ATOMIC STRUCTURE CALCULATIONS AT LISBON

FOR SPECTROSCOPY, CANCER THERAPY, AND…

… *NEUTRON STAR MERGERS?*

EMMI Rapid Reaction Task Force:
The physics of Neutron Star Mergers at GSI/FAIR
(4-15 June, 2018)

JORGE MIGUEL SAMPAIO

LIP

LABORATÓRIO DE INSTRUMENTAÇÃO
E FÍSICA EXPERIMENTAL DE PARTÍCULAS

Layout

- Motivation
- Multi-configuration Dirack-Fock (MCDF) method
- Atomic structure calculations
- The mcdfgme code
- Applications
- Large scale calculations
- Summary

Motivation

About one month ago, I came to GSI…

… to attend the **MAT Science Week**

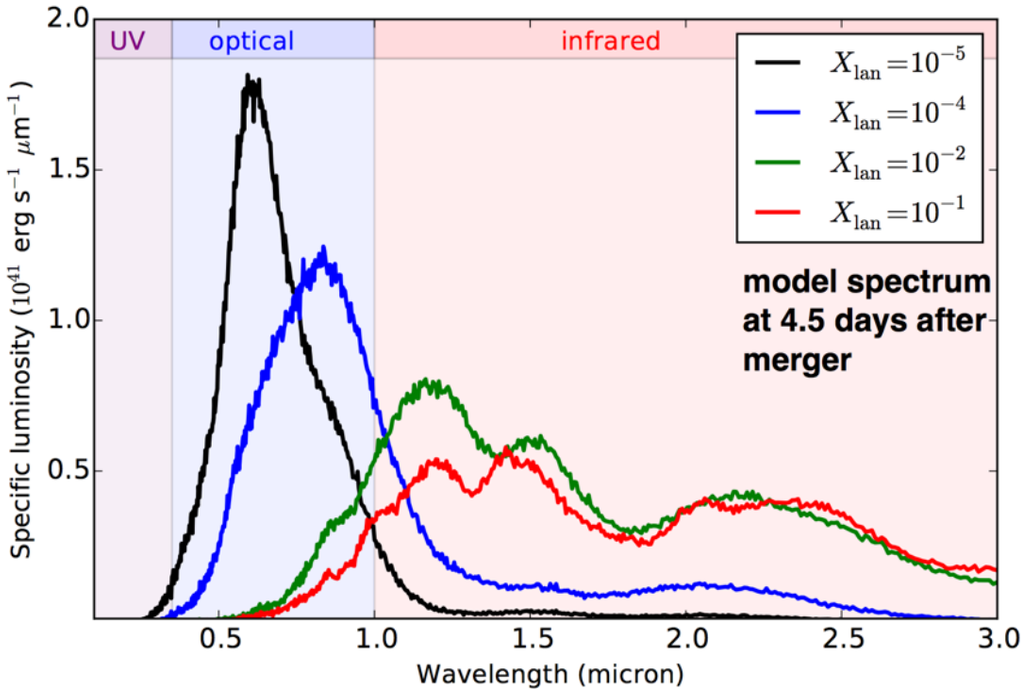
… and to talk with the **biophysics group**…

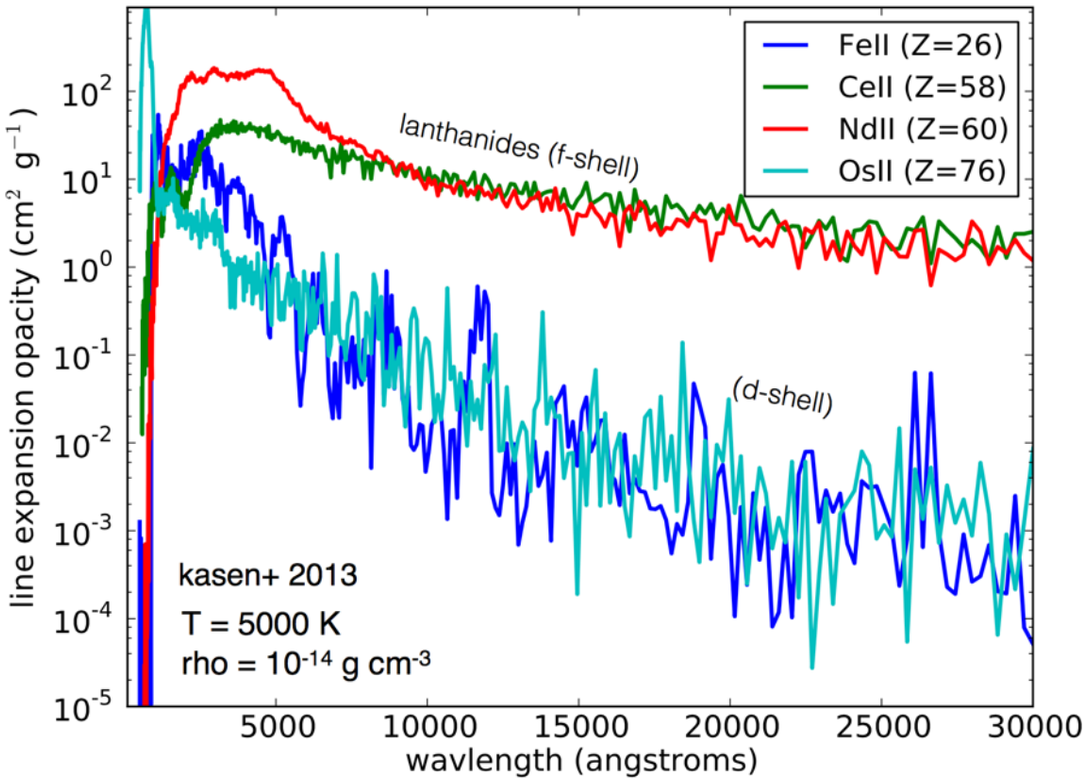
… and I payed a visit to **Gabriel** that I had not seen for **10 years.** He gave me a ride to the hotel …

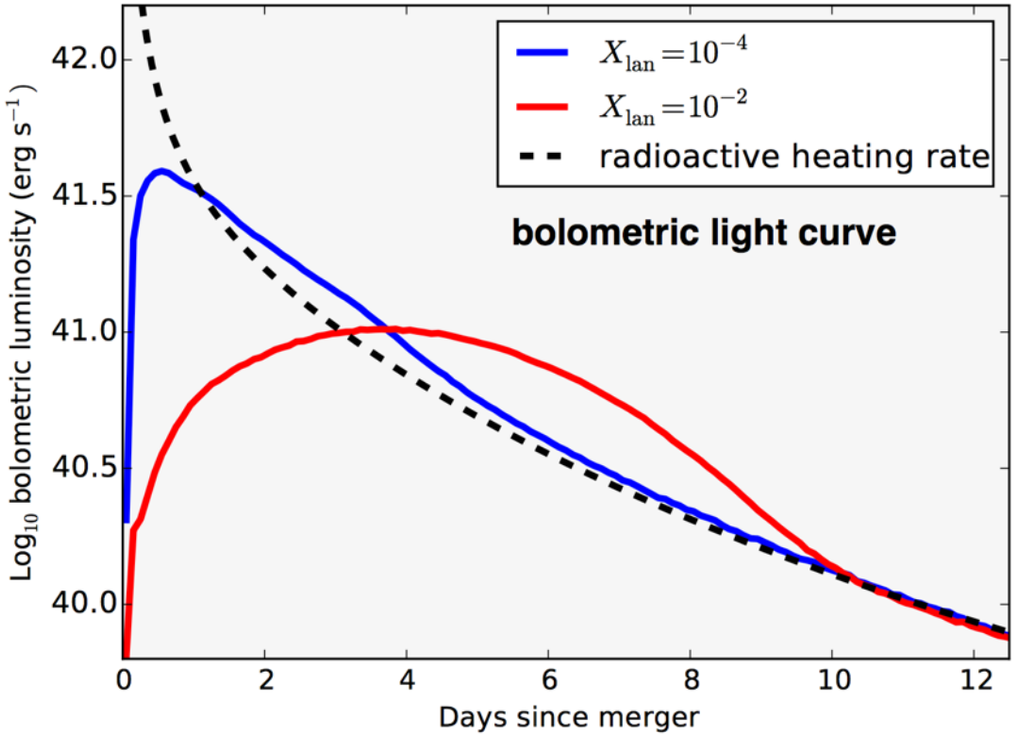
… and I told him that I have been doing **atomic structure calculations.**

