAC calculations yield higher (~factor of 2) opacities than those using HULLAC
- Effect of calibration to experimental data weaker than differences between calculations

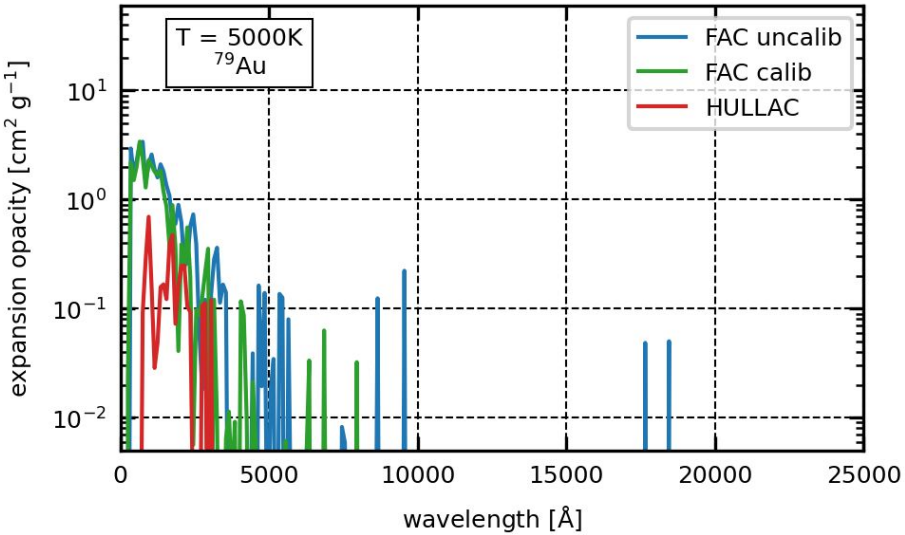


Pt And Au Atomic Data



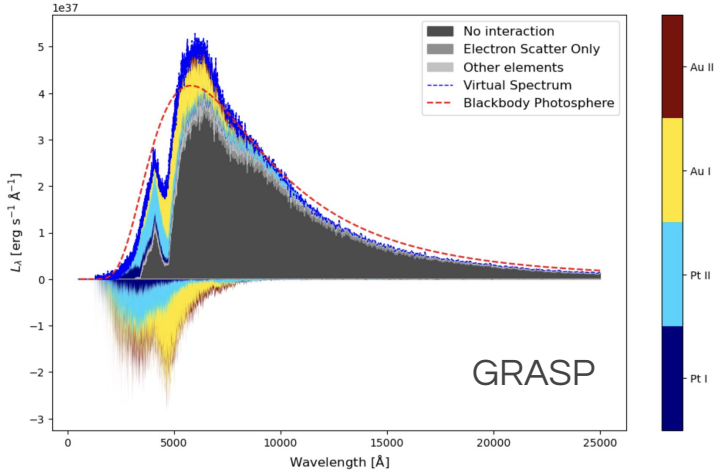
Pt And Au Atomic Data

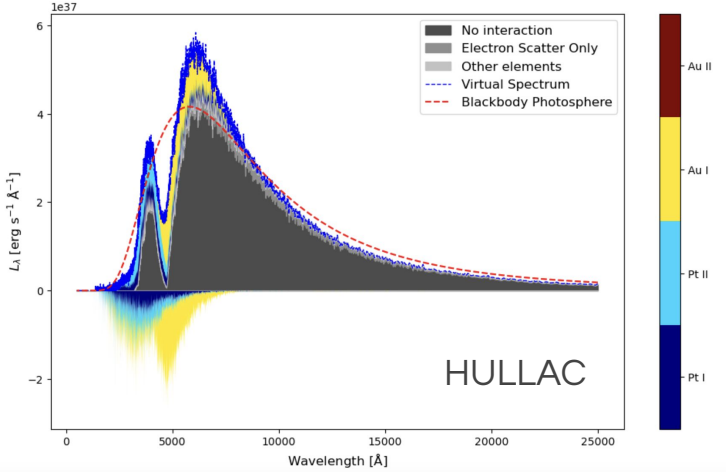


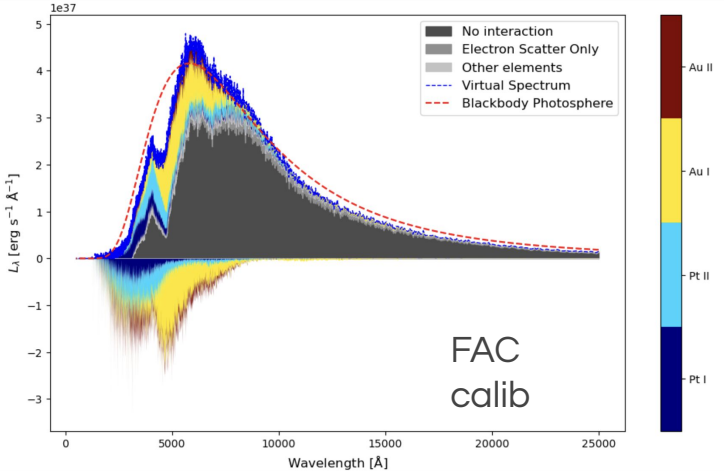


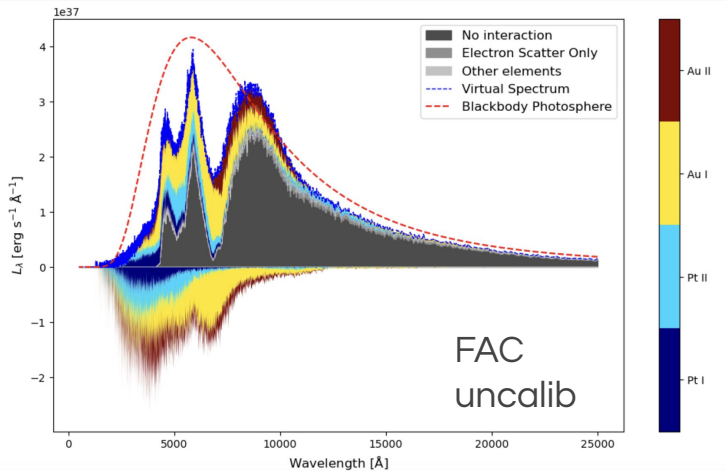
Pt And Au Radiative Transfer

similar setup as in [Gillanders+2021]

