Atomic Data for Elemental Kilonovae Identification

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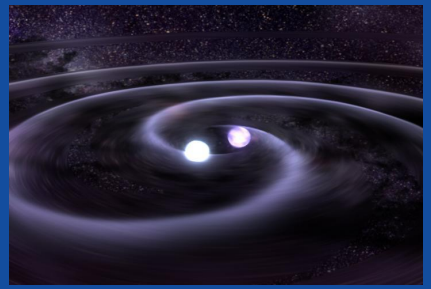
July 15th, 2026

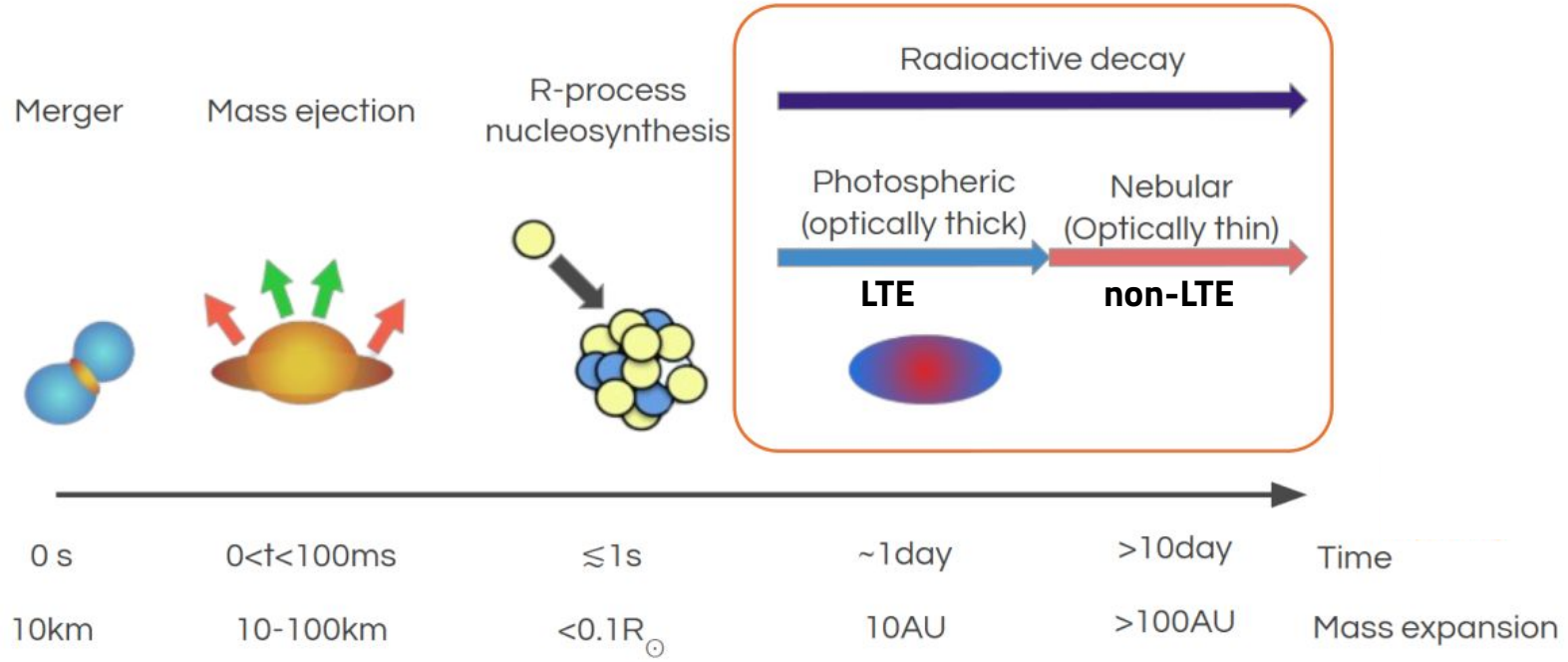
Supervisors:
Profs. Drs. José Pires Marques & Jorge Sampaio



Introduction

Astrophysical site, Atomic Data needs and Atomic Codes

Neutron Star Mergers
Kilonovae



Adapted from K. Hotokezaka


Atomic Data needs:
and our team

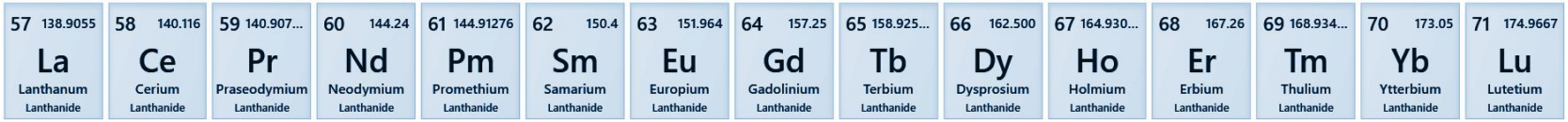
Energy levels


Radiative rates
(E1 transitions)




A.K. Pradhan and S.N. Nahar. **Atomic Astrophysics and Spectroscopy**. Cambridge University Press, 2011.

Atomic Codes:
which ones to use?



➔ **Open *f*-shells**: high amount of levels and transitions needed;

➔ Computationally fast and efficient;

➔ Able to compute a wide variety of atomic processes.

★ **The Flexible Atomic Code**

★ AUTOSTRUCTURE

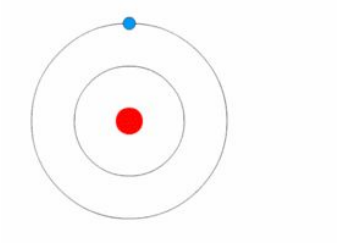
The FLEXIBLE ATOMIC CODE and AUTOSTRUCTURE

A quick overview on these atomic codes

FLEXIBLE ATOMIC CODE	AUTOSTRUCTURE
(**Relativistic**) Dirac's formalism in the Hamiltonian	**Non-relativistic** Hamiltonian with relativistic interactions as corrections
Central potential: Dirac-Fock-Slater	**Central potential**: Thomas-Fermi-Dirac-Amaldi
Configuration interaction to describe the ASF	**Configuration interaction** to describe the ASF
Distorted wave method for interactions with the continuum	**Distorted Wave** method for interactions with the continuum

PART I
Atomic Structure for Lanthanides and Actinides

Atomic Structure Calculations:
what am I calculating?

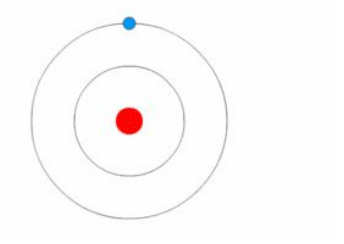


Wavefunctions:

➔ building wavefunctions for atomic systems

Atomic State Function	Configuration State Functions	Electron Wavefunctions
Linear combination of CSFs, weighted by mixing coefficients	[Xe] $4f^{12}\ 6s^{1}$ Antissymetric combinations of e⁻s wavefunctions	$\lvert n\ l\ m_l\ s\ m_s \rangle$ or $\lvert n\ l\ s\ j\ m_j \rangle$

Atomic Structure Calculations: what am I calculating?



Levels:

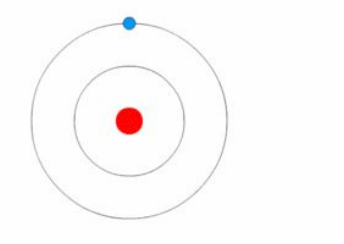
➔ Term, parity and 2*J*: level identification

➔ Ground-state and excited states

Apply the hamiltonian operator to the ASF previously built.

Use self-consistent methods (Hartree-Fock).

Atomic Structure Calculations: what am I calculating?



Transitions:

➔ Transition's wavelenght	wavel. of the emmited/absorbed photon
➔ Transition's rate	how probable is the transition
➔ Oscillator strenght	how strong is the transition

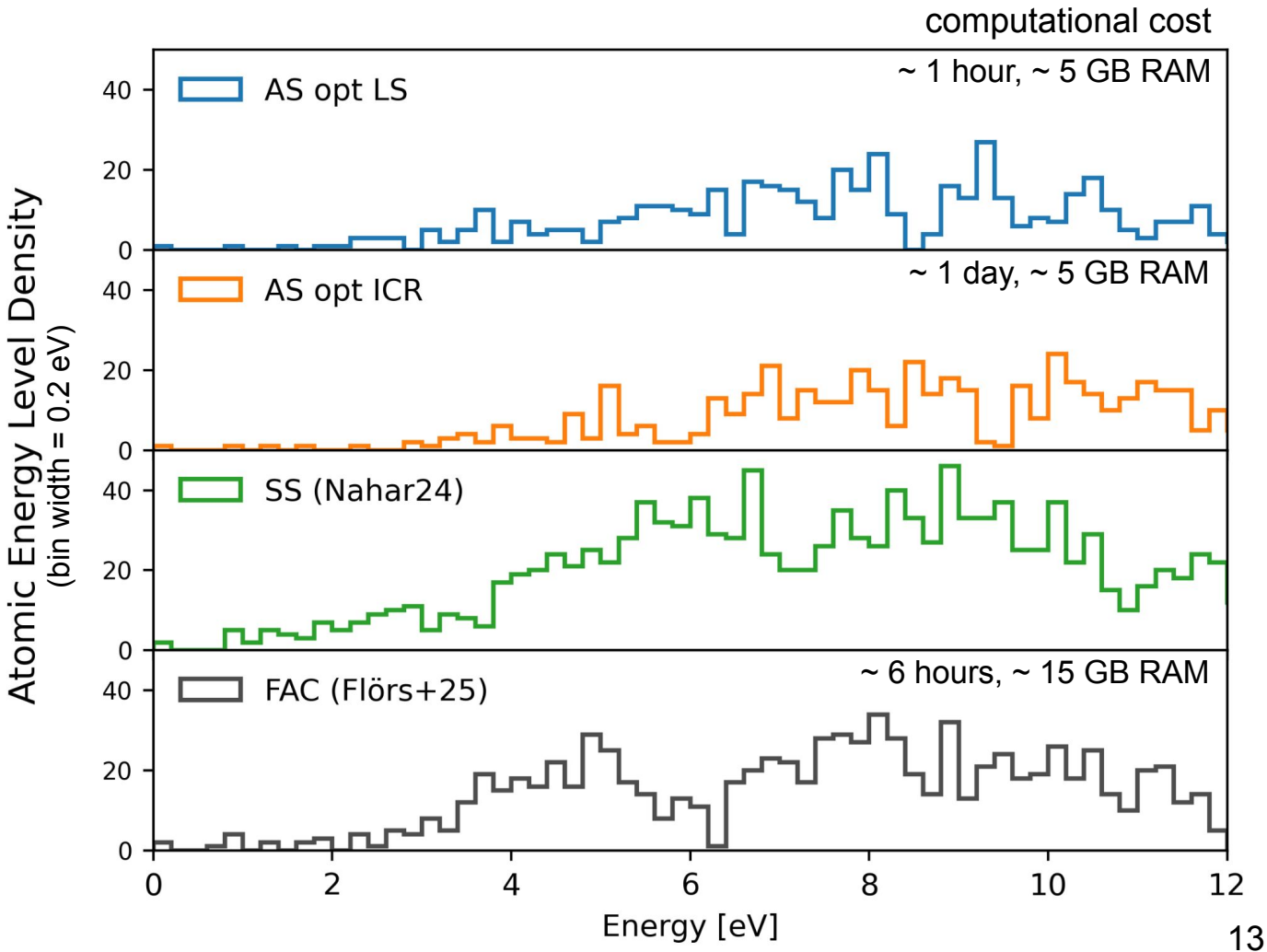
Results

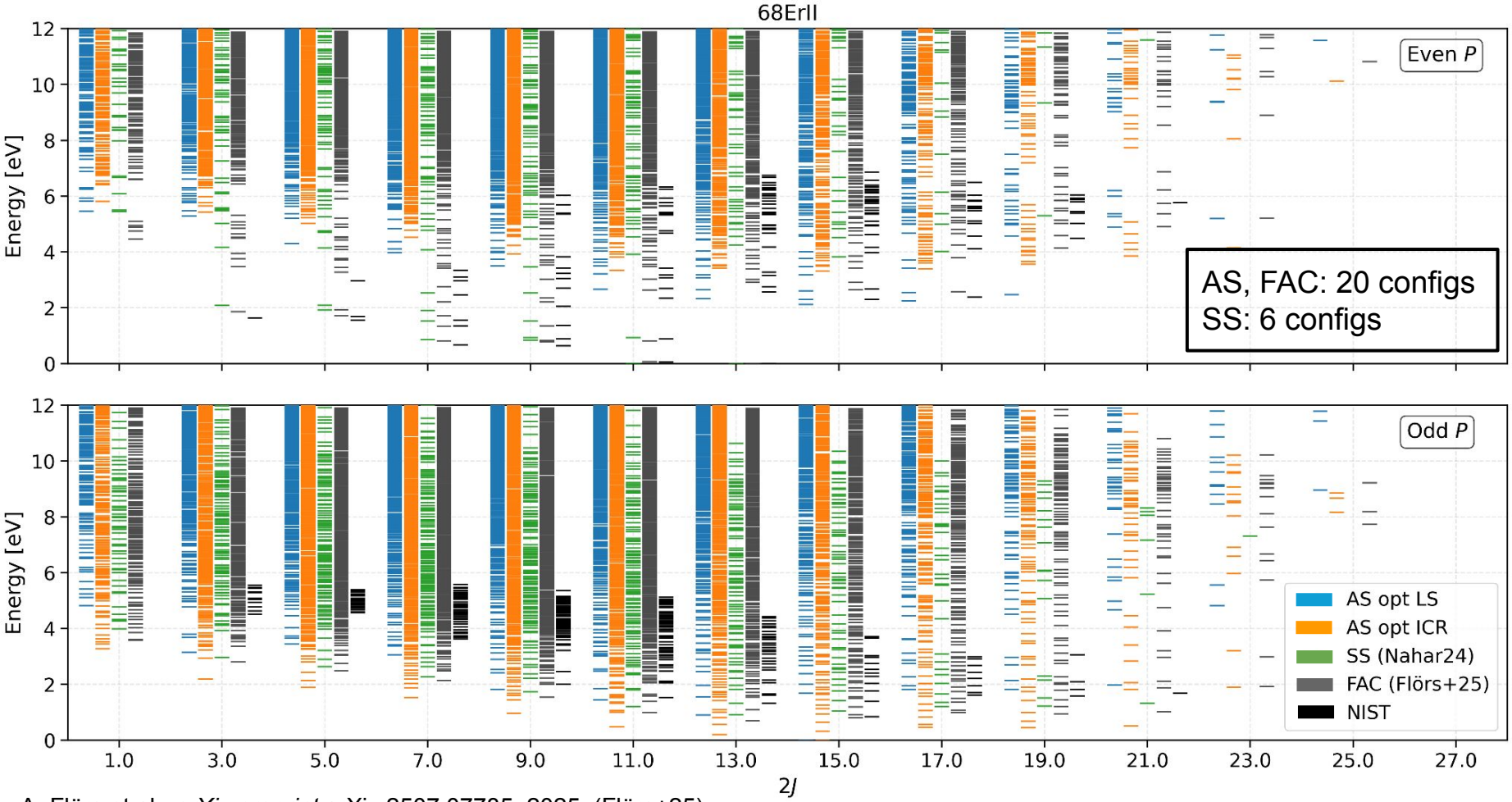
All lanthanides, focusing on the Er II case

Er II
(Z=68)

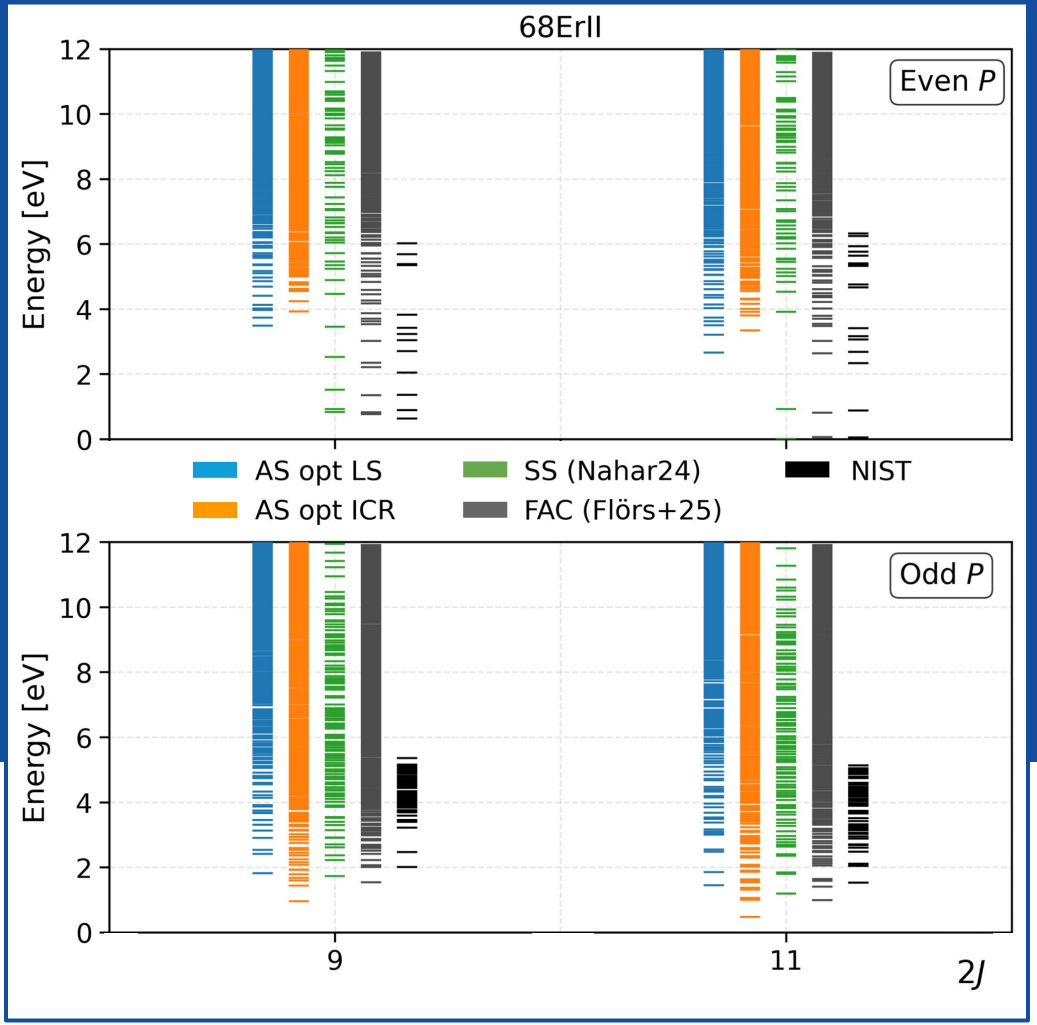
6 configurations:

$4f^{12}\,6s^{1}$
$4f^{12}\,5d^{1}$
$4f^{12}\,6p^{1}$
$4f^{11}\,6s^{1}\,5d^{1}$
$4f^{11}\,6s^{1}\,6p^{1}$
$4f^{11}\,6s^{2}$





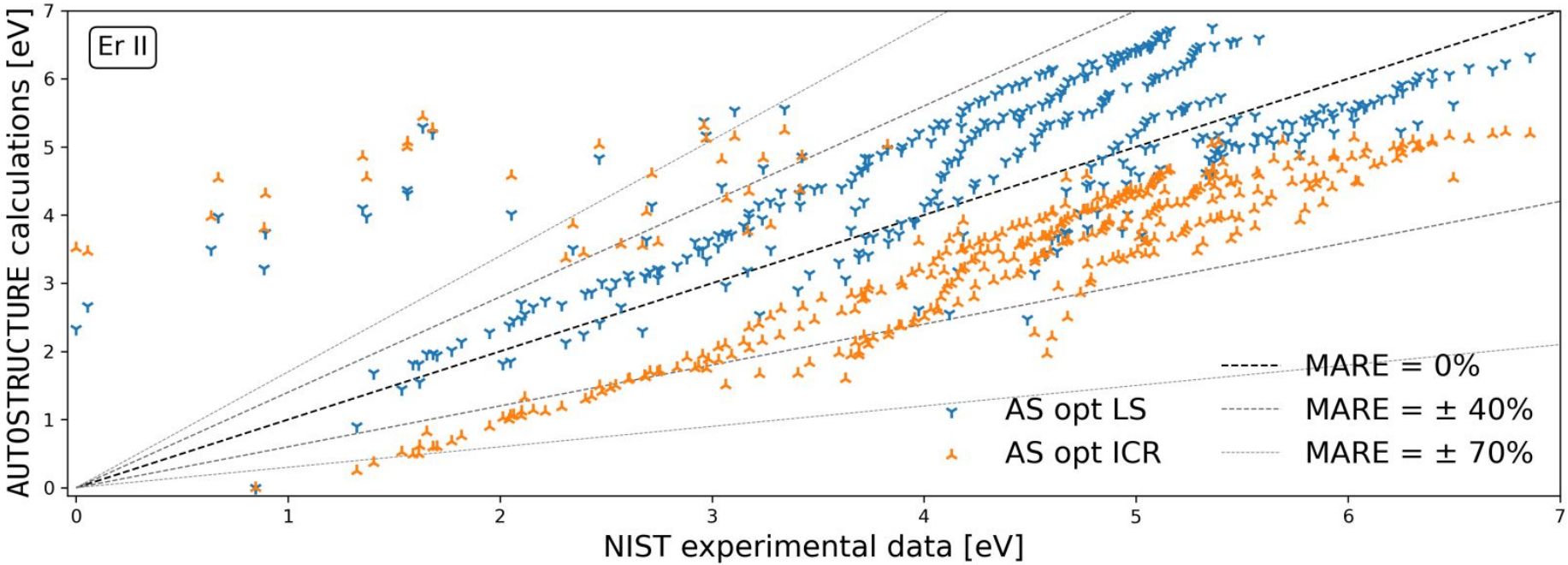
A. Flörs et al., *arXiv preprint* arXiv:2507.07785. 2025. (Flörs+25)
Sultana N. Nahar, *Atoms* 12.4: 24. 2024. (Nahar24)



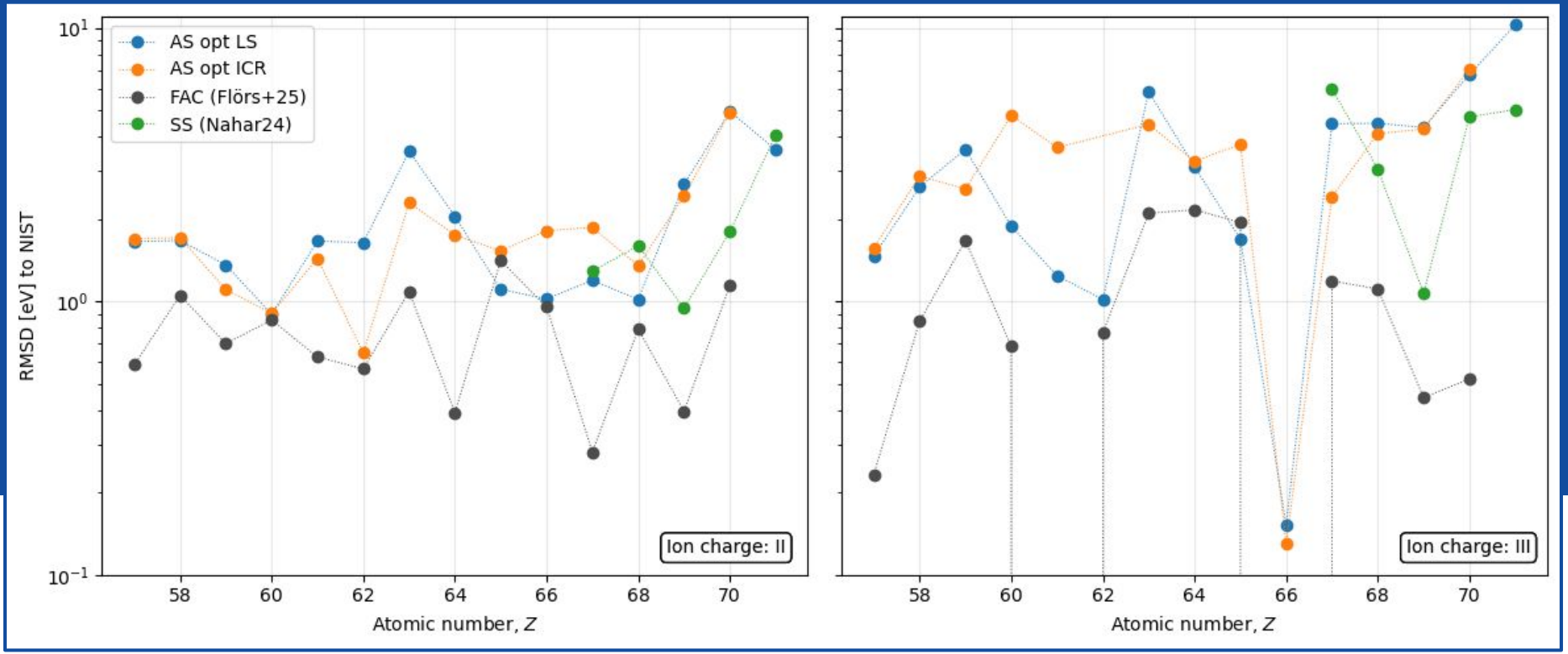
➔ Implementation of a MARE to quantify how similar calculations are to NIST.

Separation by P and $2J$.
Matching by $\min(\Delta E)$.

Energy agreement



Lanthanides



A. Flörs et al., *arXiv preprint* arXiv:2507.07785. 2025. (Flörs+25)
Sultana N. Nahar, *Atoms* 12.4: 24. 2024. (Nahar24)

TRANSITIONS

TO BE ANALISED yet…

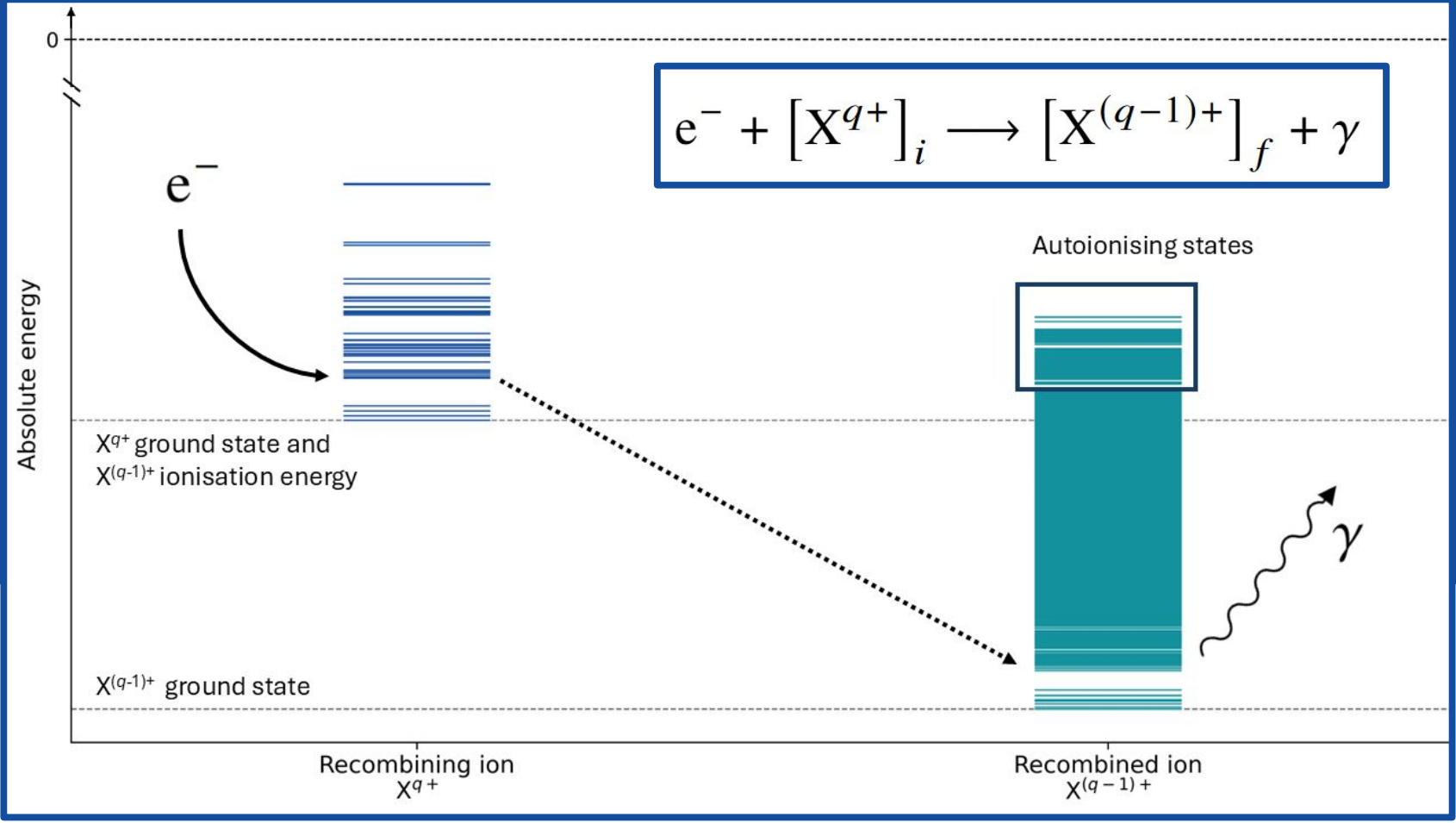
Conclusions (Part I)

➔ Complete set of **atomic energy levels** (AELs) **and E1 transitions** for **all singly and doubly ionised lanthanides** using **AS** for comparison with **FAC**.

- ➔ FAC provides AELs closer to experimental values, but relies on optimization against experimental data.
- ➔ AS can be optimized without experimental input, although with larger deviations from experiments (e.g., failing to identify ground states).
- ➔ **Now**, in the absence of experimental data, AS calculations can still be used, with a known average deviation from experimental values.

PART II
Radiative Recombination Rate Coefficients for Lanthanides

Radiative Recombination



Radiative Recombination:

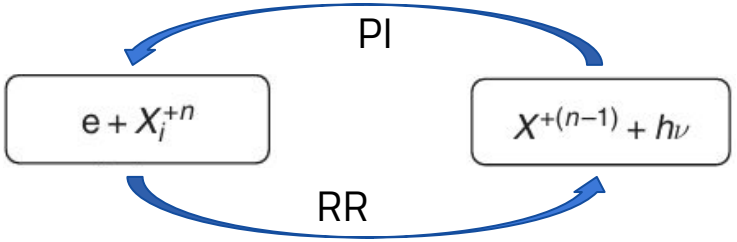
RR and DR as separate, independent processes

Both direct radiative recombination (RR) and dielectronic recombination are (DR) key for Collisional-Radiative Modelling (CRM).

The distorted wave (DW) approximation considers both processes independently, under the unified treatment of RR and DR methodology.

S.N. Nahar and A.K. Pradhan. *Physical Review A*, 49(3):1816–1835. 1994.
S.N. Nahar and A.K. Pradhan. *Radiation Physics and Chemistry*, 70(1):323–344. 2004.
A.K. Pradhan and S.N. Nahar. **Atomic Astrophysics and Spectroscopy**. Cambridge University Press, 2011.

Radiative Recombination: calculated by **atomic codes**



Quantity of interest for CRM: **RR rate coefficient**

$$\alpha_{\mathrm{RR,lev}}(T) \equiv \langle v_{\mathrm{e}} \sigma_{\mathrm{RR,lev}}(v_{\mathrm{e}}) \rangle = \int_0^\infty v_{\mathrm{e}} f_{\mathrm{MB}}(v_{\mathrm{e}}, T) \sigma_{\mathrm{RR,lev}}(v_{\mathrm{e}})\, dv_{\mathrm{e}}$$

Depends on the RR cross-sections
→ obtained via detailed balance:

$$\sigma_{\mathrm{PI}} \frac{g_f}{{p_{\mathrm{e}}}^2} = \sigma_{\mathrm{RR}} \frac{g_i}{{p_\gamma}^2}$$

M F Gu. *Canadian Journal of Physics*, 86(5):675–689, 2008.
Anil K. Pradhan and Sultana N. Nahar. **Atomic Astrophysics and Spectroscopy**. Cambridge University Press, 2011.

Radiative Recombination: choice of configurations

Explicit treatment of low-nl states:

Recombining configuration $[\mathrm{Xe}]\ 4f^4$

$$\textbf{Recombined configuration}\ [\mathrm{Xe}]\ 4f^4 + (nlj) = [\mathrm{Xe}] \begin{cases} 4f^5 \\ 4f^4\ 5d^1,\ 4f^4\ 5f^1,\ 4f^4\ 5g^1 \\ 4f^4\ 6s^1,\ 4f^4\ 6p^1,\ 4f^4\ 6d^1,\ \ldots \\ 4f^4\ 7s^1,\ \ldots \\ \ldots \end{cases}$$

$n_{\max}$=10

$l_{\max}$=5

,

For high-nl states other approximations were used.

M.B. Trzhaskovskaya, V.K.; Nikulin, Y.N. Tsarev. *Atomic Data and Nuclear Data Tables*, 139: 101389. 2021

Radiative Recombination:
The Axelrod approximation (1980)

The Axelrod approximation is often used:

$$\alpha_{\mathrm{RR}}(T) = \alpha_0 \left(\frac{T}{1 \times 10^4 \ \mathrm{K}} \right)^{-3/4} q^2$$

What is the best α_0 value to use?
Should we use the same α_0 for all lanthanides?