He exclaimed: **“I'm interested in that!”**

Motivation





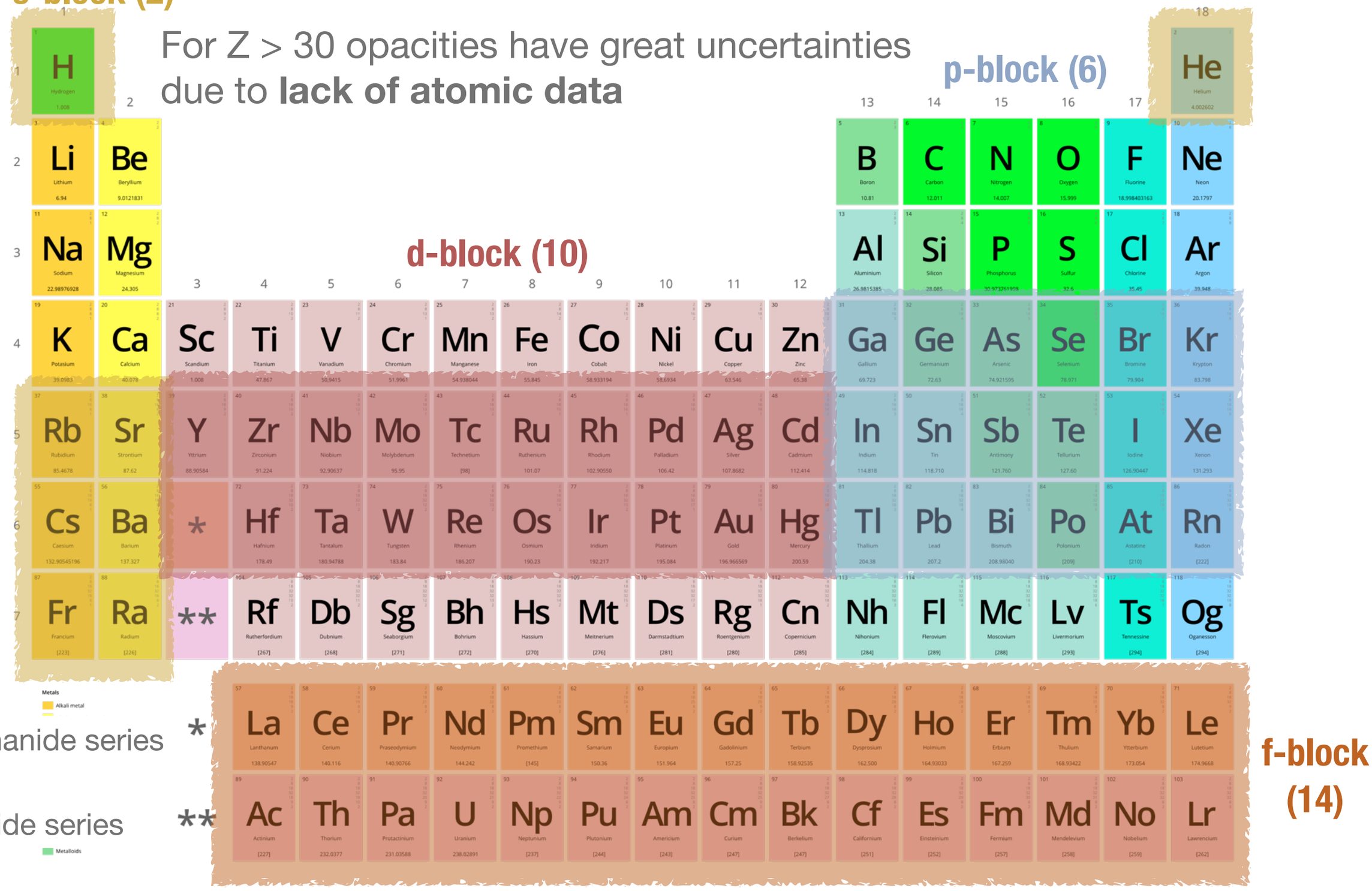


$X_{lan}<10^{-4}$: **low opacity** ejecta ($k\lesssim 1$ cm^2/g)

$X_{lan}>10^{-2}$: **high opacity** ejecta ($k\approx 10$ cm^2/g)

Kasen et al. Astrophys. J. (2013) and Nature (2017)

Motivation



For Z > 30 opacities have great uncertainties due to **lack of atomic data**

Motivation

Atomic data needs for stellar modelling

- Levels energies
- Oscillator strengths (bound-bound radiative processes)
- Photoionisation cross-sections (bound-free processes)
- Free-free scattering

Variational Relativistic Atomic Structure Calculations

$$\delta E[\Psi] = \delta \left[\frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle} \right] = 0$$

Multi-Configuration Dirac-Fock (MCDF) method

MCDF method (Hamiltonian)

- "No-pair" (np) **Dirac-Coulomb-Breit** (DCB) hamiltonian

$$H_{np} = \sum_a h_a^D + \sum_{a<b} P_{ab}^{++} V_{ab} P_{ab}^{++}$$

Projectors into positive energy states

- One-electron Dirac hamiltonian

$$h_a^D = c\boldsymbol{\alpha_a} \cdot \boldsymbol{p_a} + c^2(\beta_a - 1) + V_a^N$$

Nuclear interaction

Dirac matrices

- Two-electrons interaction (in the Coulomb gauge)

$$V_{ab} = \frac{1}{r_{ab}} - \frac{\boldsymbol{\alpha}_a \cdot \boldsymbol{\alpha}_b}{r_{ab}} \cos(\omega_{ab} r_{ab}/c) + c^2(\boldsymbol{\alpha}_a \cdot \boldsymbol{\nabla}_a)(\boldsymbol{\alpha}_b \cdot \boldsymbol{\nabla}_b) \frac{\cos(\omega_{ab} r_{ab}/c) - 1}{\omega_{ab}^2 r_{ab}}$$

Coulomb interaction

Breit interaction

MCDF method (Atomic States)

- Configuration state functions (CSF) ☞ **Configuration Interaction** (mixing) method

$$\Phi^{\nu}_{\Pi,J,M}(\vec{r}_1,\cdots,\vec{r}_a,\cdots) = \sum_q C_q \begin{vmatrix} \phi^q_{n_1\kappa_1 m_1}(\vec{r}_1) & \cdots & \phi^q_{n_a\kappa_a m_a}(\vec{r}_1) & \cdots \\ \vdots & \cdots & \vdots & \cdots \\ \phi^q_{n_1\kappa_1 m_1}(\vec{r}_a) & \cdots & \phi^q_{n_a\kappa_a m_a}(\vec{r}_a) & \cdots \\ \vdots & \cdots & \vdots & \cdots \end{vmatrix}$$