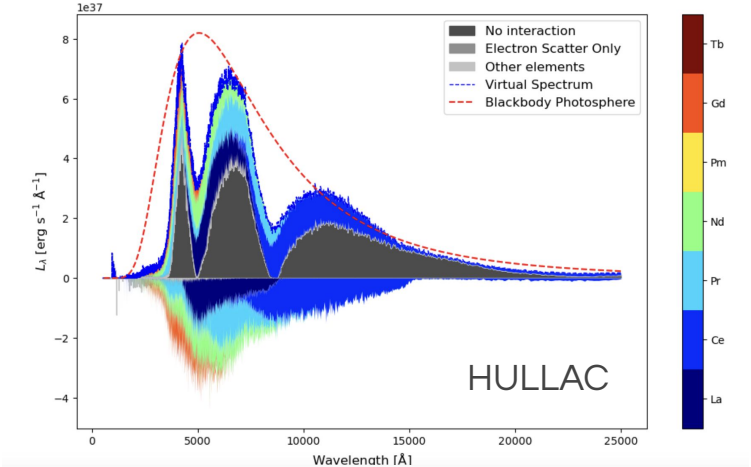


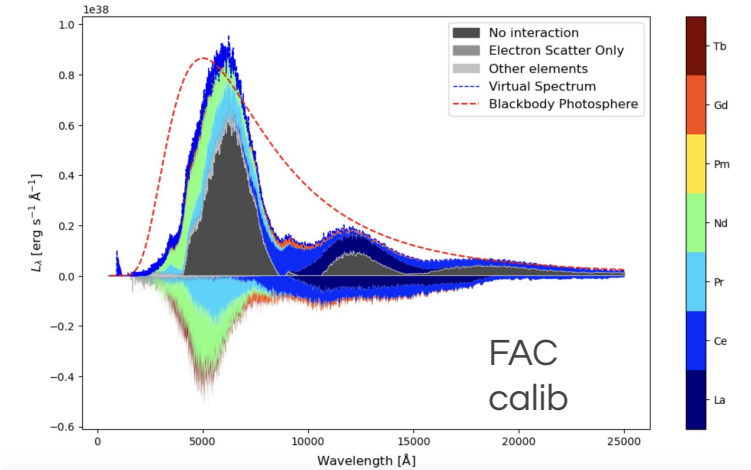


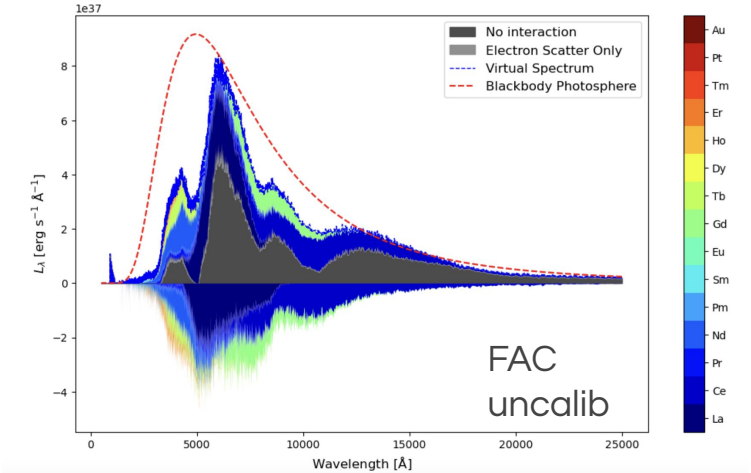




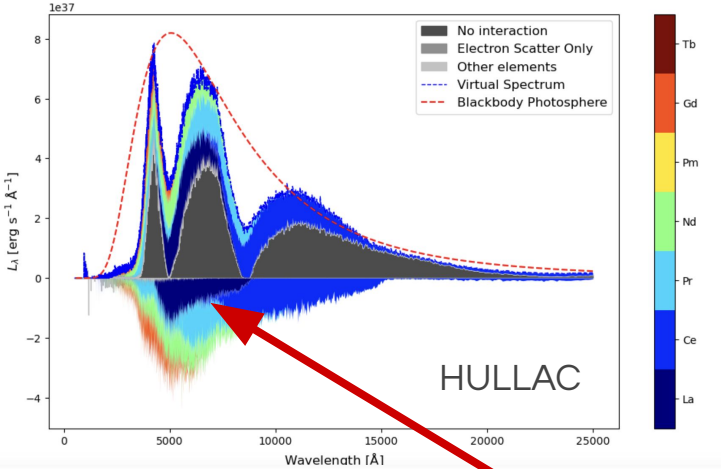
Lanthanide Radiative Transfer

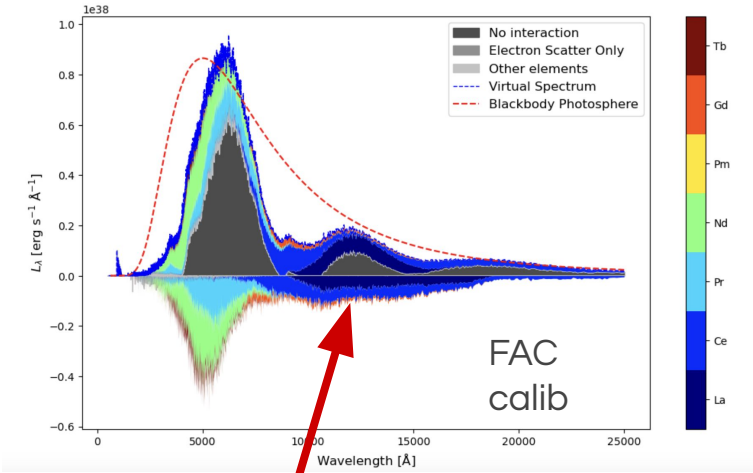


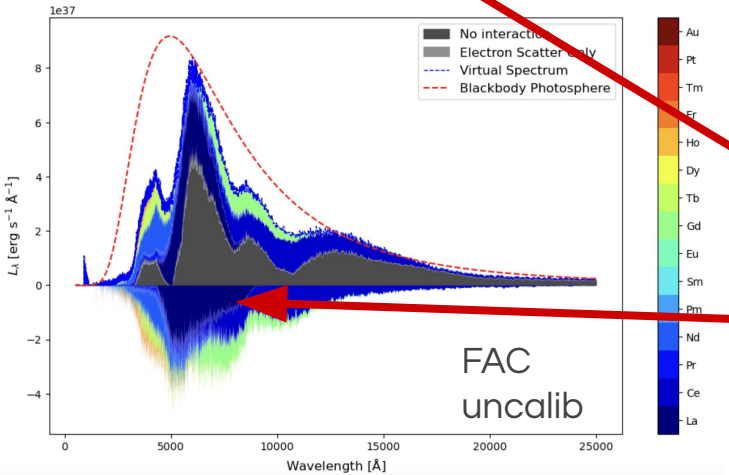




Lanthanide Radiative Transfer







[Domoto+2022]

Table 3. Summary of calibrated lines for La III. We list only lines that adopt theoretical gf-values with $\lambda > 7000$ Å and $\log gf > -3$.

	λ_{vac} [a] (Å)	λ_{air} [b] (Å)	Lower level	E_{lower} [c] (cm^{-1})	Upper level	E_{upper} [d] (cm^{-1})	$\log gf$ [e]
La III	13898.270	13894.471	$5d\ ^2D_{3/2}$	0.00	$4f\ ^2F^o_{5/2}$	7195.14	−0.749
	14100.037	14096.183	$5d\ ^2D_{5/2}$	1603.23	$4f\ ^2F^o_{7/2}$	8695.41	−0.587
	17882.977	17878.094	$5d\ ^2D_{5/2}$	1603.23	$4f\ ^2F^o_{5/2}$	7195.14	−1.938

Conclusions

- Optimisation of the mean local potential leads to very good agreement with NIST data - similar to GRASP calculations but only at a fraction of the computational cost

- Number of included configurations is not too important
  → quick convergence of level energies and opacities
  → additional configurations lead to increased opacity close to the ionisation edge (<1500Å)

- General agreement on Planck mean opacities to ±50% between codes
  → calibration to experimental data has only minor effect on grey opacity

- Radiative transfer models are sensitive to transition wavelengths
  → uncalibrated datasets easily yield features at wrong wavelengths
  → radiative transfer models using our optimised + calibrated atomic data are in extremely good agreement with GRASP (Pt + Au) and they reproduce experimentally measured La III transitions

- We will make our data publicly available after publication (Zenodo)