T.S. Axelrod. University of California, Santa Cruz, 1980

Results

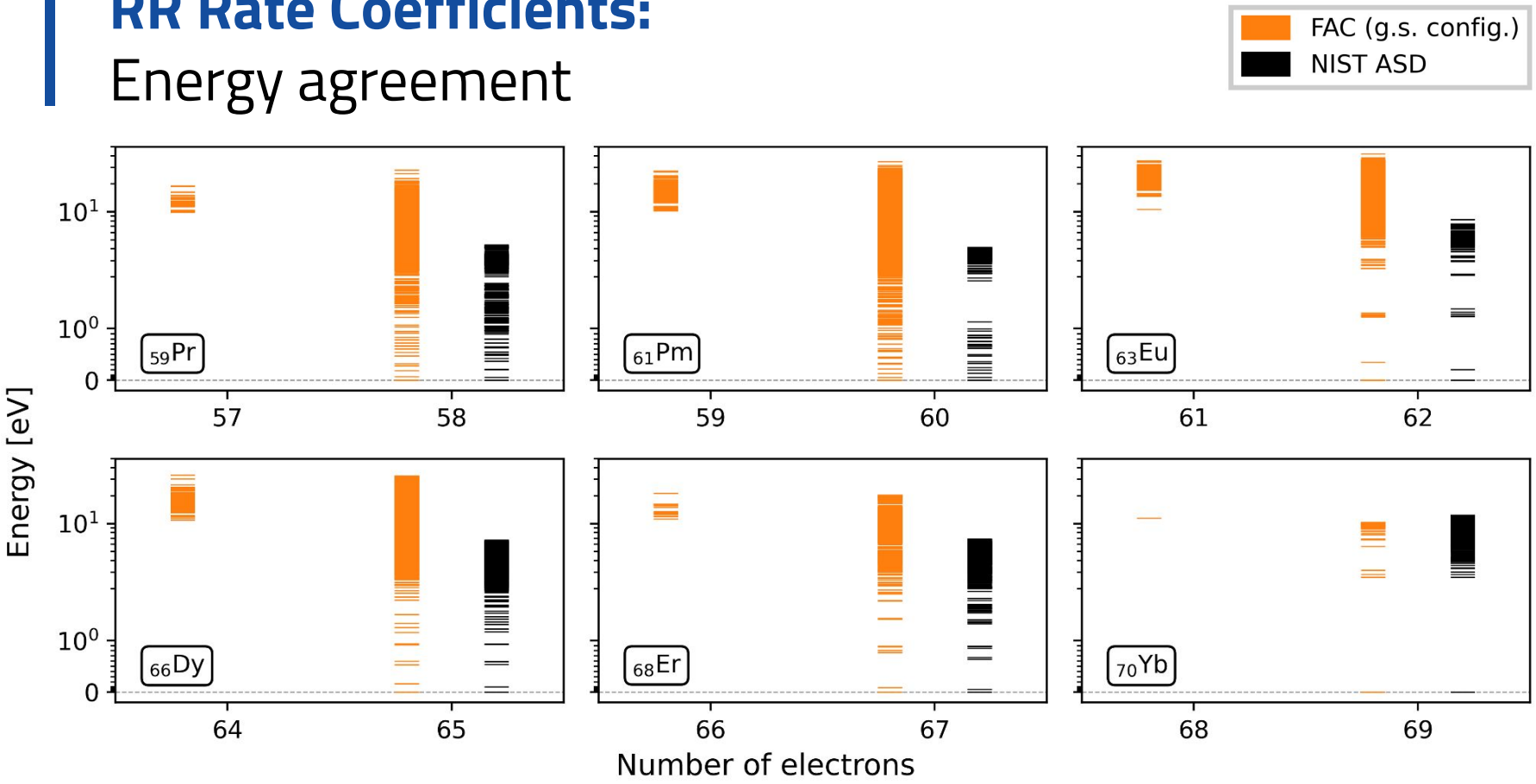
Radiative recombination (RR) rate coefficients

Ground state levels

NIST ASD =
= FAC = AS

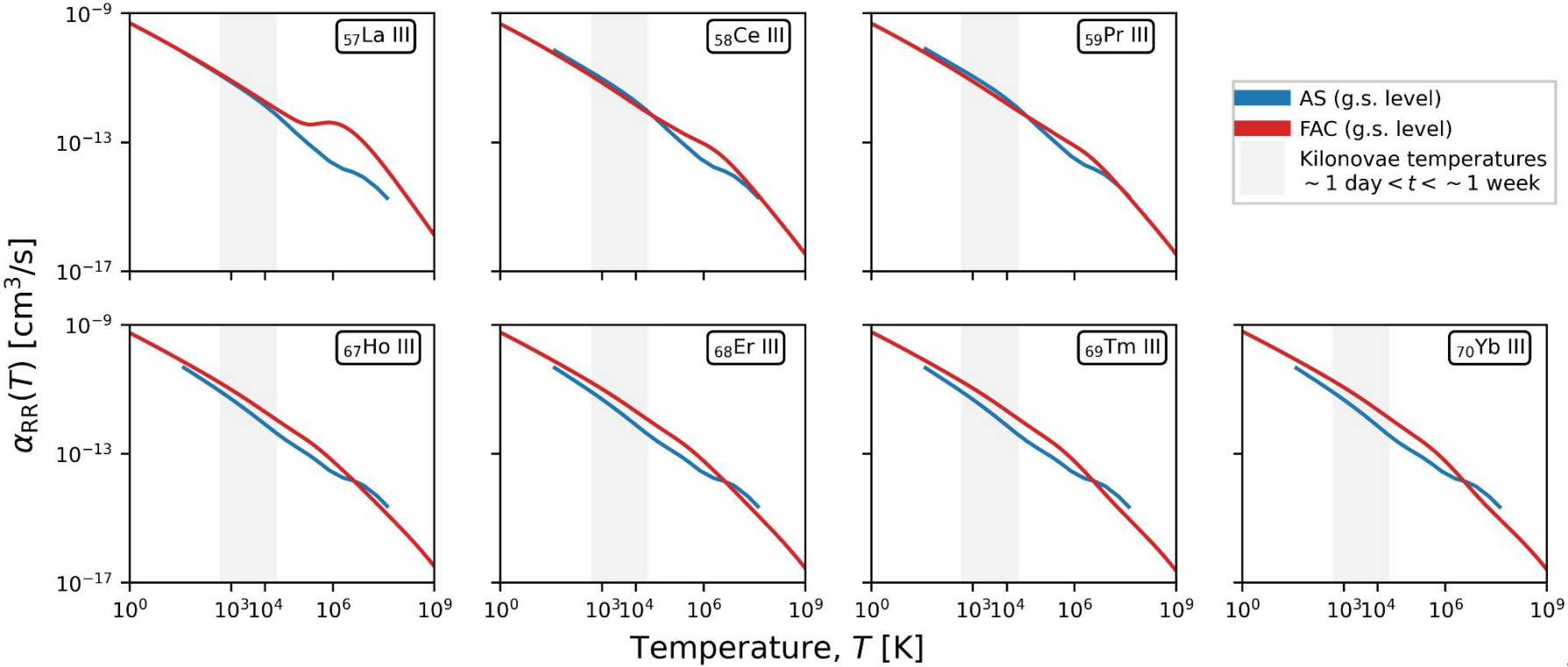
Ion	Configuration	LSJ Term	Parity
$_{57}$La III	[Xe] $5d^1$	$^2D_{3/2}$	even
$_{58}$Ce III	[Xe] $4f^2$	$^3H_4$	even
$_{59}$Pr III	[Xe] $4f^3$	$^4I_{9/2}$	odd
$_{60}$Nd III	[Xe] $4f^4$	$^5I_4$	even
$_{61}$Pm III	[Xe] $4f^5$	$^6H_{5/2}$	odd
$_{62}$Sm III	[Xe] $4f^6$	$^7F_0$	even
$_{63}$Eu III	[Xe] $4f^7$	$^8S_{7/2}$	odd
$_{64}$Gd III *	[Xe] $4f^7\,5d^1$	$^9D_2$	odd
$_{65}$Tb III	[Xe] $4f^9$	$^6H_{15/2}$	odd
$_{66}$Dy III	[Xe] $4f^{10}$	$^5I_8$	even
$_{67}$Ho III	[Xe] $4f^{11}$	$^4I_{15/2}$	odd
$_{68}$Er III	[Xe] $4f^{12}$	$^3H_6$	even
$_{69}$Tm III	[Xe] $4f^{13}$	$^2F_{7/2}$	odd
$_{70}$Yb III	[Xe] $4f^{14}$	$^1S_0$	even

RR Rate Coefficients:
Energy agreement



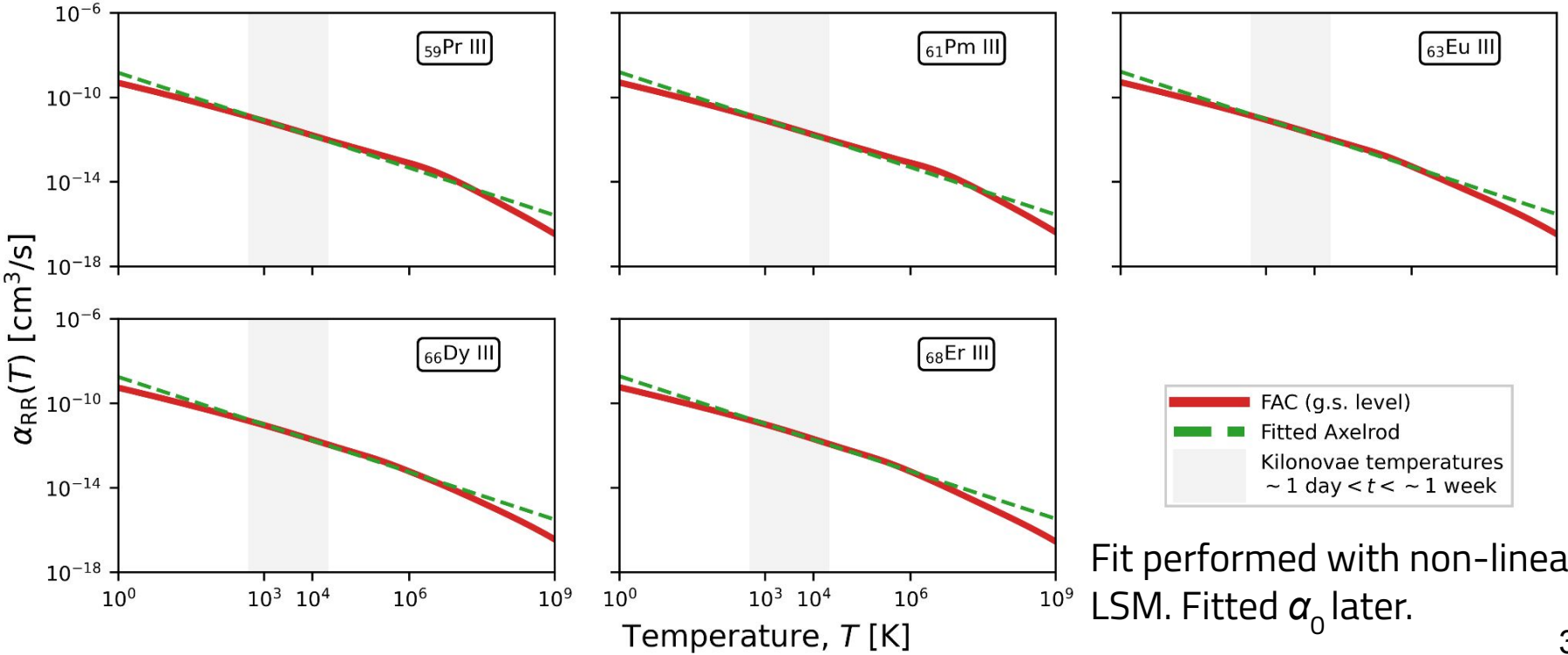
RR Rate Coefficients:

Electron captured by the **ground state level**: FAC vs AS



RR Rate Coefficients:

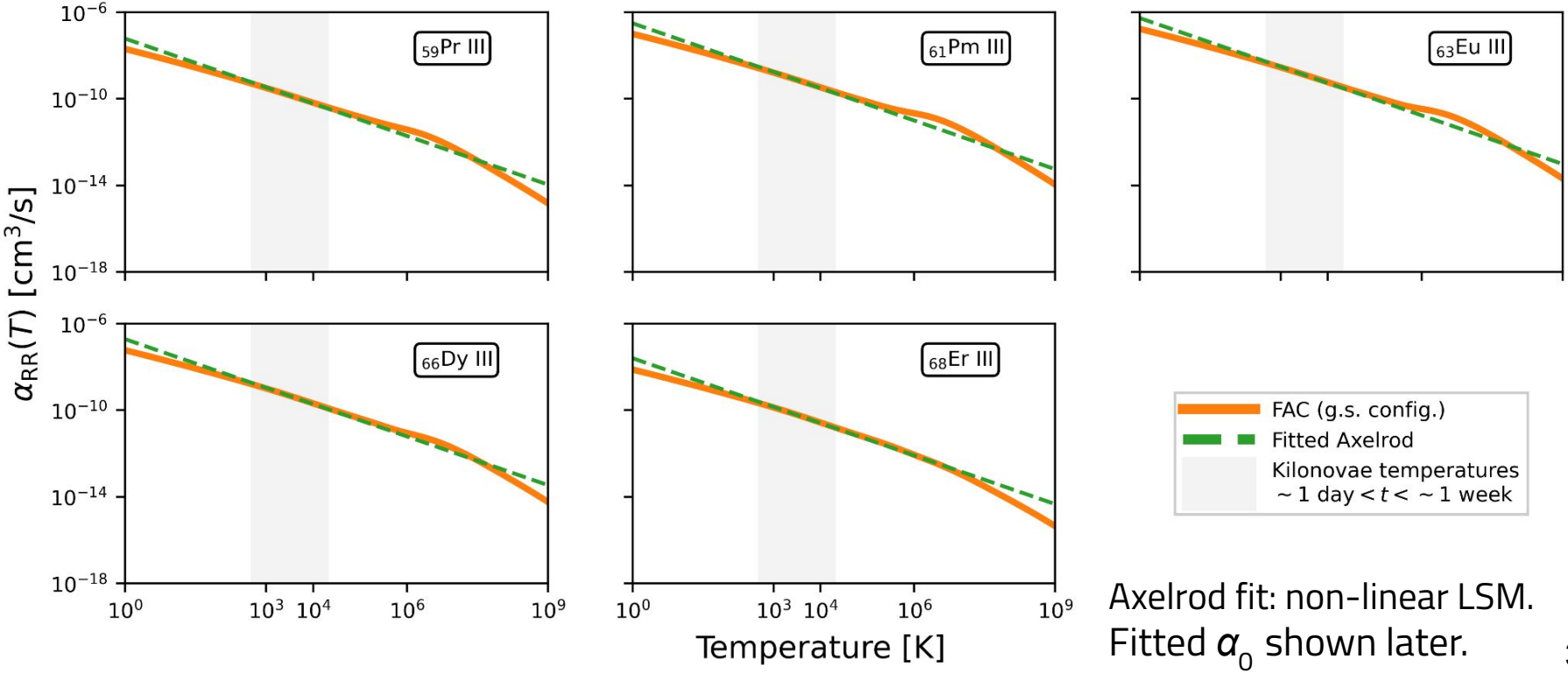
Electron captured by the **ground state level**



Fit performed with non-linear LSM. Fitted α_0 later.

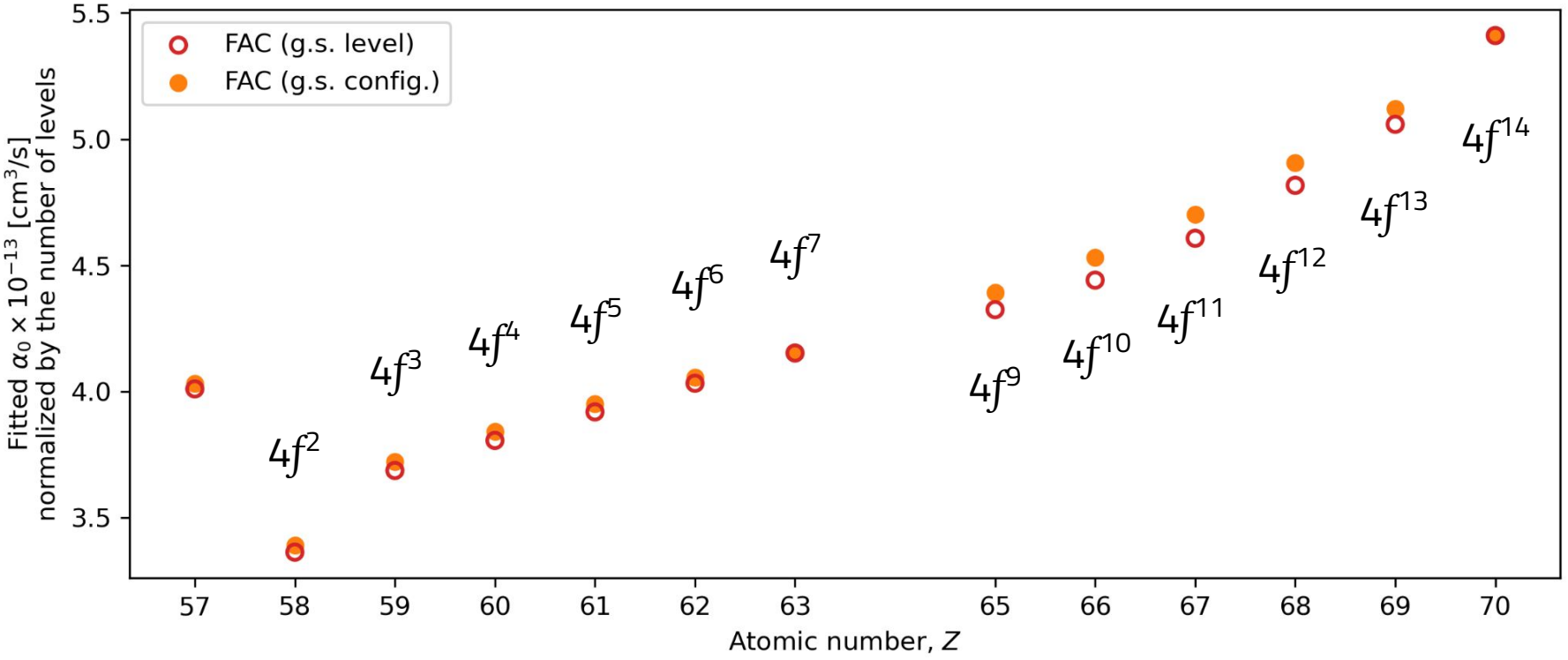
RR Rate Coefficients:

Electron captured by the **ground state configuration**



Axelrod fit: non-linear LSM.
Fitted α_0 shown later.