Dirac spinor

Mixing coefficient of different CSF

Slater determinant

- Atomic state function (ASF) ☞ **Multi-Configuration** (correlation) method

$$\Psi_{\Pi,J,M}(\vec{r}_1,\cdots,\vec{r}_a,\cdots) = \sum_{\nu=1}^{N_{CSF}} c_\nu \Phi^{\nu}(\vec{r}_1,\cdots,\vec{r}_a,\cdots)$$

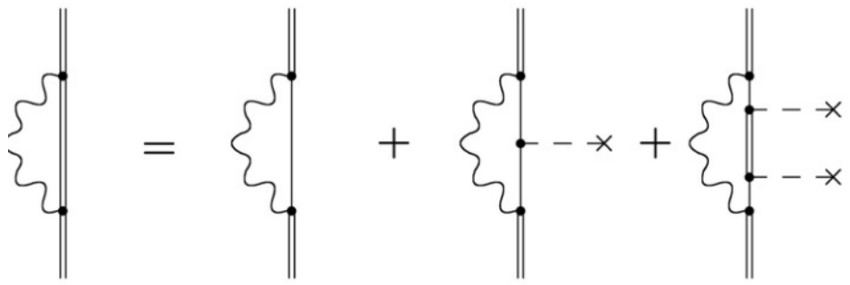
CSF

Mixing coefficient of ground and excited CSFs

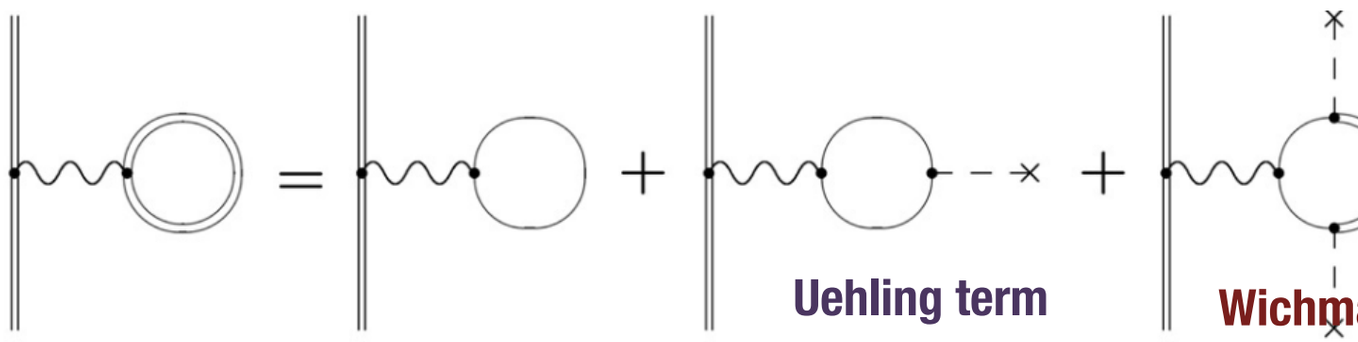
Froese Fischer, Comput. Phys. Commun. (1991)
Grant, Comput. Phys. Commun. (1994)

MCDF method (QED)

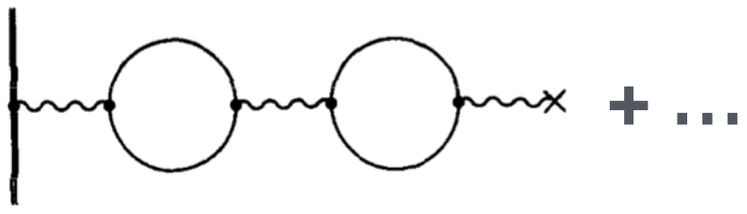
Self-energy (one-loop)



Vacuum polarisation (one-loop)



(two-loops)



P. J. Mohr et al., Phys. Rep. (1998)

Andreev et al., Phys. Rep. (2008)