RR Rate Coefficients:
Scaling



Conclusions (Part II)

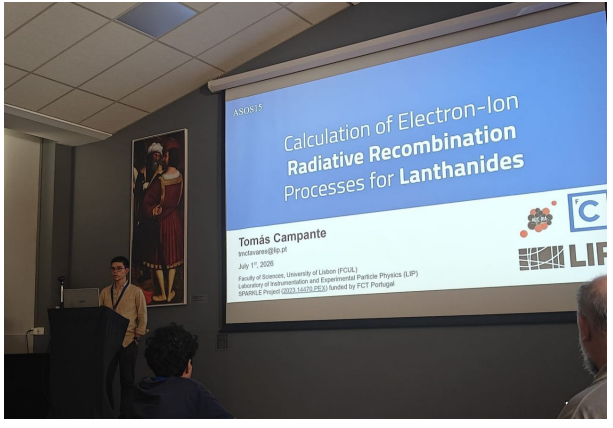
- ➔ Calculation of **RR rate coefficients** for doubly ionised **lanthanides**.
  - No Gd III ($4f^7\ 5d^1$): not enough RAM memory.

- ➔ FAC and AS are in general agreement for RR rate coefficients.

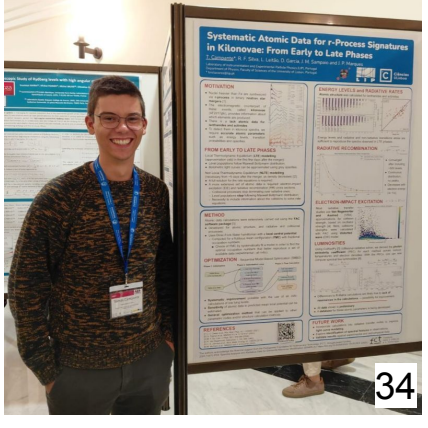
- ➔ Axelrod's α_0 scales with the atomic number.

Communications and Publications

ISAMDEC oct. 2025 – Valladolid, Spain;
IOCAT jan. 2026 – Online (MDPI);
ENEF feb. 2026 – Coimbra, Portugal;
ASOS jul. 2026 – Nice, France.



Co-author in 2 conference papers (Phys. Sci. Forum);
1st author of 1 conference paper (Phys. Sci. Forum);
1st author of 1 journal paper (to be submitted to Atoms);
1st/2nd author of 1 journal paper (in preparation).



Acknowledgments

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Daniel Garcia (MSc student)

Luis Leitão (MSc student)

Prof. Dr. **Jorge Miguel Sampaio**

Prof. Dr. **José Pires Marques**

SPARKLE Project	2023.14470.PEX
Adv. Computation Project	2025.00065.CPCA

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COMPETE 2020 PORTUGAL 2020 UNIÃO EUROPEIA Fundo Europeu de Desenvolvimento Regional

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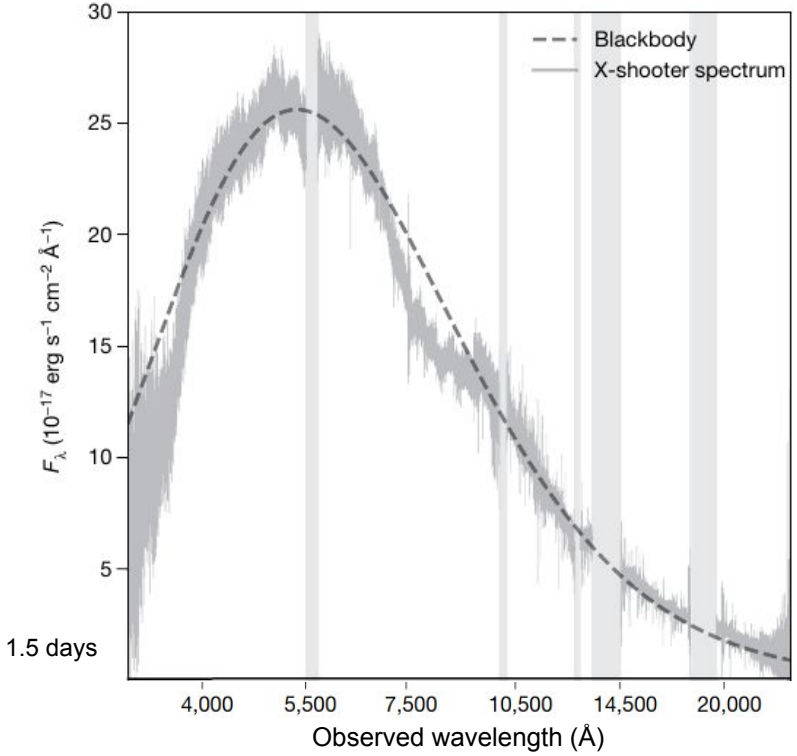
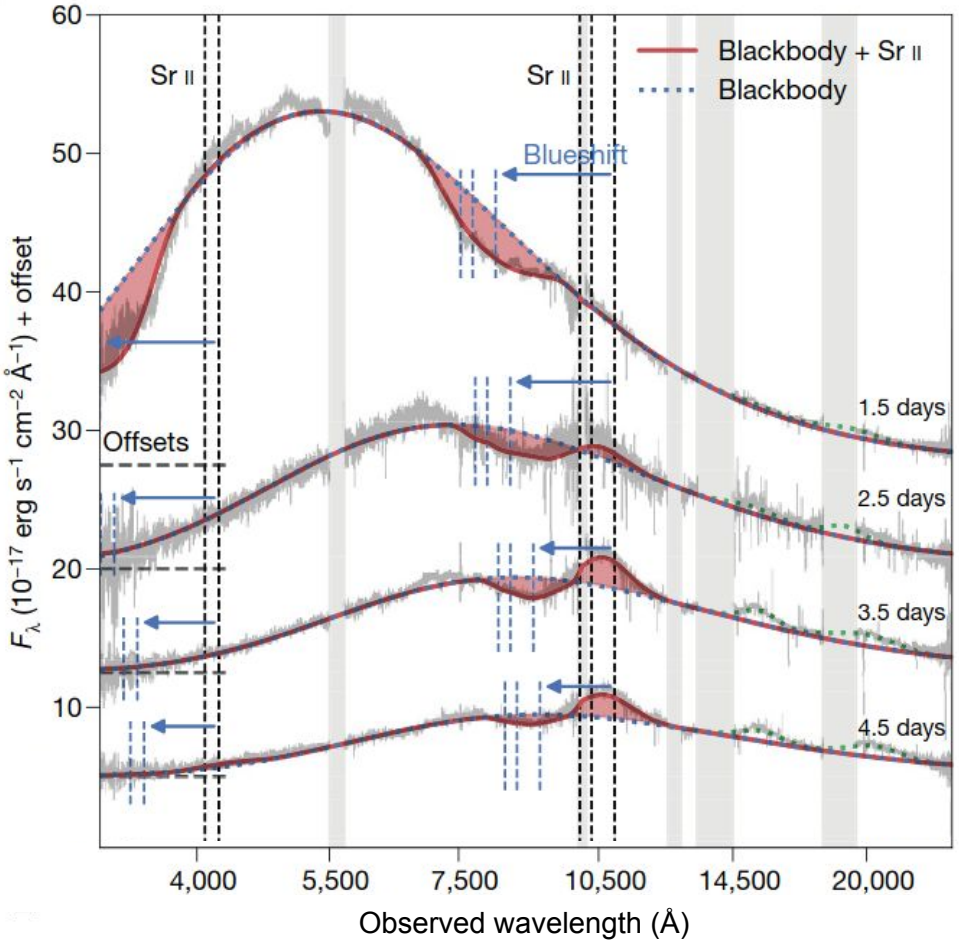
Neutron Star Mergers
Kilonovae



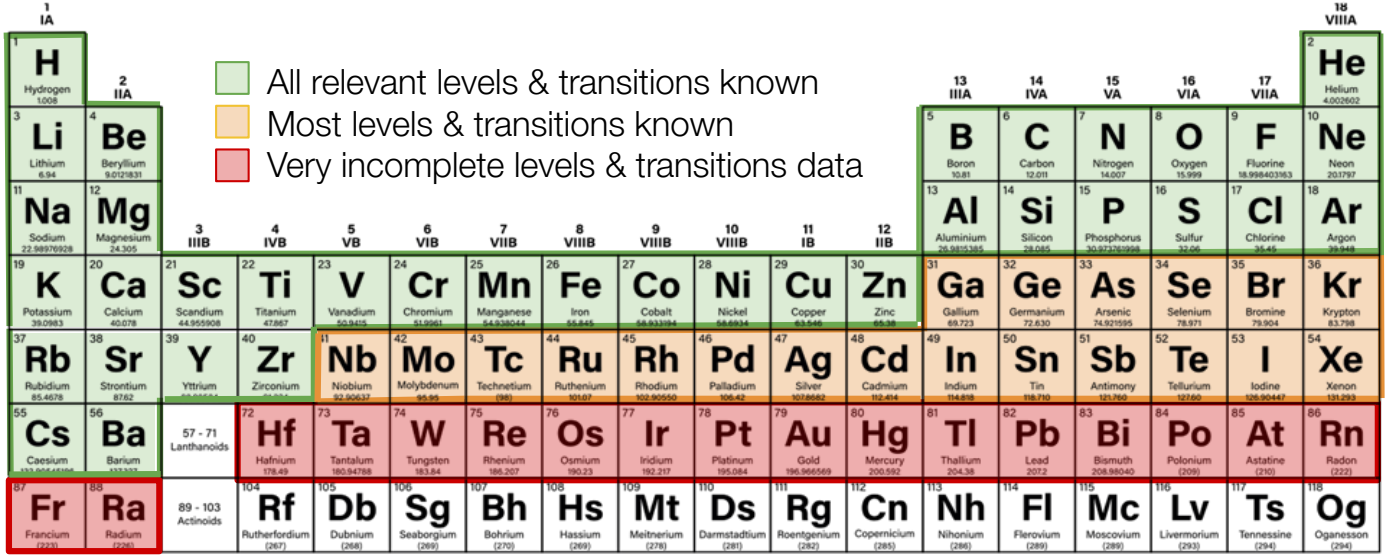


Watson, et al. *Nature*, 574.7779: 497-500. 2019.

Atomic Data needs:

Available Experimental Data

Credit: A. Flörs

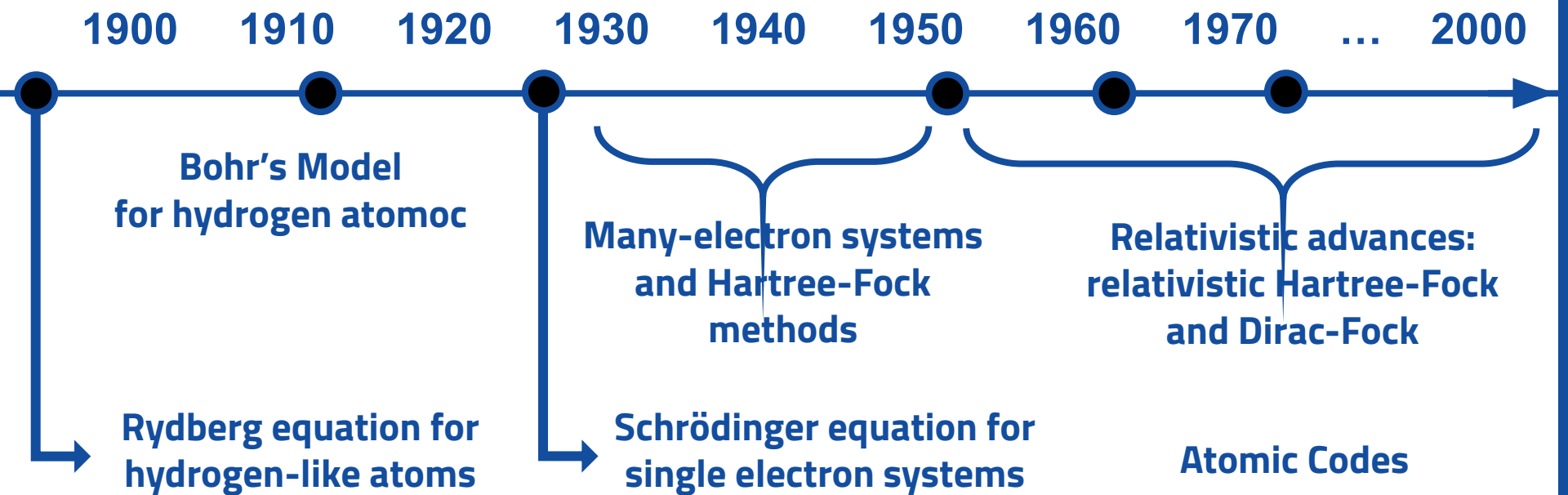


Theoretical calcs. **Flörs+25**

Even less exp. data… what now?

r-process signature elements

Atomic Structure Calculations
Chronology



Atomic Codes: which ones to use?

General use codes - multiple atomic processes

- Usually user-input dependent parameters – Central potential
- Able to calculate a large number of processes
- Limited accuracy
- Fast and efficient
  - 100 000+ levels and transitions in hours/days
- E.g. - FAC Hullac Autostructure JAC Cowan Codes

High accuracy structure codes

- Fully *ab-initio* using MC(D)HF or MBPT approaches – detalied potential for each level
- Focused on structure and some radiative properties
- High accuracy
- Computationally demanding
  - Months for large scale calculations depending on the code of one ion
- E.g. – GRASP ATSP MCDFGME AMBIT CI-MBPT

credit: R. Ferreira da Silva

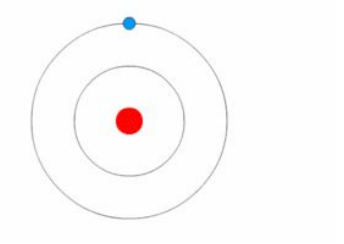
Atomic Structure Codes

- Cowan's code, 1970s
- SUPERSTRUCTURE (SS), 1974
- ★Multiconfiguration Dirac-Fock and General Matrix Elements (**MCDFGME**), 1990s
- GRASP2018
- HULLAC, 2000s
- Jena Atomic Code (JAC), 2024

★Flexible Atomic Code (**FAC**), 2010s ⟶ M. F. Gu | University of California, Berkeley

★AUTOSTRUCTURE (AS), 2013 ⟶ N. R. Badnell | University of Strathclyde, Glasgow

Atomic Structure Calculations: what am I calculating?



Wavefunctions:

➔ Building wavefunctions for atomic systems

Levels:

➔ Term, parity and 2*J*: level identification

➔ Ground and excited states

Lines:

➔ Transition wavelength

➔ Transition rate

➔ Oscillator strengths

Atomic Structure Calculations:
main ingredients

(central)
potential

Self-consistent methods
(Hartree-Fock)

hamiltonian

QED corrections

wavefunctions

Einstein radiation
theory

One-electron atoms

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r}) = E\psi(\vec{r})$$

- Bohr's model for hydrogen atom (1913);

- Schrödinger's equation for one electron recovers Bohr's model;

$$\begin{aligned} E_n &= -13.6\frac{Z^2}{n^2}\left(\frac{\mu}{m}\right)\text{eV} \\ &= -\frac{Z^2}{n^2}\left(\frac{\mu}{m}\right)\text{Ry} \\ &= -\frac{Z^2}{2n^2}\left(\frac{\mu}{m}\right)\text{a.u.} \end{aligned}$$

Bohr's model solutions are recovered

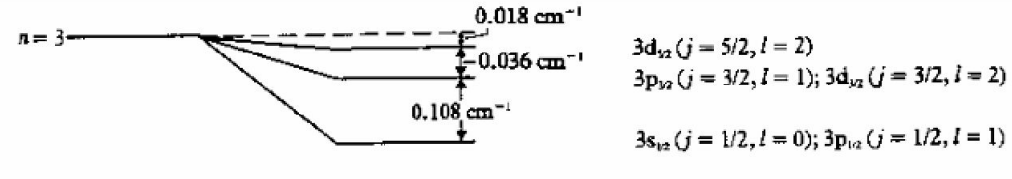
Fine and Hyperfine Structure:
What is the difference between them?

Fine

Orbitals split due to **different j**:

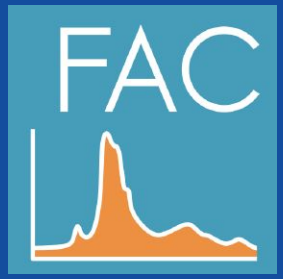
Example: l=2 (s=1/2)

j = 3/2 , 5/2



Hyperfine

Orbitals split due to interaction between j and the **nuclear spin**: the magnetic field generating for the moving electrons affects the spin of the nucleus. The magnitude of this spliting is much smaller than fine structure effets, hence *hyper*fine.



The Flexible Atomic Code

A quick overview

The Flexible Atomic Code (FAC): a **fully-relativistic** atomic code

$$\mathcal{H}_{\mathrm{FAC}} = \sum_{i=1}^{N} \mathcal{H}_{\mathrm{Dirac}}(\vec{r}) + \sum_{i<j}^{N} \frac{1}{r_{ij}}$$

$$\mathcal{H}_{\mathrm{Dirac}} = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta c^2 + V_C(r)$$

- ➔ Dirac's formalism in the Hamiltonian;
- ➔ Includes Breit interaction and QED corrections;
- ➔ Relativistic configuration interaction;
- ➔ Distorted Wave (DW) approximation for interactions with the continuum.

M.F. Gu, *Canadian Journal of Physics*, 86, 675. 2008.

The Flexible Atomic Code (FAC):
Potential Optimization

→ Central potential:

A unique potential — one potential for all orbitals.