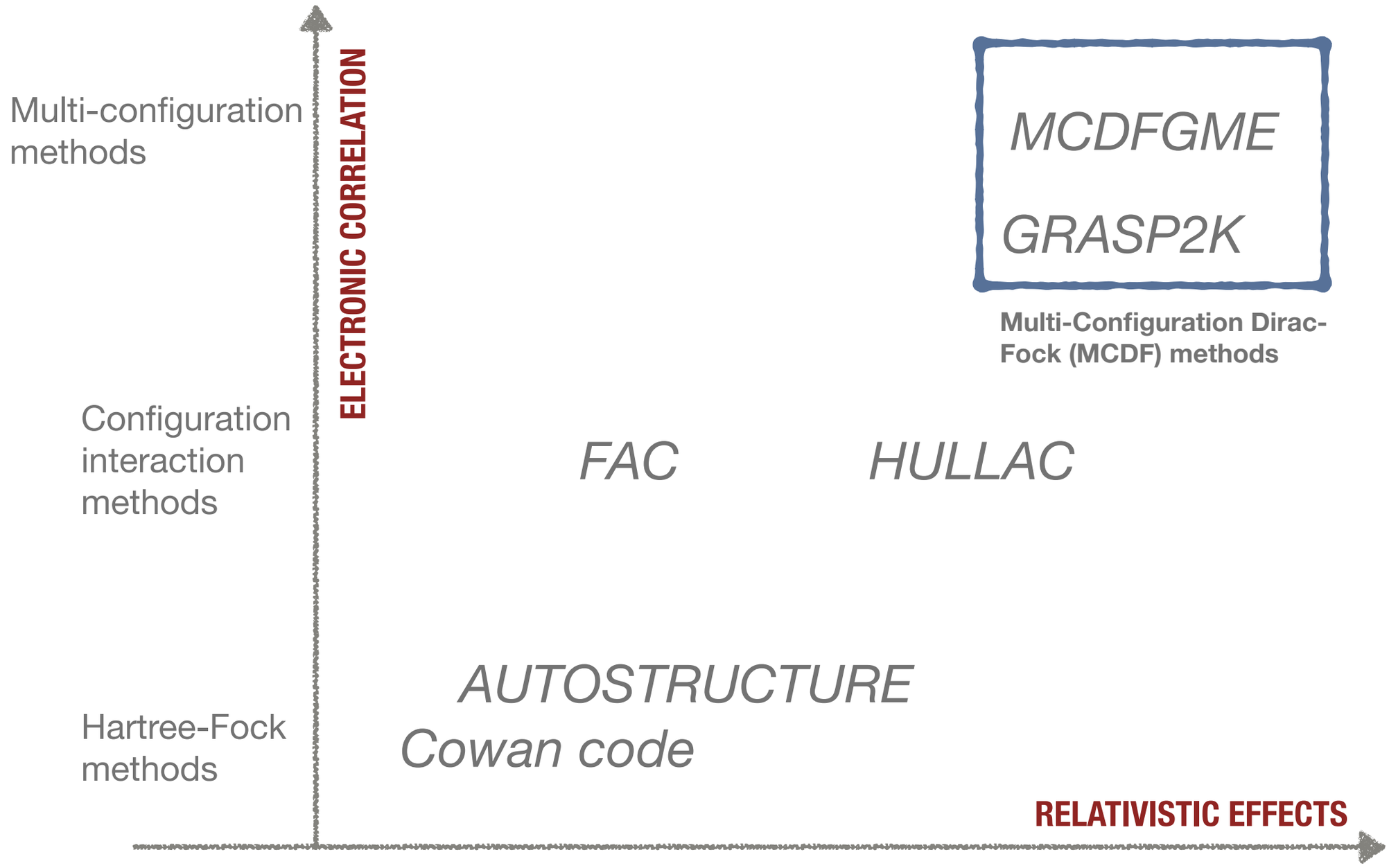
Atomic structure calculations

Effects on atomic levels

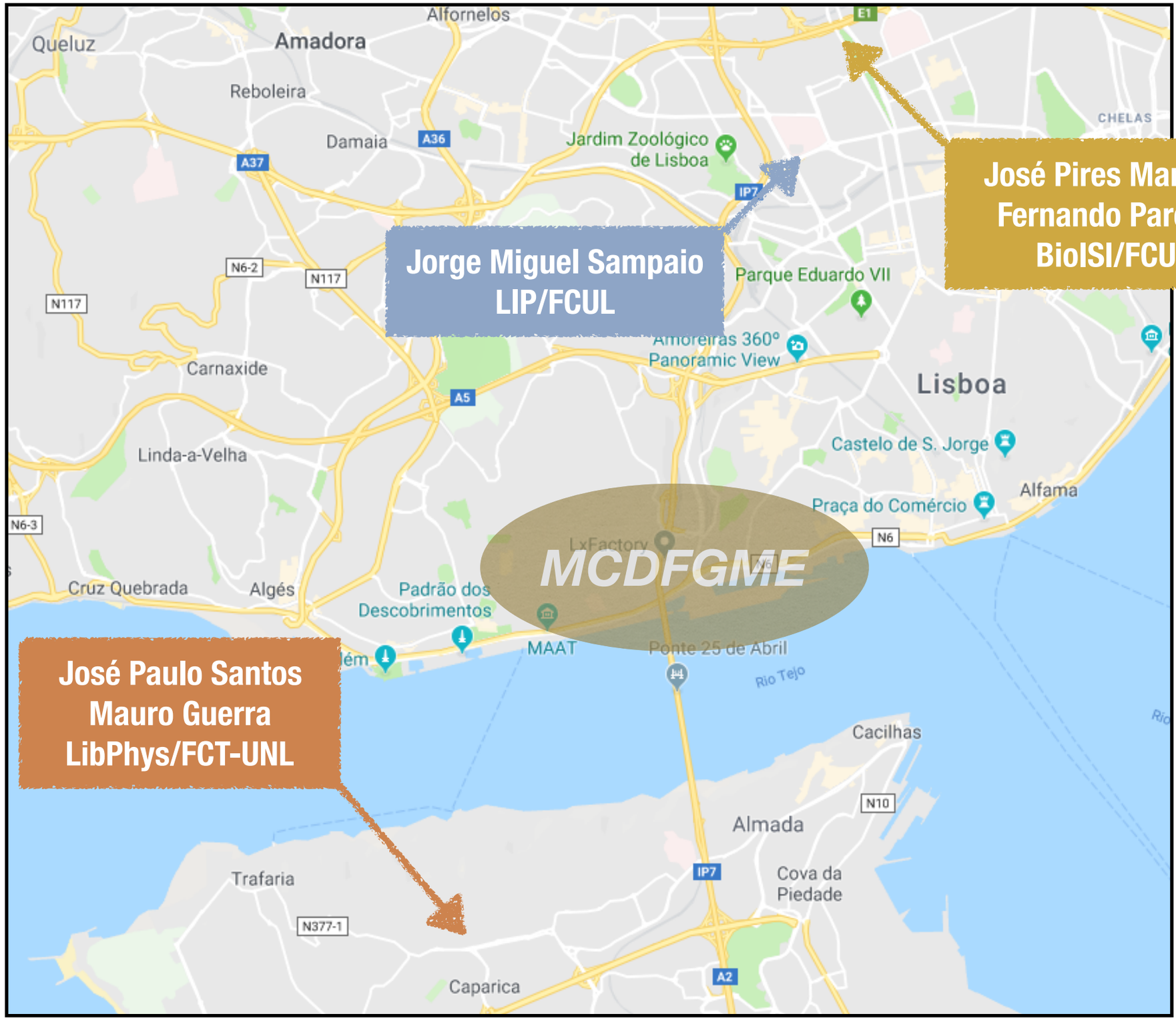
	$Z_{eff}(nl) \leq 20$	$20 \leq Z_{eff}(nl) \leq 60$	$Z_{eff}(nl) \geq 60$
Correlation	**Dominant**	**Important**	Needed
Relativity	Needed	**Important**	**Dominant**
QED	Marginal	Needed	**Important**

$$Z_{eff}(nl) = Z - \langle \#\ core\ electrons \rangle_{nl}$$

Atomic structure calculations



The “atomic group” at Lisbon



The *MCDFGME* code

The ***MCDFGME*** code developed by Desclaux and Indelicato implements the **MCDF method,** including:

- Low-order Coulomb-Breit interaction ($\omega_{ab} = 0$)
- Uehling vacuum polarisation term
- Self-energy

} **Self-consistent field**

- High-order Coulomb-Breit interaction ($\omega_{ab} > 0$)
- Wichmann-Koll and Källén-Sabry terms

} **As perturbations**

Nuclear mass models options:

- Point nucleus, uniform charge, exponential, gaussian and Fermi distributions.

The *MCDFGME* code

Current version (2017) computes:

- **Level energies** (configuration state or multi-configuration state levels)
- **Radiative transition probabilities and oscillator strengths**
- Radiationless transition probabilities (Auger and Coster-Kronig)
- **Photoionisation cross-sections**
- **Electron excitation cross-sections**
- Hyperfine splitting including nuclear mass (isotopic and specific) shifts, and field shifts
- Overlap integrals for calculation of shake processes (shake-up and shake-off)…

… and more…

Fundamental atomic parameters

International initiative on X-ray fundamental parameters:

- Mass absorption coefficients (photoionisation cross-sections)
- Fluorescence yields (radiative and radiationless transitions)
- Line intensities (radiative and radiationless transitions, shake processes)
- Electron ionisation cross-sections

- Structure of high-resolution K $\beta_{1,3}$ x-ray emission spectra for the elements from Ca to Ge, I*to et al., Phys. Rev. A* (2018)
- Theoretical and experimental determination of K - And L -shell x-ray relaxation parameters in Ni, *M. Guerra, J M. Sampaio et al.,* Phys. Rev. A (2018)
- Relativistic calculations of K-, L- and M-shell X-ray production cross-sections by electron impact for Ne, Ar, Kr, Xe, Rn and Uuo, *J. M. Sampaio et al., J. Quant. Spectrosc. Radiat. Transfer* (2016)
- Calculations of photo-induced X-ray production cross-sections in the energy range 1–150 keV and average fluorescence yields for Zn, Cd and Hg, *J. M. Sampaio et al., At. Data. Nucl. Data Tables* (2016)

Fundamental atomic parameters

Example: K-shell (1s) fluorescence yield and photoionisation cross-sections in **Fe**

- Level energies calculated: **5933** (without correlation)
- Radiative transition probabilities: **38871**
- Radiationless transition probabilities: **309234**
- Photoionisation cross-sections (one energy): **2142**