In FAC, we can use an average configuration to optimize the potential

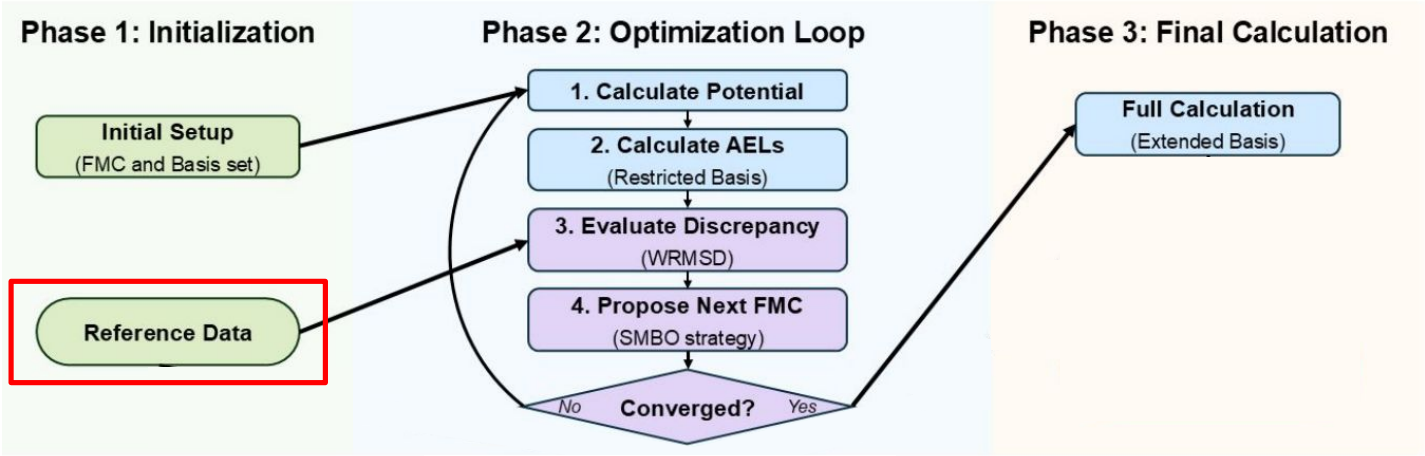
Er II: [Xe] $4f^{\mathbf{11.72}}\ 5d^{\mathbf{0.42}}\ 6s^{\mathbf{0.86}}\ 6p^{0.00}$

This configuration has fractional occupations number, and it is called **Fictitious Mean Configuration** (FMC).

Sampson, Zhang and Fontes. *Physics Reports*, 477.4-6: 111-214. 2009.

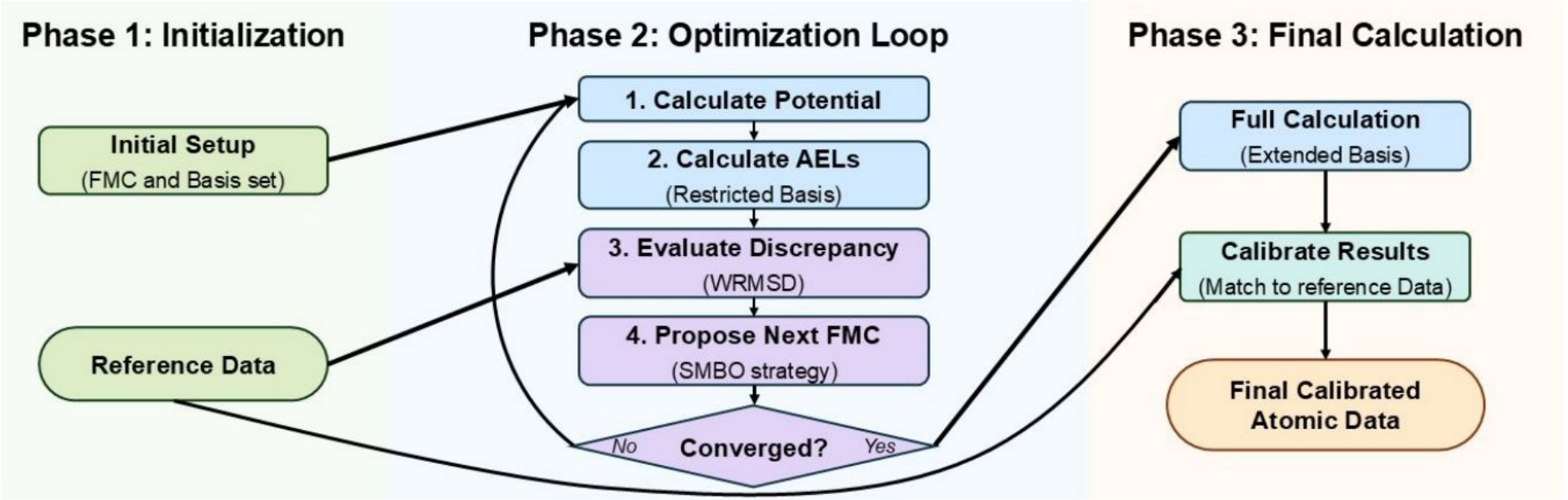
The Flexible Atomic Code (FAC):
Potential Optimization

Using an **optimization method external to FAC**, we vary the occupation numbers and get the FMC that provides atomic energy levels closer to the experimental NIST values.



R. Ferreira da Silva et al., Physical Review A, 112(1), 012802. 2025.

The Flexible Atomic Code (FAC):
Potential Optimization



R. Ferreira da Silva et al., Physical Review A, 112(1), 012802. 2025.

Flexible Atomic Code (FAC):
a **fully-relativistic** atomic code

Eletrostatic interaction:

$$\mathcal{H}_{\mathrm{FAC}} = \sum_{i=1}^{N} \mathcal{H}_{\mathrm{Dirac}}(\vec{r}) + \sum_{i<j}^{N} \frac{1}{r_{ij}}$$

jj-coupling scheme and spin-orbit interaction

Better for high Z atoms, where spin-orbit interactions dominate over the eletrostatic ones

Spin-orbit interaction:

$$\mathcal{H}_{S-O} = f(r)\vec{S}\cdot\vec{L}$$

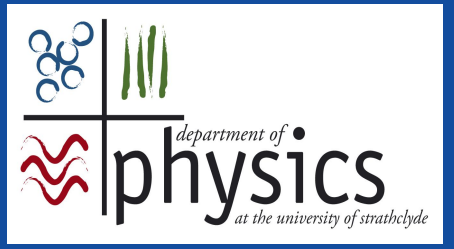
$$f(r) = \frac{1}{4\pi\varepsilon_0}\frac{Zq_e{}^2}{2m^2c^2}\frac{1}{r^3}$$

$$\vec{S}\cdot\vec{L} = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$$

It doesn't make sense to talk about **l** and **s** separetely when S-O dominates

$$\mathbf{j}_i = \mathbf{l}_i + \mathbf{s}_i$$

$$\mathbf{J} = \sum_{i=1}^{N} \mathbf{j}_i$$



AUTOSTRUCTURE

A quick overview

AUTOSTRUCTURE (AS) Code:
a **semi-relativistic** atomic code

- ➔ Non-relativistic Hamiltonian; $\mathcal{H}_{\rm AS} = \sum_{i=1}^{N}\left(-\frac{{\nabla_i}^2}{2} - \frac{Z}{r_i}\right) + \sum_{i<j}^{N}\frac{1}{r_{ij}} + \mathcal{H}_{\rm rel.\ corr}$
- ➔ Uses Breit-Pauli interaction. Can also include QED and other relativistic corrections;
- ➔ Also a configuration interaction code;
- ➔ Distorted Wave (DW) approximation for interactions with the continuum.

N.R. Badnell, *Astrophysics Source Code Library,* ascl:1612.014. 2016.
W. Eissner, M. Jones, and H. Nussbaumer. *Computer Physics Communications*, 8(4):270–306, 1974.

AUTOSTRUCTURE (AS) Code:
Potential Optimization

➔ A different **central potential for each orbital.**

$$\left[\frac{1}{2}\frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{nl}(\lambda_{nl}, r) + E_j\right] P_{nl}(r) = 0\,,$$

λ_{nl} is scale parameter chosen to minimize the potential for each orbital: **Variational Principle**

$$E[\Psi] = \frac{\langle\Psi|H_{BP}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0$$

$$E_{AS}^{opt} = \min_{\{\lambda\}}\langle\Psi(\{\lambda\})|H_{BP}|\Psi(\{\lambda\})\rangle$$

M.P.A. Mendez, PhD thesis. 2021.
M.M. Bluteau, PhD thesis. 2018.

AUTOSTRUCTURE (AS) Code:
Potential Optimization

Two different optimizations in AS

Two-step optimization: **LS** → IC(R)

- ➔ Optimize λ_{nl} in LS coupling.
- ➔ Use the LS-optimized λ_{nl} in a final calculation in intermediate coupling, including relativistic corrections.

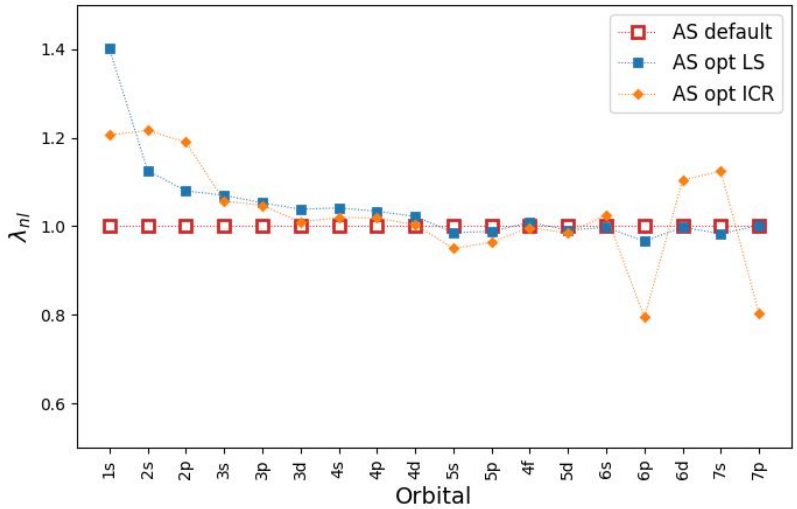
One-step optimization in **IC**(**R**)

- ➔ Optimize λ_{nl} directly in intermediate coupling.
- ➔ Perform the final calculation in the same run, including relativistic corrections.

$$\left[\frac{1}{2}\frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{nl}(\lambda_{nl}, r) + E_j\right] P_{nl}(r) = 0\,,$$

$$E[\Psi] = \frac{\langle\Psi|H_{BP}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0$$

$$E_{AS}^{opt} = \min_{\{\lambda\}} \langle\Psi(\{\lambda\})|H_{BP}|\Psi(\{\lambda\})\rangle$$

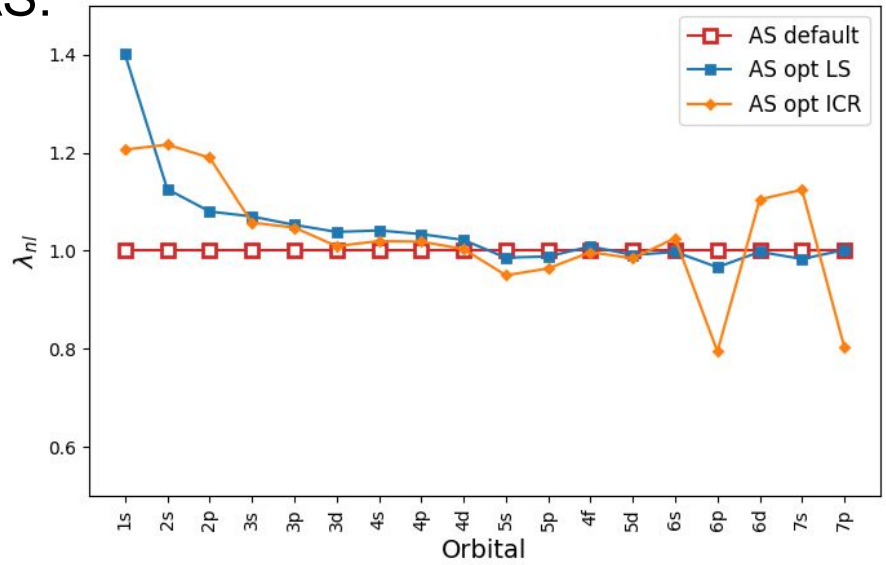


Calculations

The specific case of ^{68}Er II

20 configurations: ground state + SE until 7p + lower energy DE

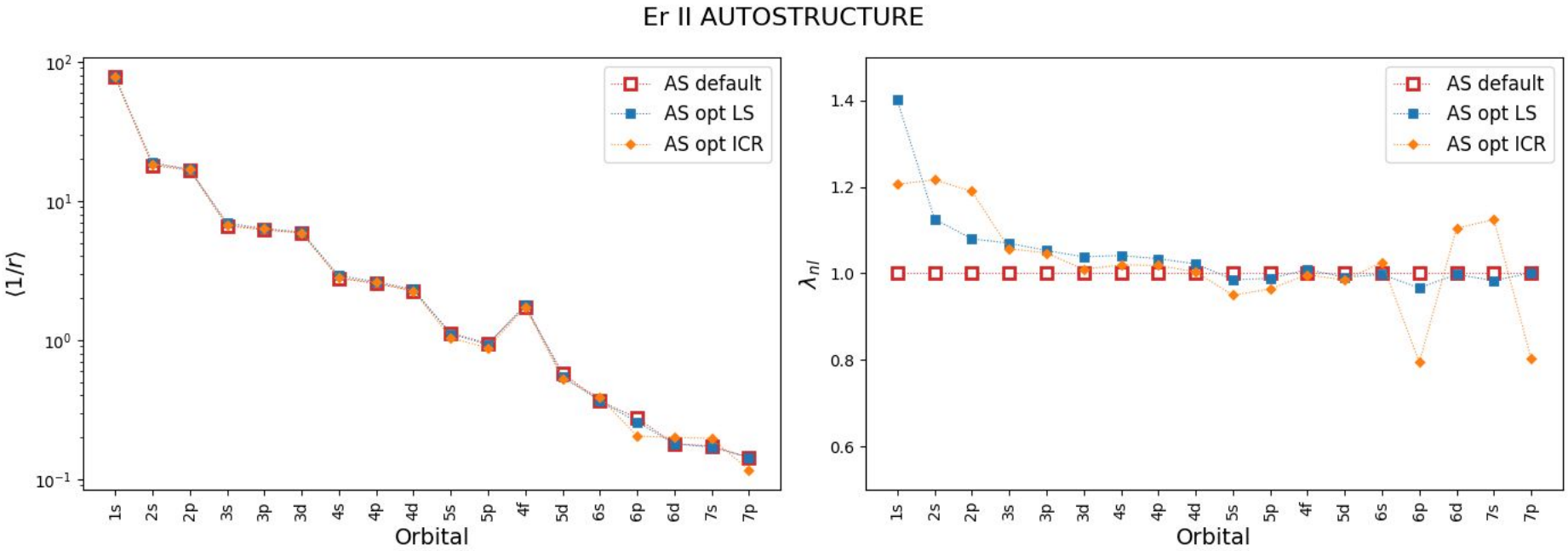
AS:



FAC:

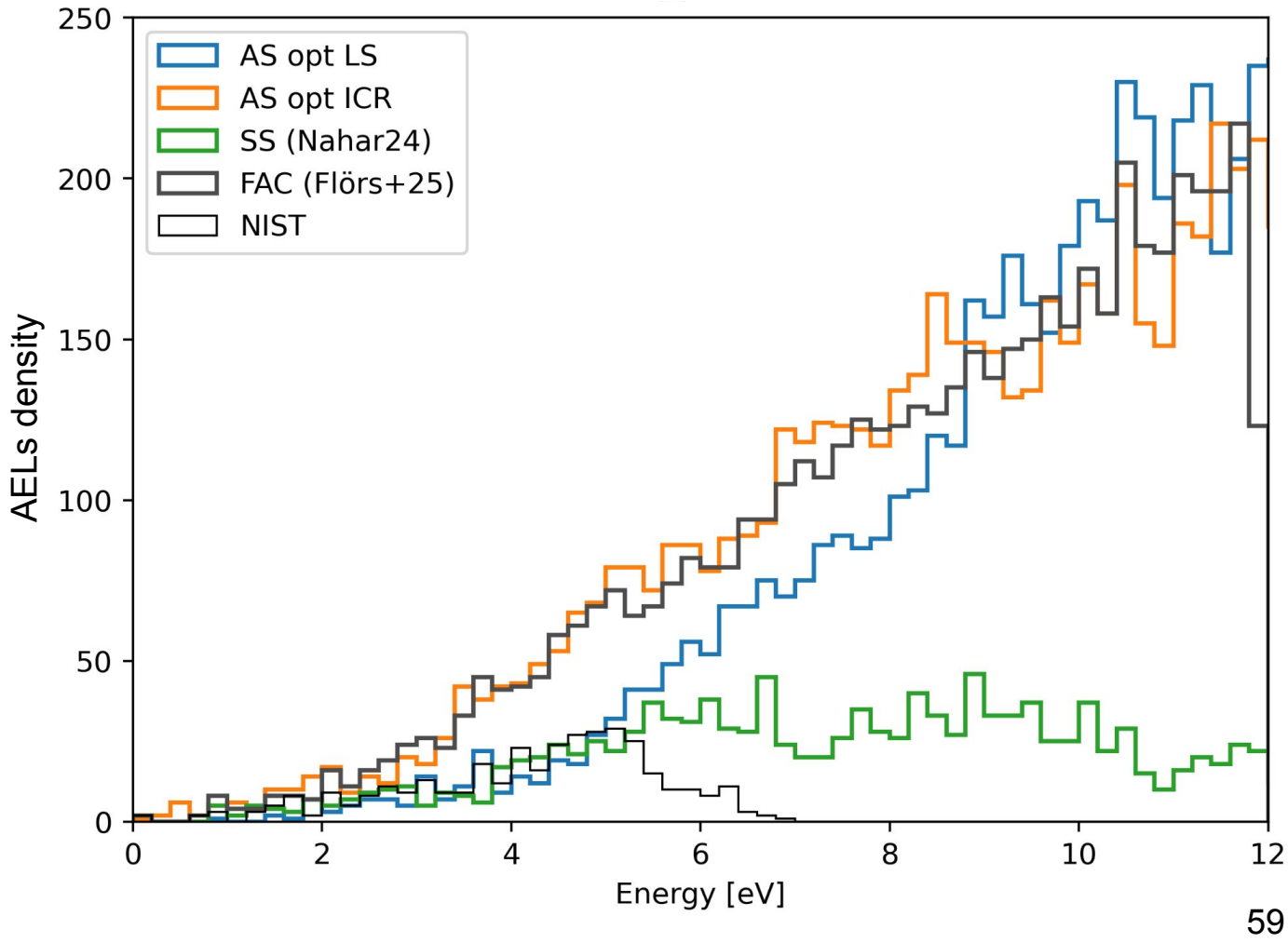
orbital	occupation
4f	11.72
5d	0.42
6s	0.86
6p	0.00