CPU time per transition: ~3-20 seconds (4-CPU, 64-bits, 2.8 GHz)
Data storage: ~ 24 GB ☞ ~69 kB/transition

Thus,

- Cross-section (one energy): **~7 CPU hours**
- Fluorescence yield: **~1.5 CPU months**

Auger emitters for cancer therapy

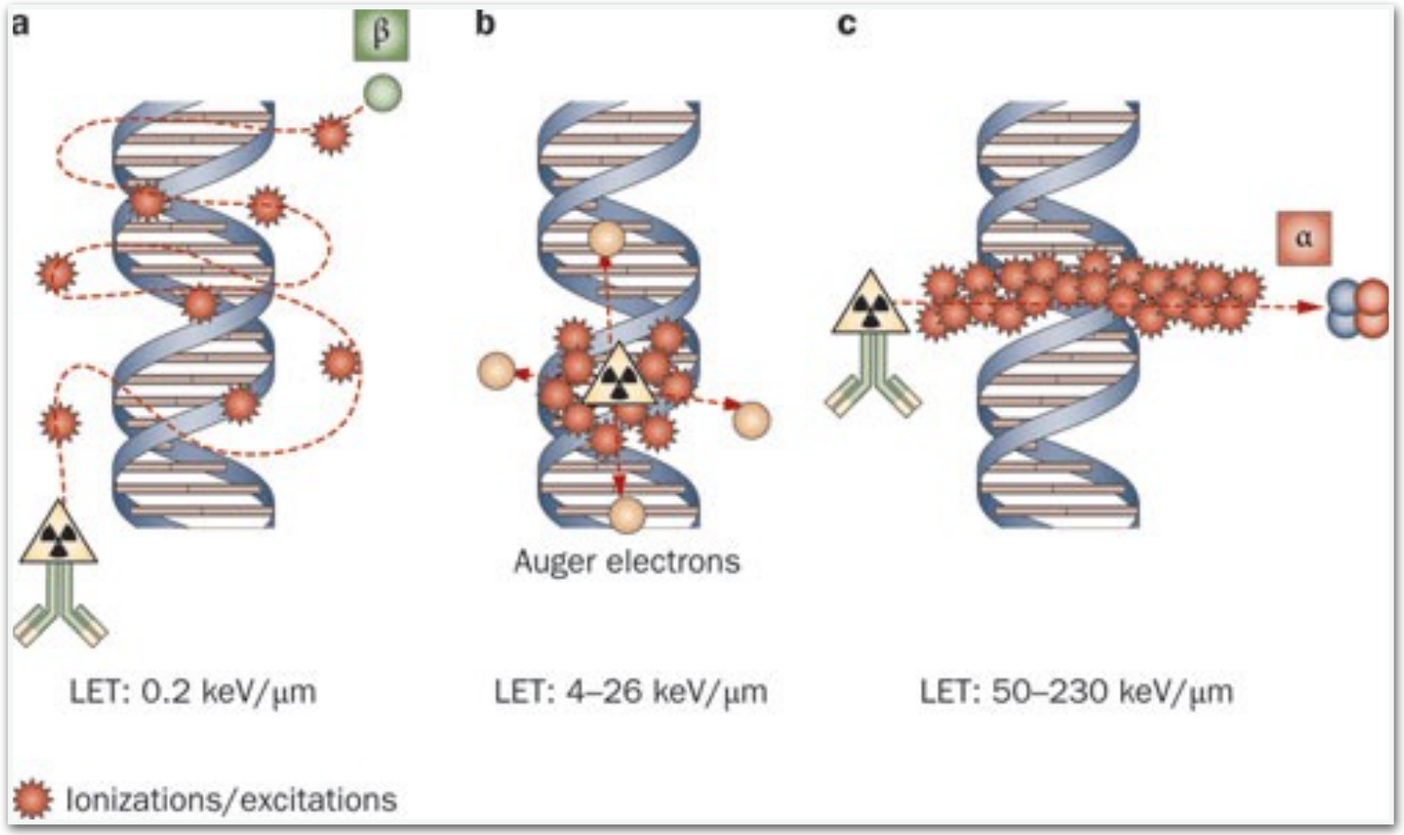
targeted

Auger electrons:

- Energy: ~20 - 500 ev
- Range ~1 - 10 nm

***LET*~ 2 - 30 keV/µm**

High RBE

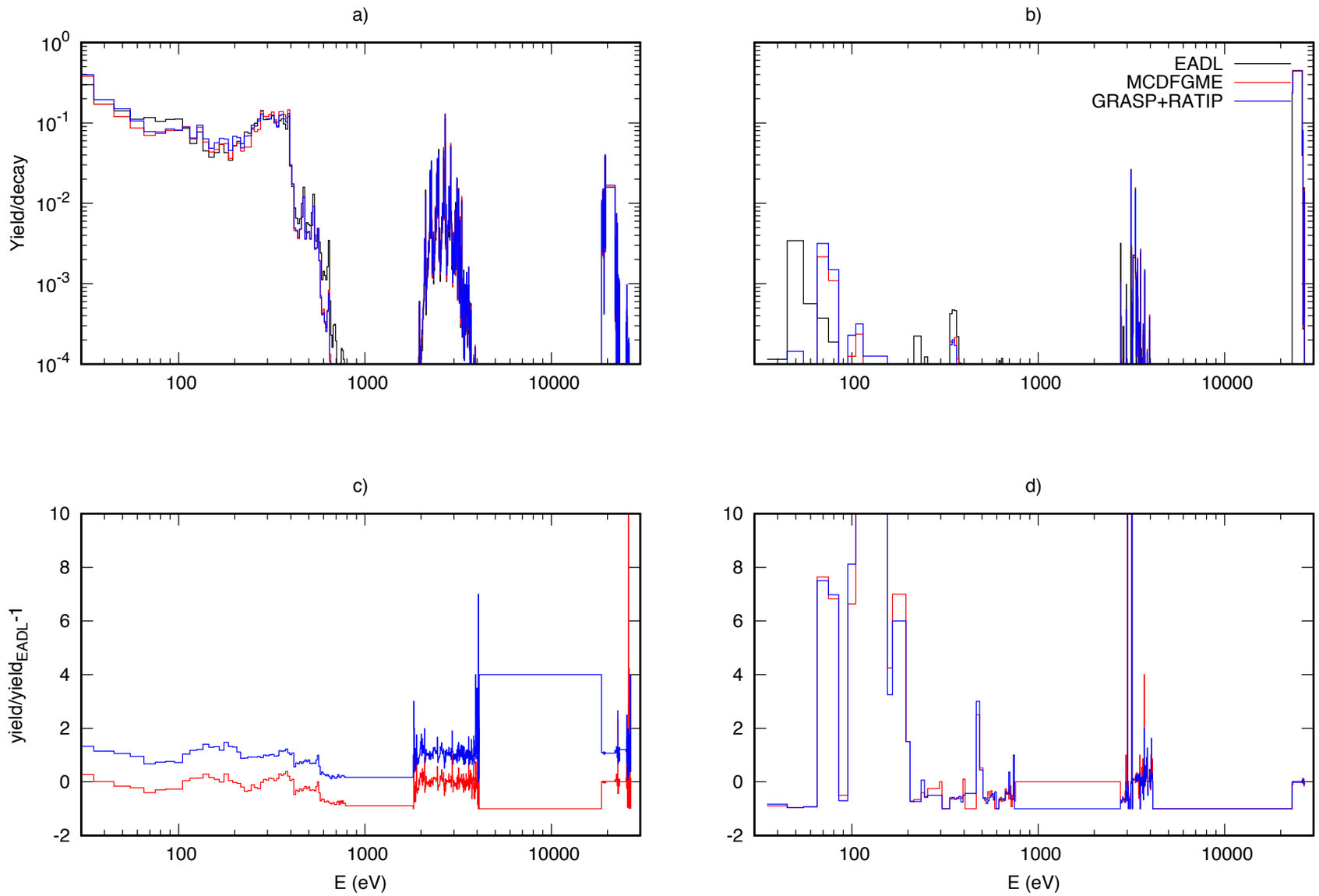


☞ Auger-emitters can trigger clusters of ionisations near the DNA molecule

Auger emitters for cancer therapy

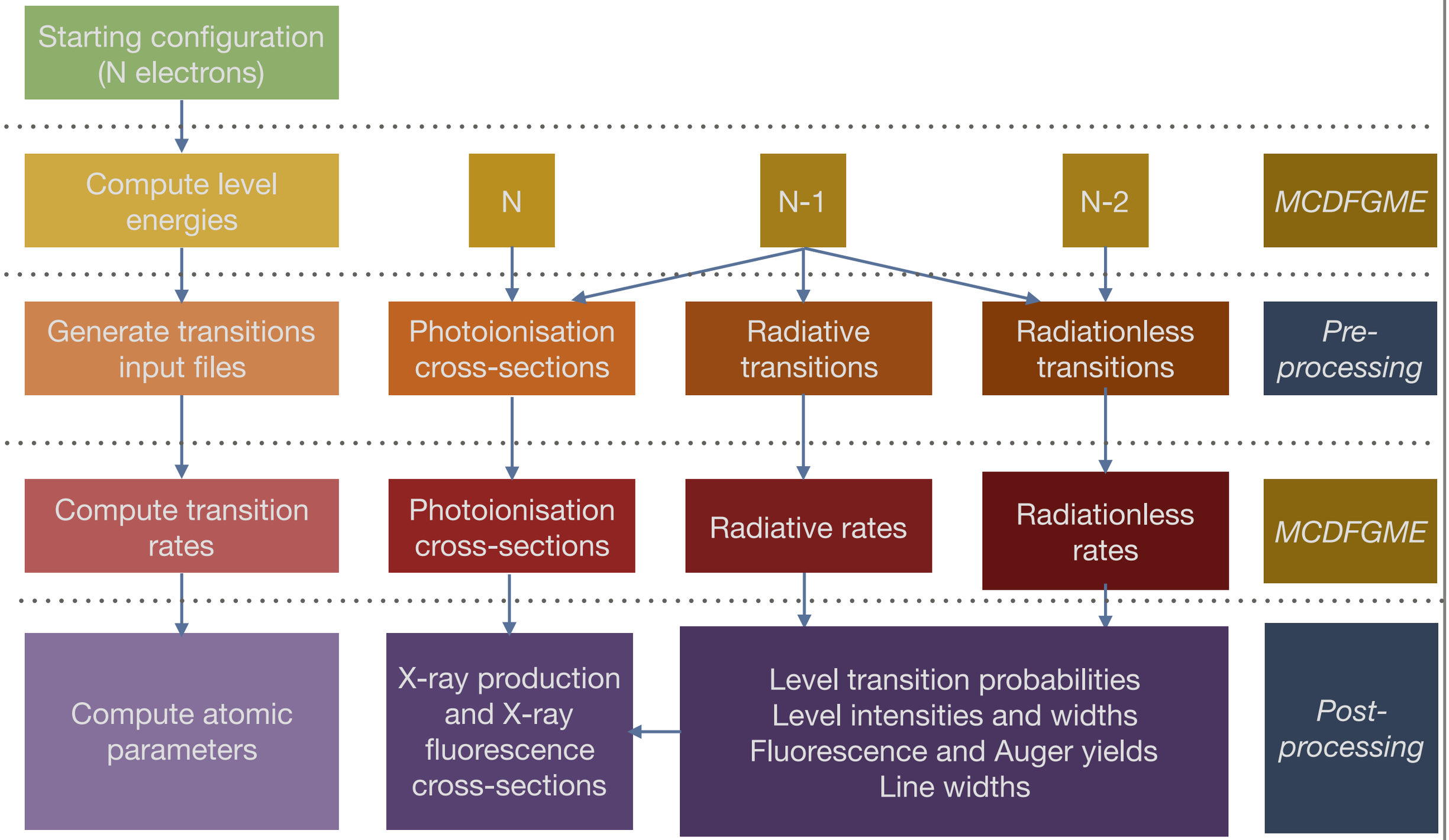
targeted

Work in progress



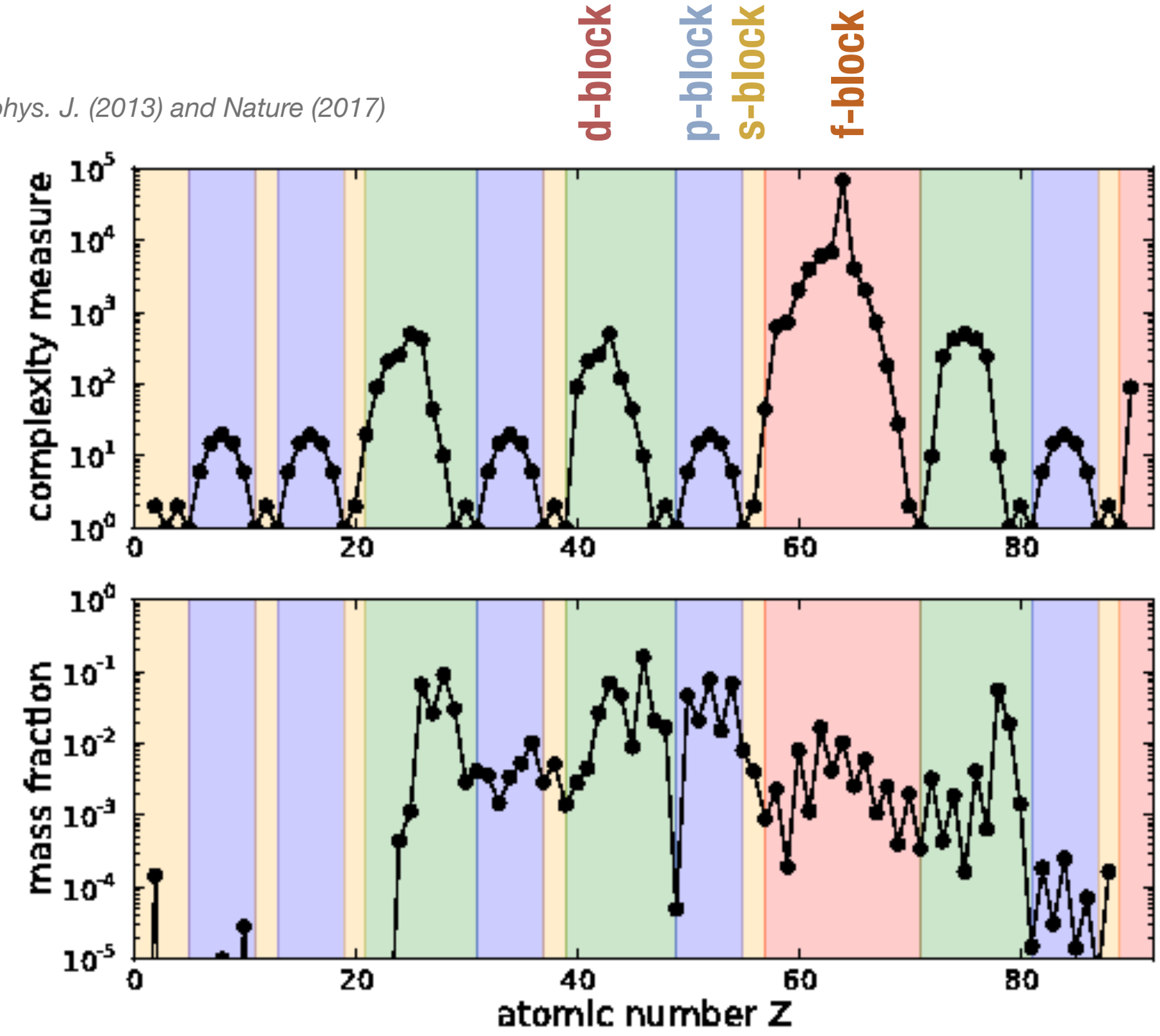
T. Kibedi, A. Stuchbery, B. Lee (ANU) and J. Ekman, P. Jönsson (GRASP2K) and J. M. Sampaio, J. P. Marques (MCDFGME)