Optimization effect on the wavefunction (AS)

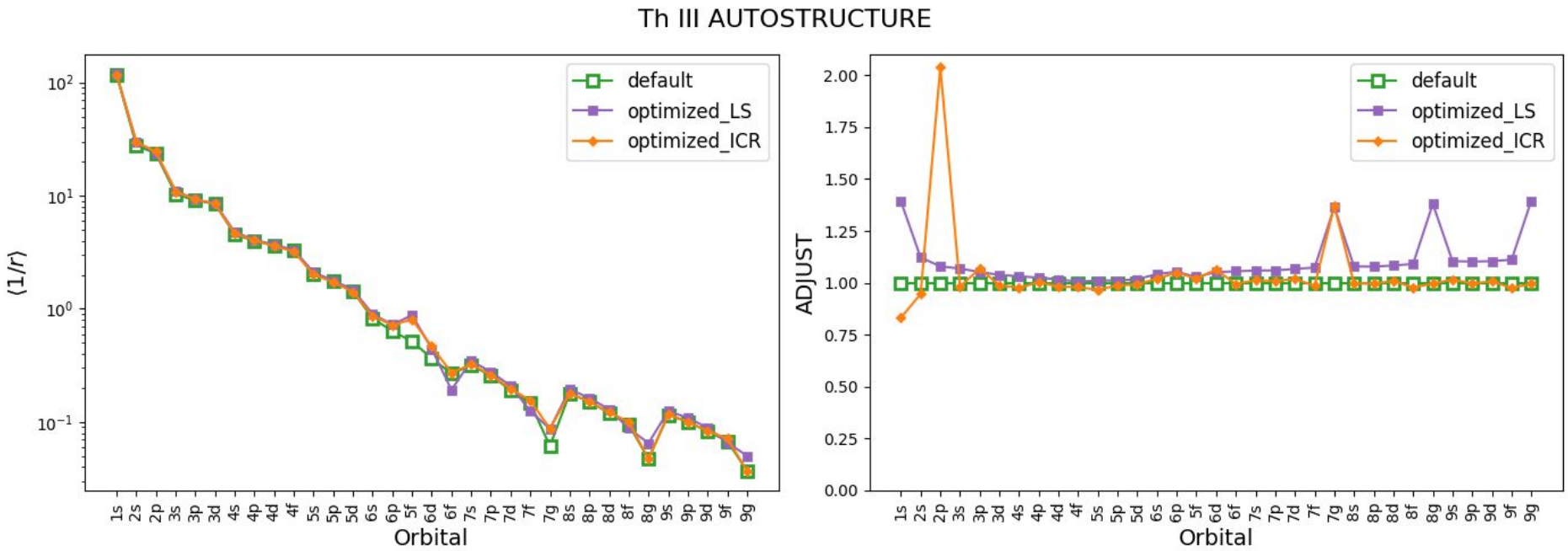


Er II
(Z=68)

AS, FAC: 20 configs
SS: 6 configs



Optimization effect on the wavefunction (AS)



AUTOSTRUCTURE (AS) Code:
a **semi-relativistic** atomic code

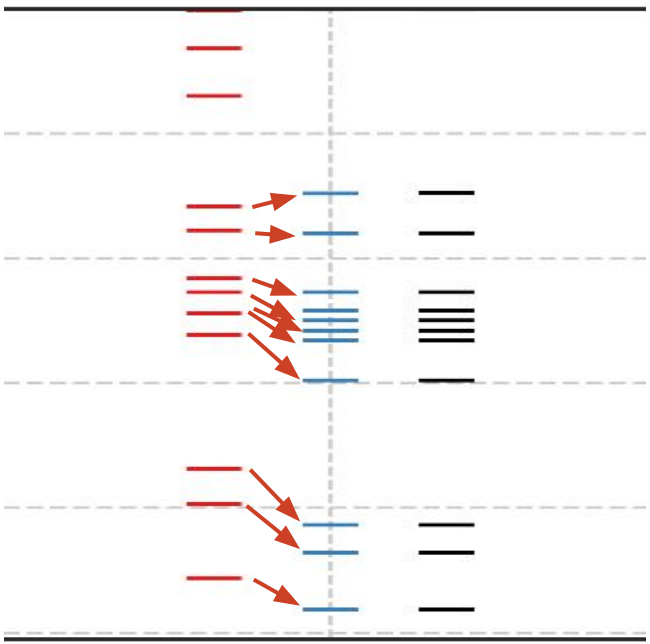
LS-coupling scheme and spin-orbit interaction

Better for low Z atoms, where eletrostatic interactions dominate over the spin-orbit

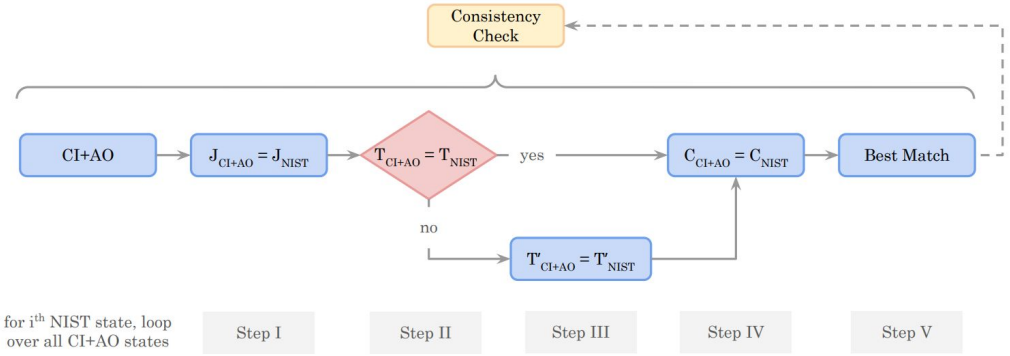
$$\mathbf{L} = \Sigma\, \mathbf{l} \qquad \mathbf{S} = \Sigma\, \mathbf{s}$$

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

Calibration



- P, J & spectroscopic term known for FAC & some NIST levels (using the grasp/jj2lsj module by G. Gaigalas)
- Match NIST levels with corresponding FAC levels
- FAC levels without NIST data: use combination of mean correction from P-J group and mean correction from configuration

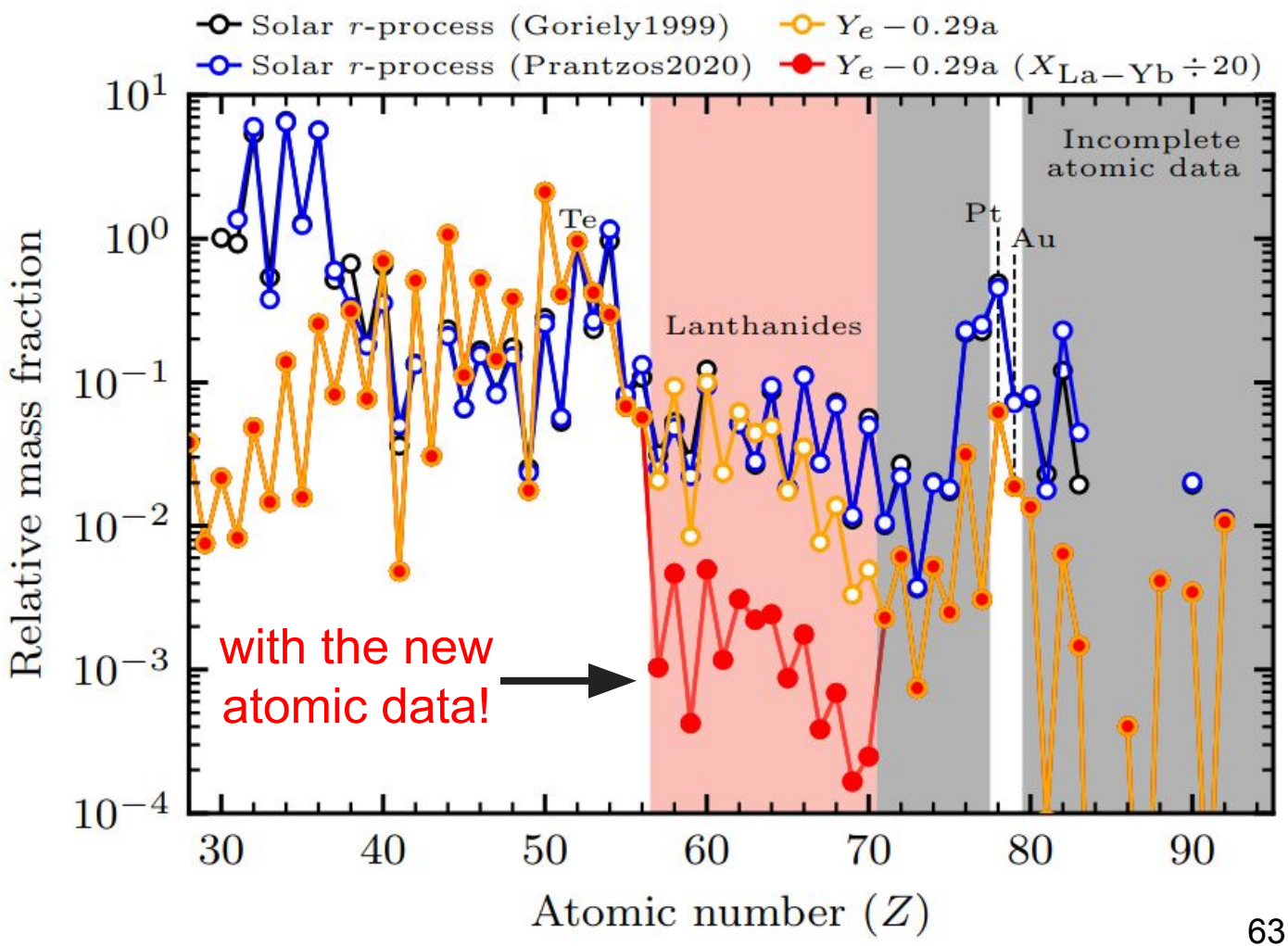


A. Kiruga et al. arXiv:2506.08170

slide by R. Ferreira da Silva

Implications:

Lanthanide mass constraints in kilonovae



Gillanders, J. H., Flörs, A., & Ferreira da Silva, R. (2025). *arXiv preprint arXiv:2512.24257*.

RR vs DR

N.C. Sterling, *Astronomy & Astrophysics*, 533:A62, 2011

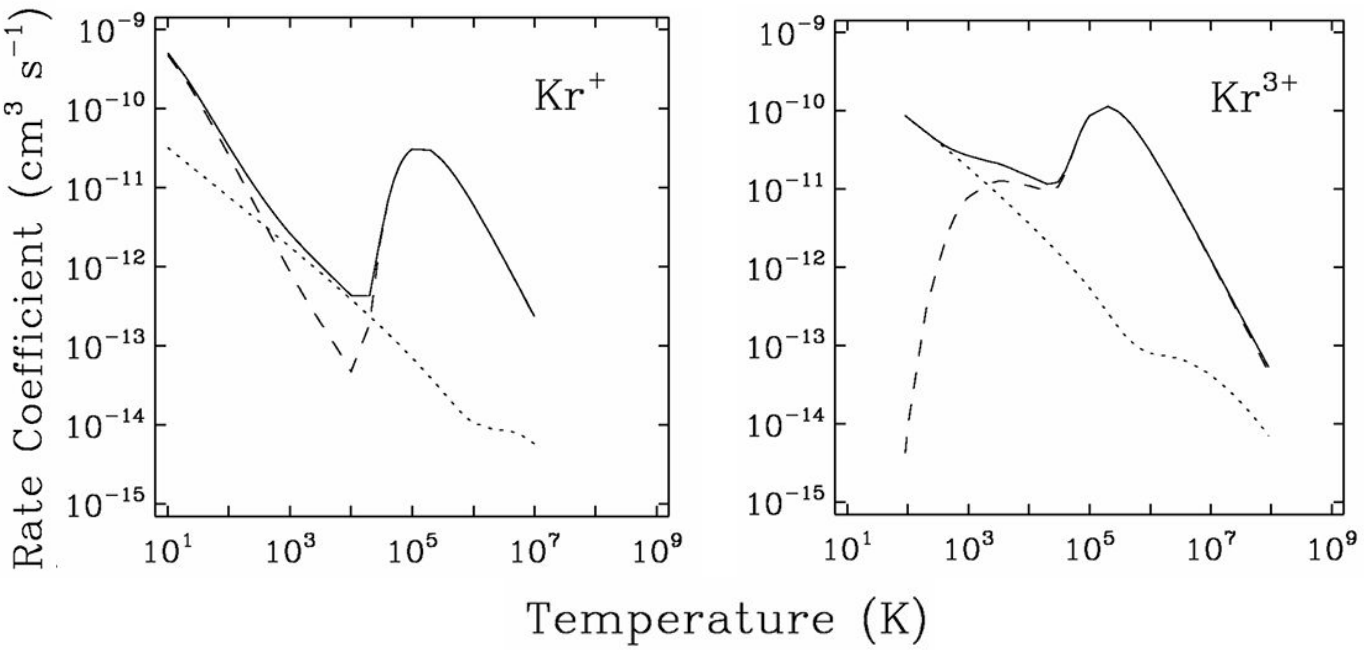


Fig. 8. Comparison of the radiative (dotted curves), dielectronic (dashed curves), and total recombination rate coefficients (solid curves) for the ground state of the first six Kr ions.

W XIV

D. Garcia *et al.*. *Physical Sciences Forum* (MDPI), 13(1), 9. 2026.

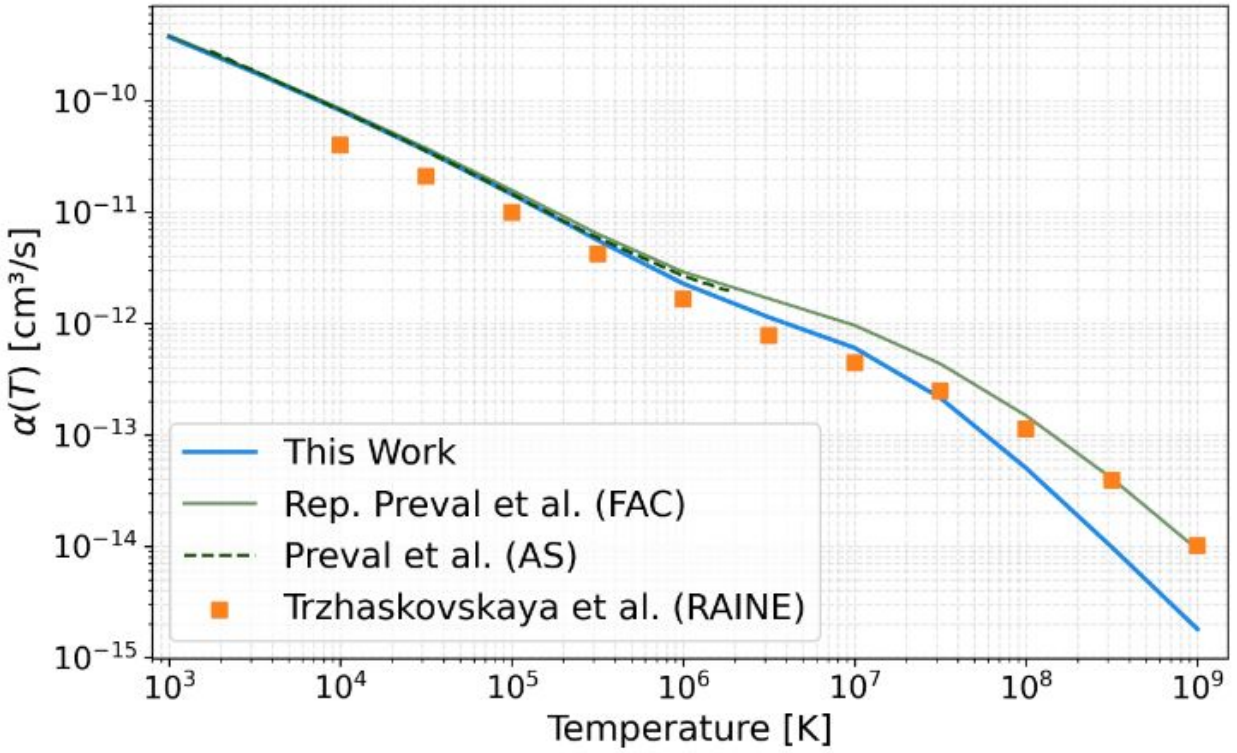
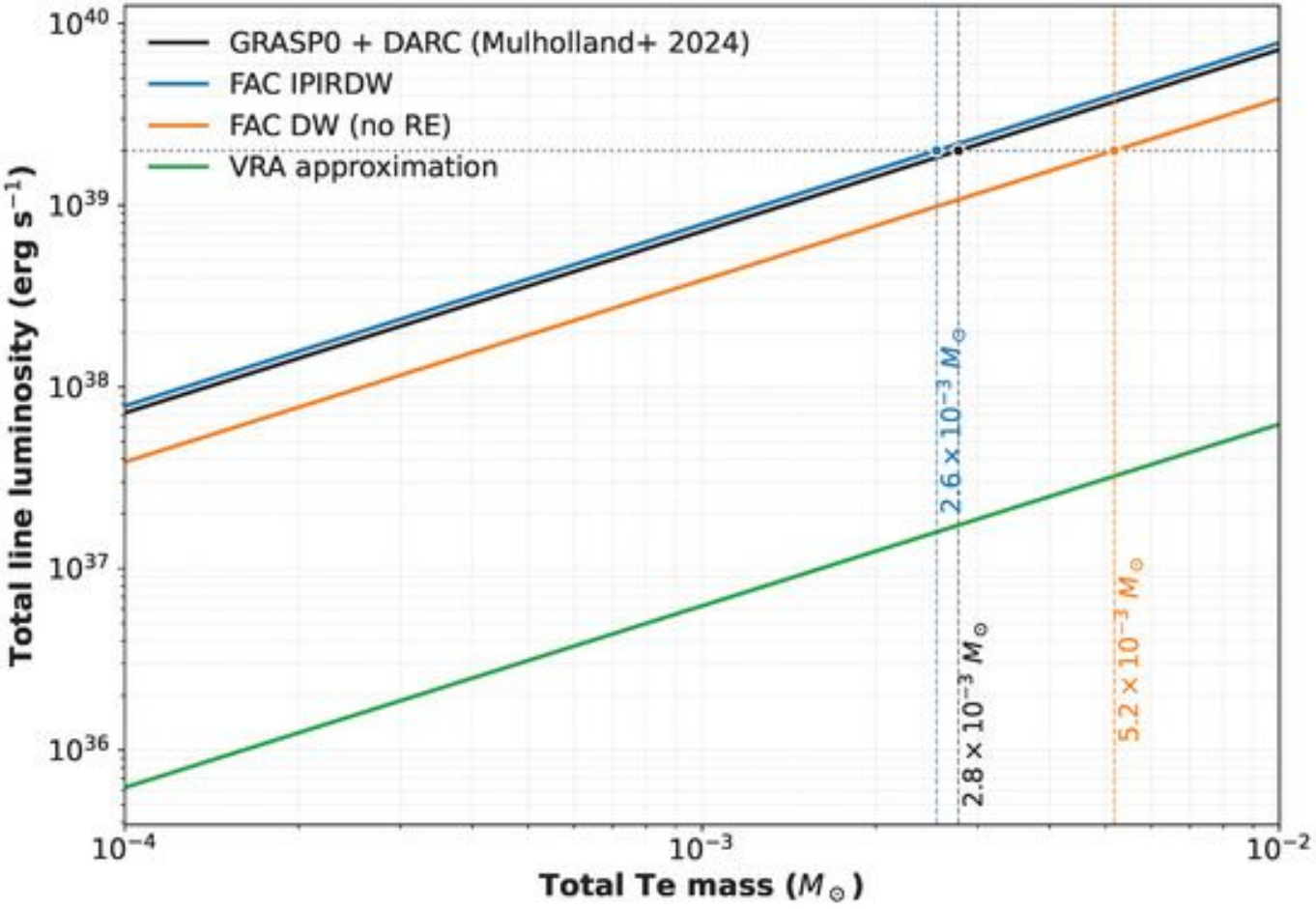


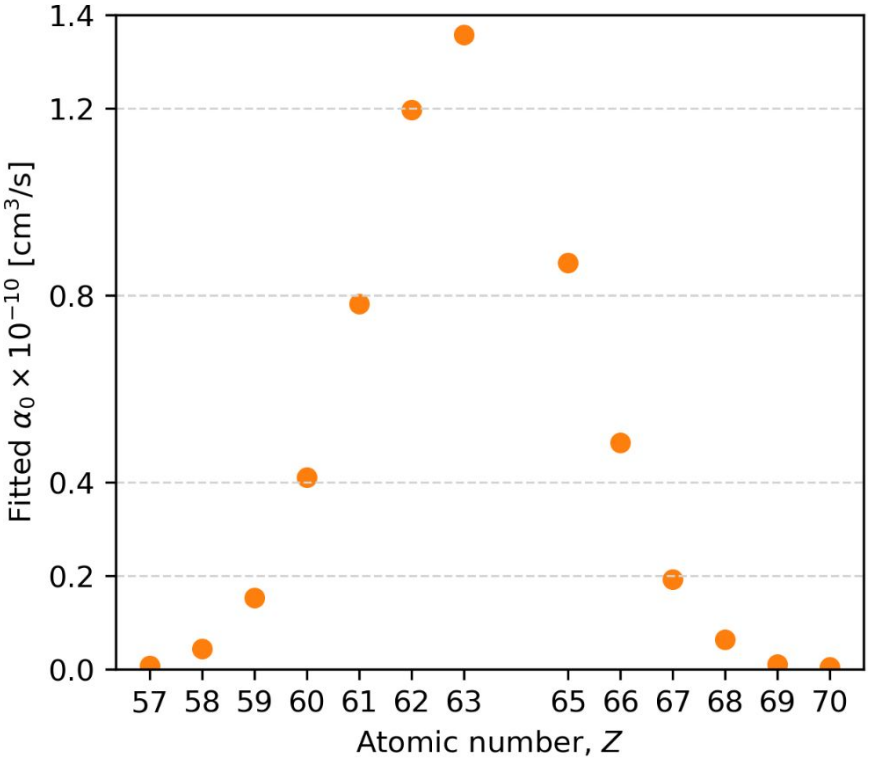
Figure 2. RR rate coefficients for W XIV as a function of temperature. The green dashed line is the original data from Preval *et al.* [24] (AUTOSTRUCTURE), with the solid green line being our FAC reproduction. The blue line shows the rates obtained in this work from the low-lying states calculation, including hydrogenic extrapolation up to $n = 1000$. The orange squares denote the data from Trzhaskovskaya *et al.* [25] (RAINE).

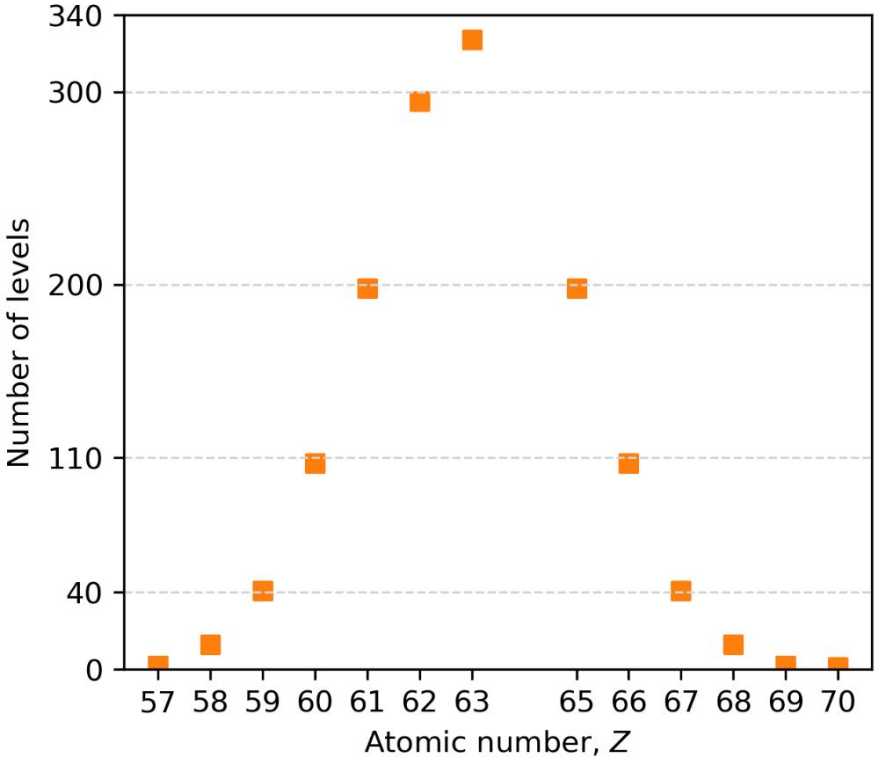
(VR)A

R. Ferreira da Silva *et al.*. *Physical Sciences Forum* (MDPI), 13(1), 5. 2026.



RR Rate Coefficients:
Scaling





Radiative Recombination:
The Verner and Ferland fit (1996)

For data replication, it is common to use the Verner and Ferland fit

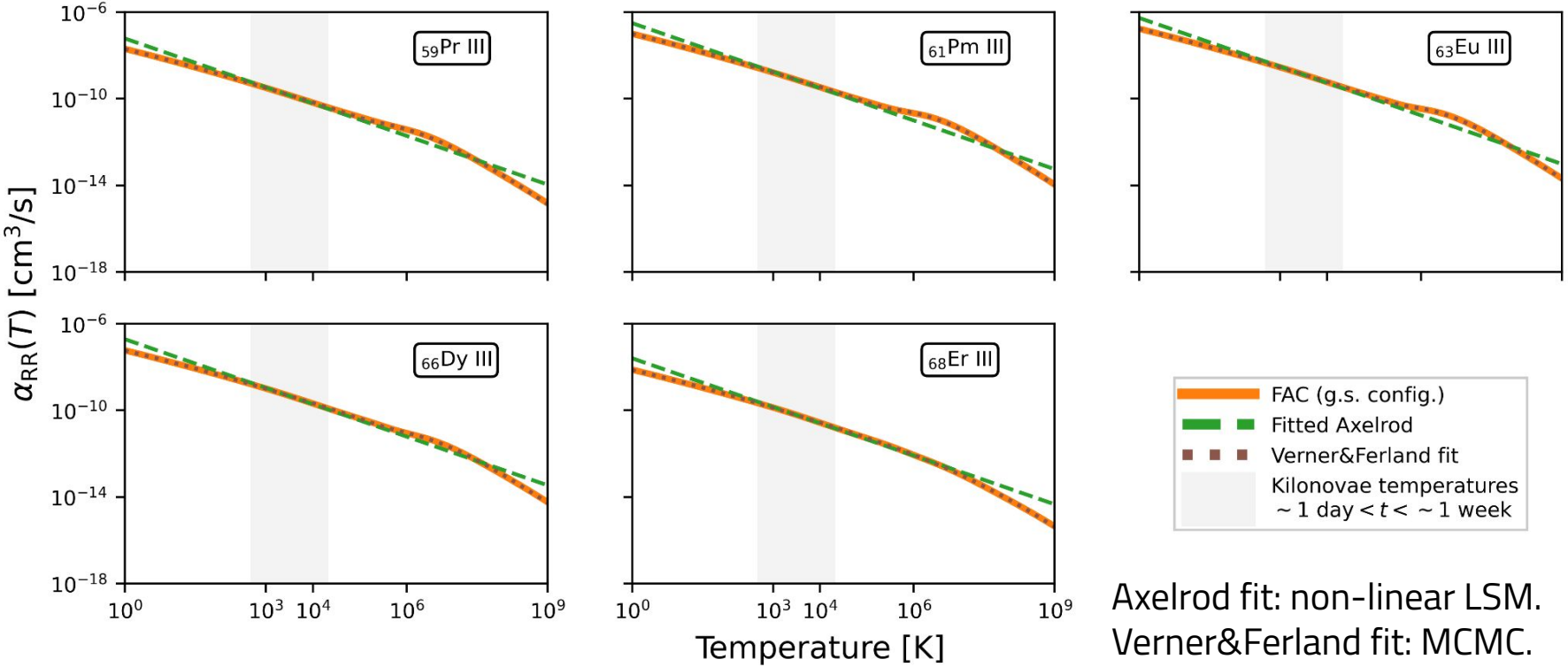
$$\alpha_{\mathrm{RR}}(T) = \frac{A}{\sqrt{\frac{T}{T_0}}\left(1+\sqrt{\frac{T}{T_0}}\right)^{1-B}\left(1+\sqrt{\frac{T}{T_1}}\right)^{1+B}}$$

$B \to B + C\exp\left(-T_2/T\right)$, for low-charge ions.

D.A. Verner and G.J. Ferland. *The Astrophysical Journal Supplement Series*, 103:467.1996.

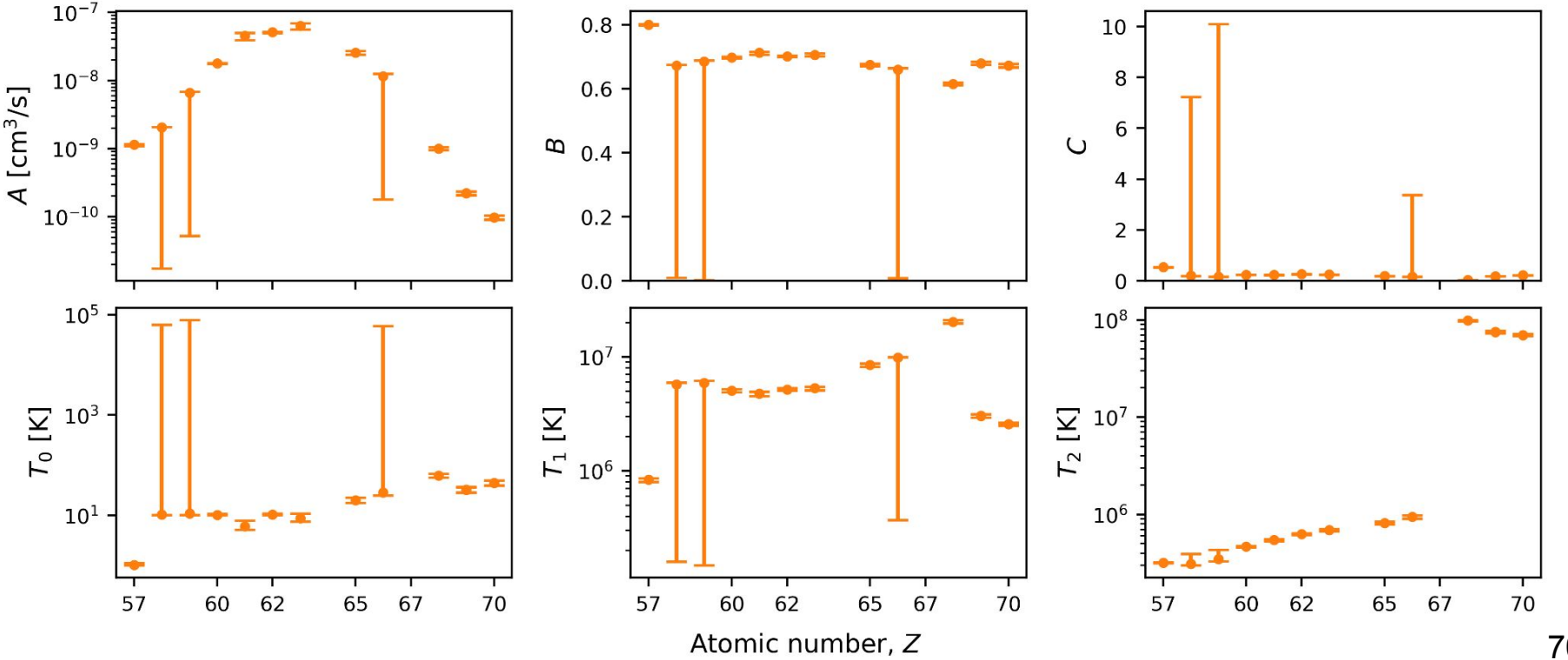
RR Rate Coefficients:

Electron captured by the **ground state configuration**



Axelrod fit: non-linear LSM.
Verner&Ferland fit: MCMC.