Large-scale calculations



Large-scale calculations

Kasen et al. Astrophys. J. (2013) and Nature (2017)

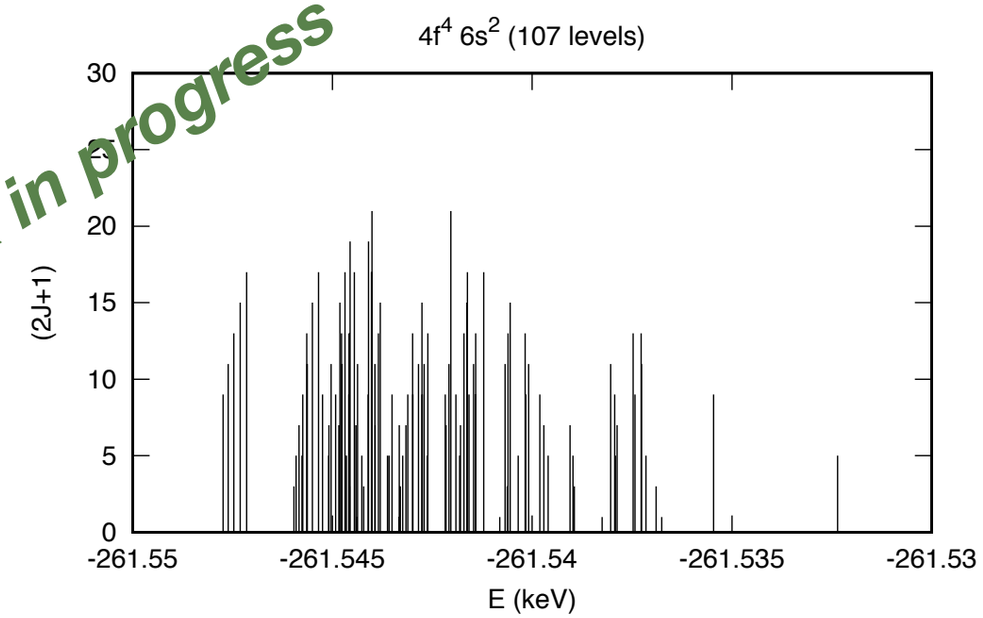


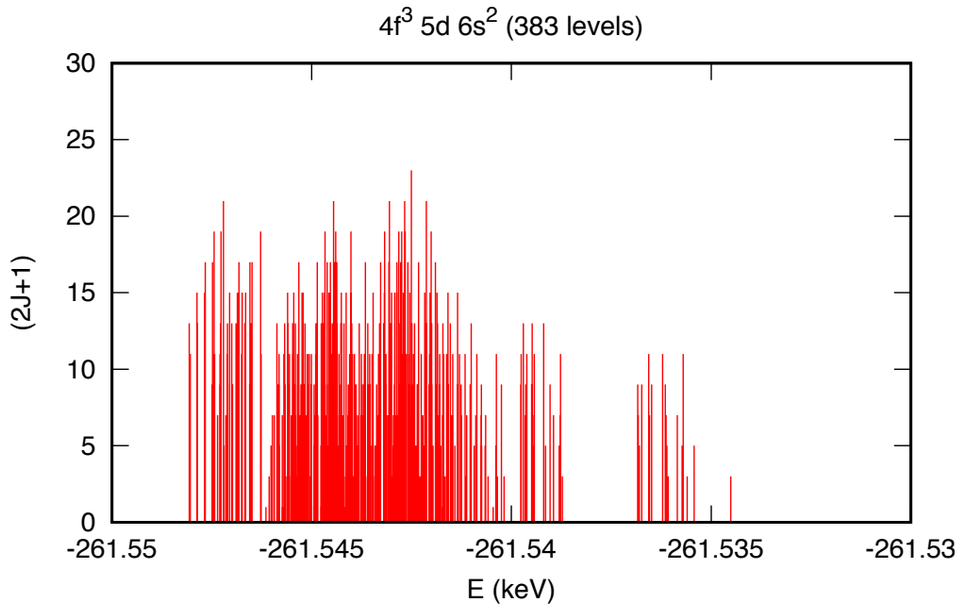
Number of levels increases drastically for f-block elements with open shells