RR Rate Coefficients:
Scaling



RR Rate Coefficients:

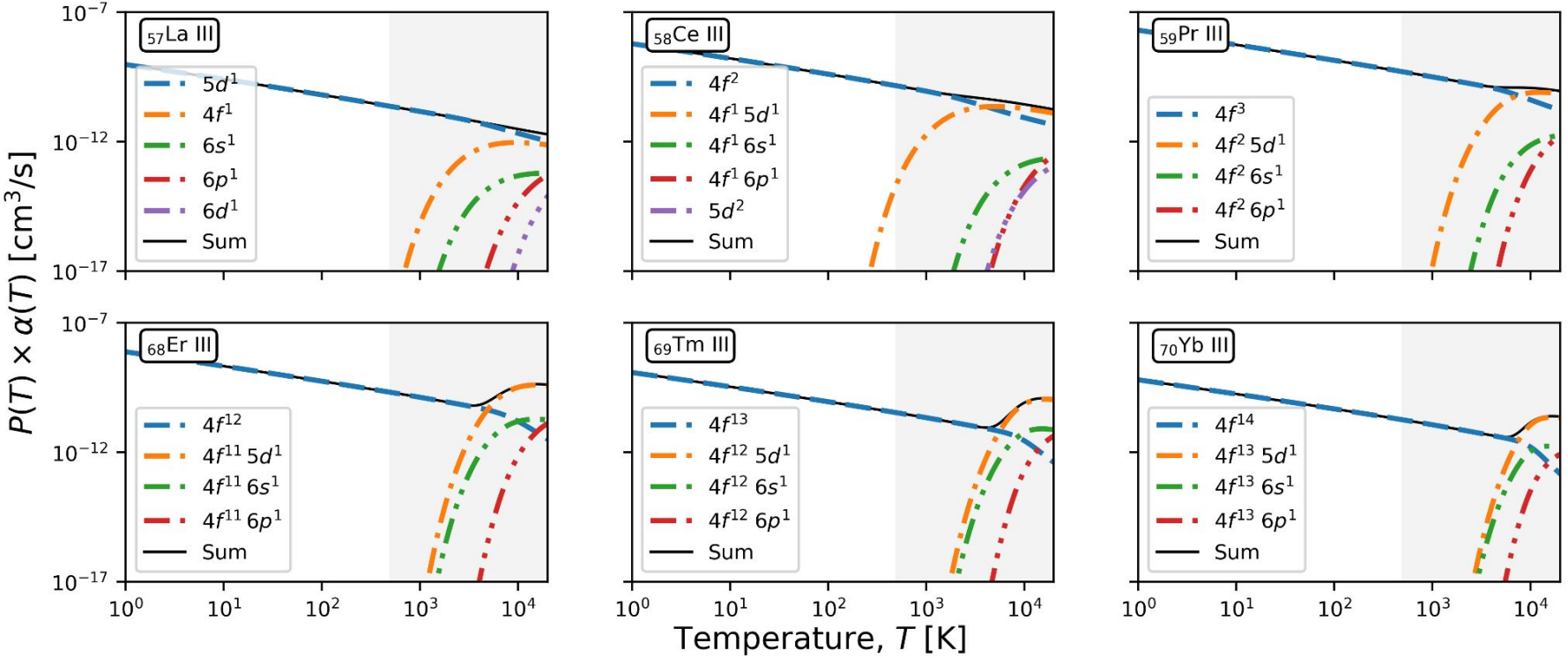
Electron captured by **excited configurations**

However, there are more levels populated besides the ground state level. Assuming LTE conditions, the populations, P, are given by

$$P_{\mathrm{lev}}(T) = \frac{g_{\mathrm{lev}} e^{-E_{\mathrm{lev}}/k_B T}}{\sum_{\mathrm{lev}} g_{\mathrm{lev}} e^{-E_{\mathrm{lev}}/k_B T}} \qquad P_{\mathrm{cfg}}(T) = \sum_{\mathrm{lev} \in \mathrm{cfg}} P_{\mathrm{lev}}(T)$$

RR Rate Coefficients:

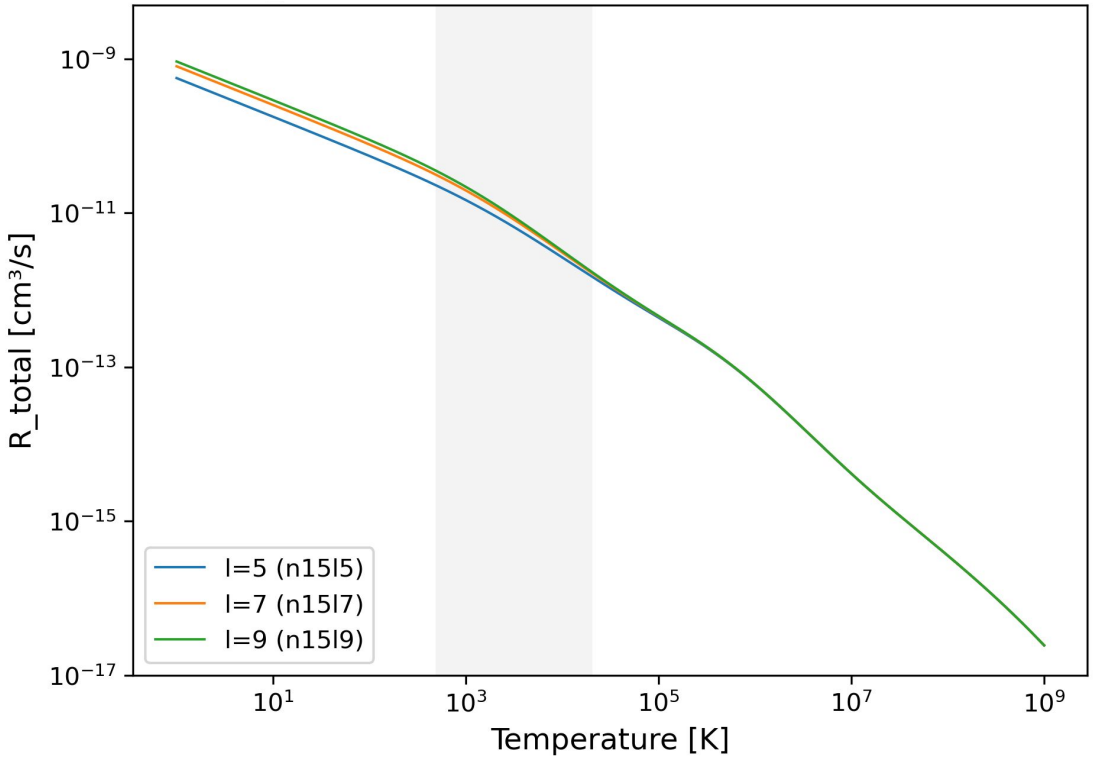
Electron captured by **excited configurations**



Radiative Recombination:

Explicit treatment of low-nl states

Within the same n value, the contribution of configurations with increasing l is residual



Private communication with M.F. Gu, may 2026

Radiative Recombination:
Approximation for high-nl states

FAC:

- Kramers' formula for high-n states.

AS:

- Top-up approximation for high-n states.

H. A. Kramers. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 46(275):836–871. 1923.
E. Zerrad and Y. Hahn. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 59(6):637–651. 1998.

A Burgess and VB Sheorey. *Journal of Physics B: Atomic and Molecular Physics*, 7(17):2403–2416. 1974.
A Burgess, DG Hummer, and JA Tully. *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 266(1175):225–279. 1970.

(Non-)relativistic Milne Relation

$$\sigma_{\mathrm{PI}} \frac{g_f}{{p_\mathrm{e}}^2} = \sigma_{\mathrm{RR}} \frac{g_i}{{p_\gamma}^2} \quad , \qquad p_\gamma = \frac{E_\gamma}{c} = \frac{\hbar\omega}{c}$$

$$p_\mathrm{e} = \sqrt{2 m_\mathrm{e} \varepsilon}$$

$$\sigma_{\mathrm{RR}} = \sigma_{\mathrm{PI}} \frac{g_f}{g_i} \frac{{E_\gamma}^2}{2 m_\mathrm{e} \varepsilon c^2}$$

$${E_\mathrm{e}}^2 = {p_\mathrm{e}}^2 c^2 + {m_\mathrm{e}}^2 c^4$$

$$(\varepsilon + m_\mathrm{e} c^2)^2 = {p_\mathrm{e}}^2 c^2 + {m_\mathrm{e}}^2 c^4$$

$${p_\mathrm{e}}^2 = \frac{1}{c^2}\left(\varepsilon^2 + 2 m_\mathrm{e} \varepsilon c^2\right)$$

$$\sigma_{\mathrm{RR}} = \sigma_{\mathrm{PI}} \frac{g_f}{g_i} \frac{{E_\gamma}^2}{\varepsilon\left(\varepsilon + 2 m_\mathrm{e} c^2\right)}$$

Atomic Data Needs:
and our team


non-LTE

LTE

Energy levels

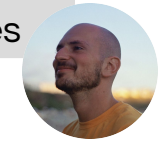

Recombination rates


Central potential → Wavefunctions

Calibration

Radiative rates (M1, E2 transitions)

Radiative rates (E1 transitions)

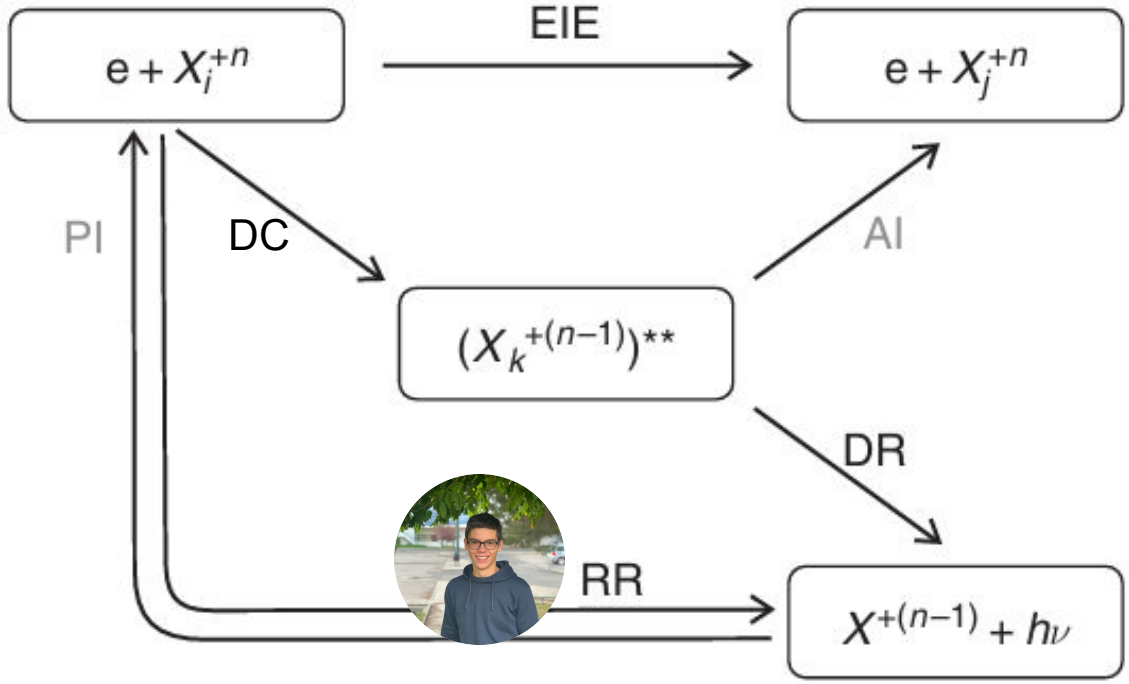

Electron-impact excitation rates


Detail in Modelling

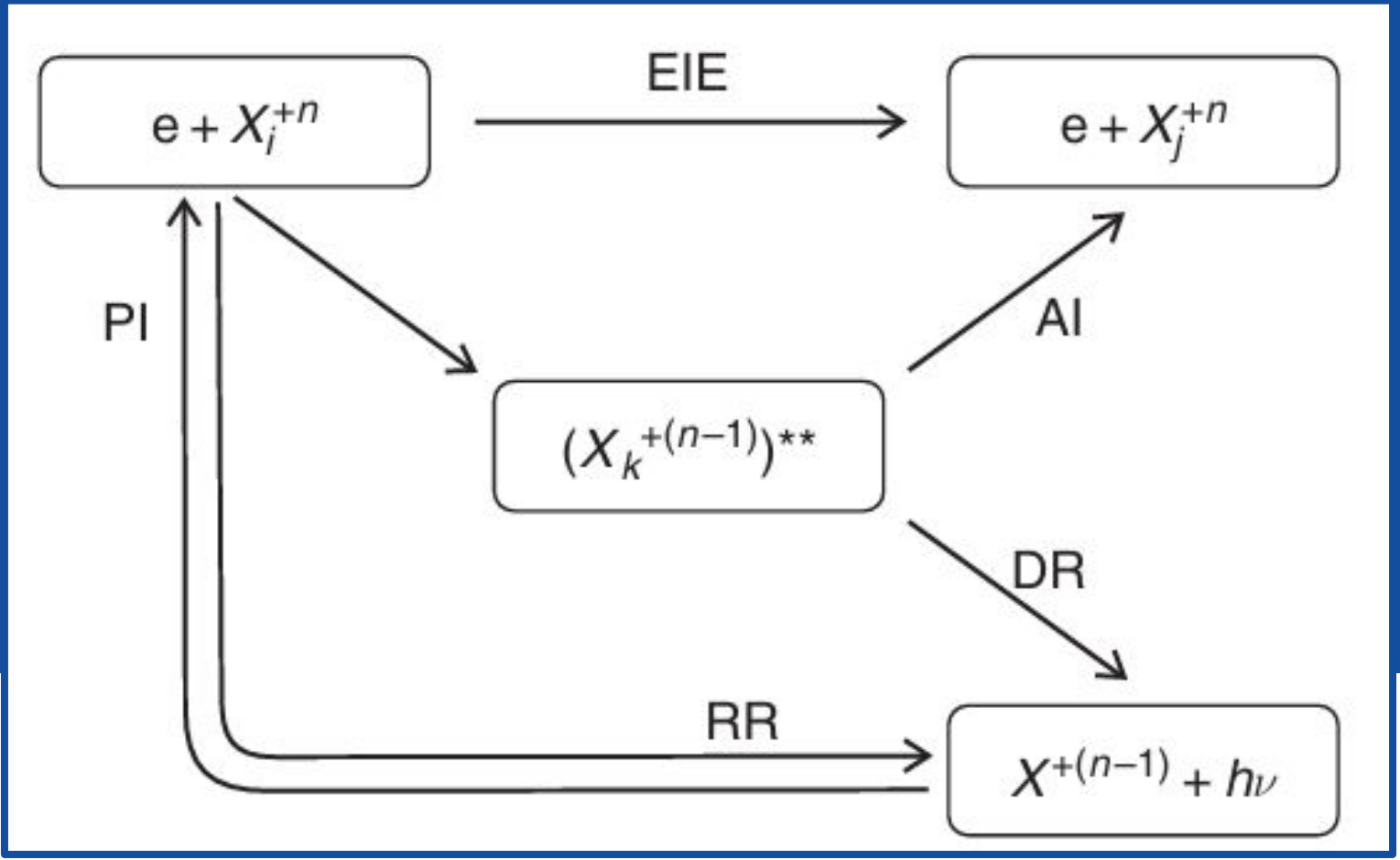
Atomic Data needs:
for astrophysical plasmas

Energy levels

Radiative rates
(E1 transitions)



A.K. Pradhan and S.N. Nahar. **Atomic Astrophysics and Spectroscopy**. Cambridge University Press, 2011.



Anil K. Pradhan and Sultana N. Nahar. **Atomic Astrophysics and Spectroscopy**. Cambridge University Press, 2011.

Breit

Interactions

W. Eissner, M. Jones, and H. Nussbaumer. *Computer Physics Communications*, 8(4):270–306, 1974.

3. Relativistic corrections

3.1. The Breit–Pauli hamiltonian

The Breit–Pauli hamiltonian H_{BP} can be written

$$H_{\mathrm{BP}} = H_{\mathrm{nr}} + H_{\mathrm{rc}}\,, \tag{43}$$

where H_{nr} has been defined in (2) and H_{rc} is a sum of relativistic correction operators:

$$H_{\mathrm{rc}} = \sum_{i=1}^{N} \{f_i(\mathrm{mass}) + f_i(\mathrm{d}) + f_i(\mathrm{so})\} + \sum_{i>j} \{g_{ij}(\mathrm{so} + \mathrm{so}') + g_{ij}(\mathrm{ss}') + g_{ij}(\mathrm{css}') + g_{ij}(\mathrm{d}) + g_{ij}(\mathrm{oo}')\}\,. \tag{44}$$

In (44) the various operators are:

(i) The one-body terms

$$f_i(\mathrm{mass}) = -\tfrac{1}{4}\alpha^2\nabla_i^4, \quad f_i(\mathrm{d}) = -\tfrac{1}{4}Z\alpha^2\nabla_i^2(1/r_i), \quad f_i(\mathrm{so}) = (Z\alpha^2/r_i^3)\,\boldsymbol{l}(i)\cdot\boldsymbol{s}(i). \tag{45}$$

(ii) The two-body fine structure terms

$$g_{ij}(\mathrm{so}+\mathrm{so}') = -\alpha^2\left\{\left(\frac{\boldsymbol{r}_{ij}}{r_{ij}^3}\times\boldsymbol{p}_i\right)\cdot(\boldsymbol{s}(i)+2\boldsymbol{s}(j)) + \left(\frac{\boldsymbol{r}_{ij}}{r_{ij}^3}\times\boldsymbol{p}_j\right)\cdot(\boldsymbol{s}(j)+2\boldsymbol{s}(i))\right\}, \tag{46}$$

$$g_{ij}(\mathrm{ss}') = 2\alpha^2\left\{\frac{\boldsymbol{s}(i)\cdot\boldsymbol{s}(j)}{r_{ij}^3} - 3\,\frac{(\boldsymbol{s}(i)\cdot\boldsymbol{r}_{ij})(\boldsymbol{s}(j)\cdot\boldsymbol{r}_{ij})}{r_{ij}^5}\right\}'.$$

(iii) The two-body non-fine structure terms

$$g_{ij}(\mathrm{css}') = -\frac{16\pi}{3}\,\alpha^2\,\boldsymbol{s}(i)\cdot\boldsymbol{s}(j)\,\delta^3(\boldsymbol{r}_{ij}), \quad g_{ij}(\mathrm{d}) = \tfrac{1}{2}\alpha^2\nabla_i^2\left(\frac{1}{r_{ij}}\right), \quad g_{ij}(\mathrm{oo}') = -\frac{\alpha^2}{r_{ij}}\left(\boldsymbol{p}_i\cdot\boldsymbol{p}_j + \frac{\boldsymbol{r}_{ij}\cdot(\boldsymbol{r}_{ij}\cdot\boldsymbol{p}_j)\boldsymbol{p}_i}{r_{ij}^3}\right). \tag{47}$$