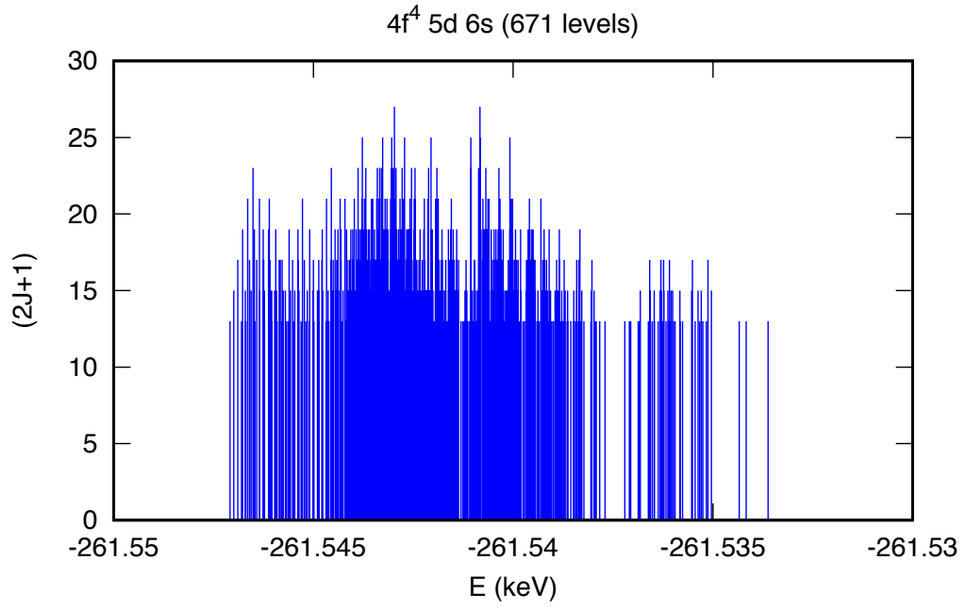
Large-scale calculations

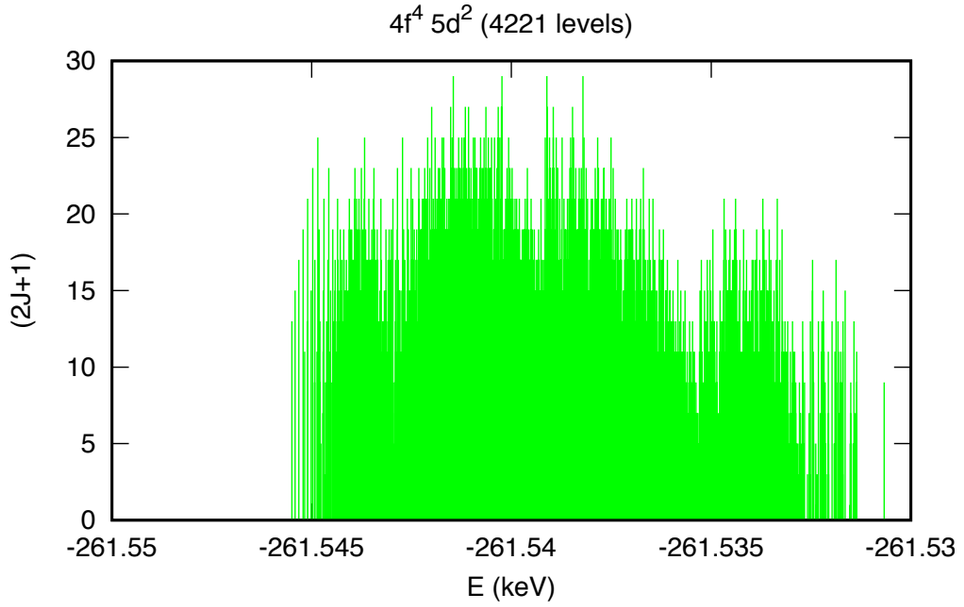
Level energies for Nd I configurations: **$4f^4 6s^2$**, $4f^3 5d\ 6s^2$, $4f^4 5d\ 6s$, $4f^4 5d^2$, …

Work in progress









Large-scale calculations

Ion	Configurations included	# levels	# lines	χ (eV)
FeI	$\mathbf{3d^6 4s^2}, 3d^7 4s, 3d^6 4s4p, 3d^7 4p, 3d^7 4d, 3d^7 4f, 3d^7 5s, 3d^7 5p, 3d^7 5d, 3d^6 4s4d$	1784	326,519	7.90
FeII	$\mathbf{3d^6 4s}, 3d^7, 3d^6 4p, 3d^6 4d, 3d^6 4f, 3d^6 5s, 3d^6 5p, 3d^6 5d, 3d^5 4s^2, 3d^5 4s4p$	1857	355,367	16.18
FeIII	$\mathbf{3d^6}, 3d^5 4s, 3d^5 4p, 3d^5 4d, 3d^5 4f, 3d^5 5s, 3d^5 5p, 3d^5 5d, 3d^4 4s4p$	2050	420,821	30.65
FeIV	$\mathbf{3d^5}, 3d^4 4s, 3d^4 4p, 3d^4 4d, 3d^4 4f, 3d^4 5s, 3d^4 5p, 3d^4 5d$	1421	217,986	54.91
CoI	$\mathbf{3d^7 4s^2}, 3d^8 4s, 3d^7 4s4p, 3d^9, 3d^8 4p, 3d^8 4d, 3d^8 5s, 3d^7 4s4d, 3d^7 4s5s$	778	62,587	7.88
CoII	$\mathbf{3d^8}, 3d^7 4s, 3d^6 4s^2, 3d^7 4p, 3d^6 4s4p, 3d^7 5s, 3d^7 4d$	757	58,521	17.08
CoIII	$\mathbf{3d^7}, 3d^6 4s, 3d^6 4p, 3d^6 4d, 3d^6 5s$	601	34,508	33.50
CoIV	$\mathbf{3d^6}, 3d^5 4s, 3d^5 4p, 3d^5 4d, 3d^5 5s$	728	48,254	51.27
NiI	$\mathbf{3d^8 4s^2}, 3d^{10}, 3d^8 4s4p, 3d^9 4s, 3d^9 4p, 3d^9 4d, 3d^9 4f, 3d^9 5s, 3d^9 5p, 3d^9 6s$	174	2,776	7.64
NiII	$\mathbf{3d^9}, 3d^8 4s, 3d^8 4p, 3d^8 4d, 3d^8 4f, 3d^8 5s, 3d^8 5p, 3d^8 6s, 3d^7 4s4p, 3d^7 4s^2$	520	25,496	16.18
NiIII	$\mathbf{3d^8}, 3d^7 4s, 3d^7 4p, 3d^7 4d, 3d^7 4f, 3d^7 5s, 3d^7 5p, 3d^7 6s, 3d^6 4s^2$	1644	61,108	35.19
NiIV	$\mathbf{3d^7}, 3d^6 4s, 3d^6 4p, 3d^6 4d, 3d^6 4f, 3d^6 5s, 3d^6 5p, 3d^6 6s, 3d^5 4s4p, 3d^5 4s^2$	751	258,305	54.92
NdI	$\mathbf{4f^4 6s^2}, 4f^3 5d6s^2, 4f^4 5d6s, 4f^4 5d^2, 4f^3 5d6s6p, 4f^4 5d6p$	18104	24,632,513	5.52
NdII	$\mathbf{4f^4 6s}, 4f^4 5d, 4f^4 6p, 4f^3 5d^2, 4f^3 5d6s, 4f^3 5d6p, 4f^3 6s6p$	6888	3,873,372	10.7
NdIII	$\mathbf{4f^4}, 4f^3 5d, 4f^3 6s, 4f^3 6p, 4f^2 5d^2, 4f^2 5d6s, 4f 5d^2 6s$	1650	232,715	22.14
NdIV	$\mathbf{4f^3}, 4f^2 5d, 4f^2 6s, 4f^2 6p$	241	5780	40.4
CeII	$\mathbf{4f5d^2}, 4f5d6s, 4f^2 6s, 4f^2 5d, 4f6s^2, 4f5d6p, 4f^2 6p, 5d^3, 4f6s6p, 4f^3$	5,637	4,349,351	10.8
CeIII	$\mathbf{4f5d}, 4f6s, 5d^2, 4f6p, 5d6s$	3,069	868,640	20.19
OsII	$\mathbf{5d^6 6s}, 5d^6 5f, 5d^6 5g, 5d^6 6s, 5d^6 6p, 5d^6 6d, 5d^6 6f, 5d^6 6g$	3271	1,033,972	17.0
SnII	$\mathbf{5s^2 5p}, 5s^2 4f, 5s^2 5d, 5s^2 6s, 5s^2 6p, 5s5p^2, 5s5p6s, 5s5p6p$	47	371	14.63

Kasen et al. Astrophys. J. (2013)

Summary

- Atomic data needed to model light-curves from neutron star mergers are missing or have large uncertainties
- The most relevant elements are lanthanides and actinides (f-block elements) which have a large valence space
- There are atomic structure codes that can compute atomic parameters with high precision, namely including configuration mixing, multi-configuration correlation, relativistic and QED effects
- These codes can handle calculations in the order of hundreds of thousands of transitions in an acceptable computational time (months)
- Calculations of large open shells beyond configuration mixing method seem to me impracticable at the current computational capabilities
- Calculations with different codes/methods are useful for intercomparison

THANK YOU