Optimization of atomic data for improved kilonova modelling

Ricardo F. Silva

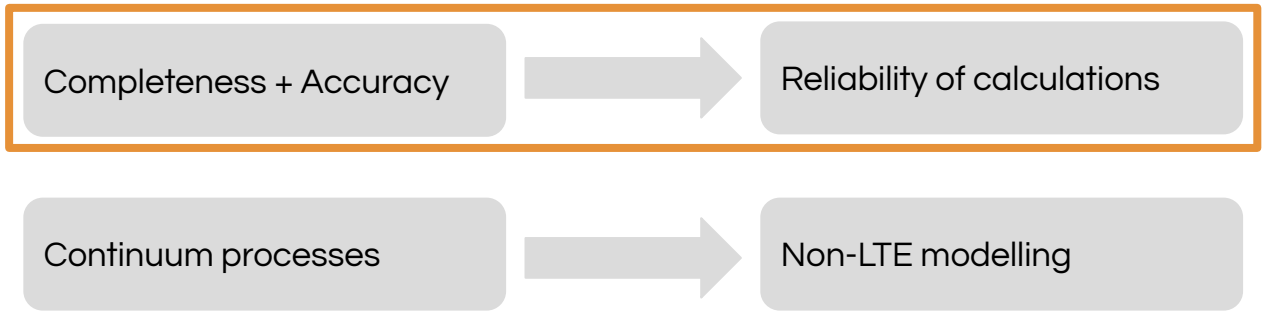
The Radiative Transfer and Atomic Physics of Kilonovae

Status of Calculations for Kilonova

Many recent published calculations:

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 - Ln and Ac (II-IV) + Pt + Au- (optimized potential where exp. data is available)
...

What is missing:



Atomic codes

General use codes - multiple atomic processes

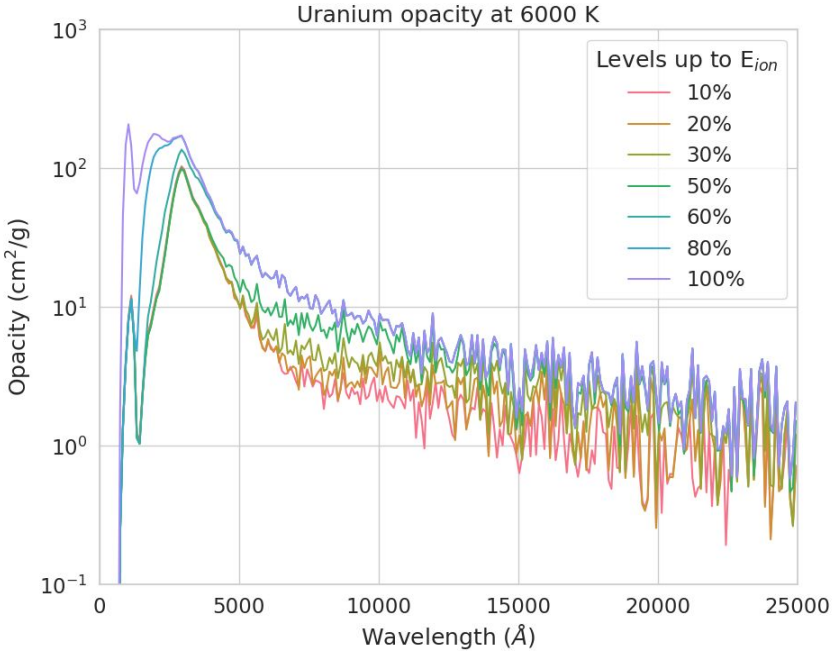
- Usually user-input dependent parameters
- Able to calculate a large number of processes
- Limited accuracy
- Fast and efficient
  - 100 000+ levels and transitions in hours/days
- E.g. - FAC, Hullac, Autostructure, Los Alamos Suite, JAC …

High accuracy structure codes

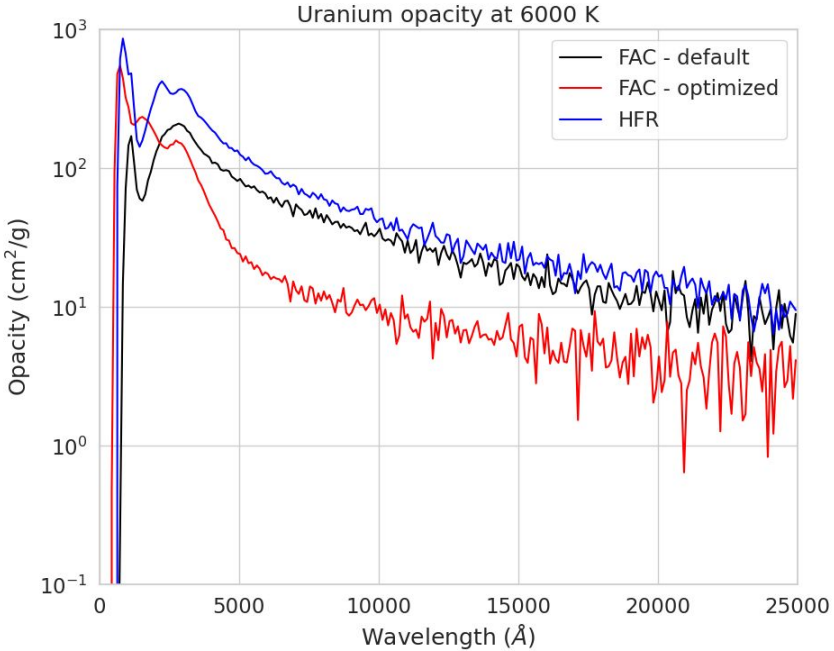
- Fully *ab-initio* using MC(D)HF or MBPT approaches
- Focused on structure and some radiative properties
- High accuracy
- Computationally demanding
  - Months for large scale calculations depending on the code of one ion
- E.g. - GRASP*, ATSP*, MCDFGME*, AMBiT, CI-MBPT…

*Can be (usually) coupled to R-matrix codes for computation of other properties

Completeness/Accuracy Duality



- Necessary to ensure convergence



- Differences in atomic data can have significant effect in opacity

Method - FAC

For the atomic data calculations we make extensive use of the FAC software package:

- Allows for a complete set of data for plasma modelling with speed and utility in mind
  - ➢ Structure, radiative and collisional processes

- Uses a Dirac-Fock-Slater Hamiltonian with a local central potential, computed for a fictitious mean configuration (FMC) with fractional occupation numbers

  - ➢ Orthogonality is ensured automatically → Speed increase

  - ➢ Potential not optimized for a single configuration → Accuracy issues

  - ➢ Choice of FMC is mostly arbitrary and usually constructed by hand → Major source of uncertainty

Method - FAC

Set of configurations $(c_1, c_2, \ldots, c_n)$

Set of weights $(w_1, w_2, \ldots, w_n)$

Mean configuration with fractional occupation numbers

$$\alpha_{Ln} = [\mathrm{Xe}]\ 4f^{\xi_1}\ 5d^{\xi_2}\ 6s^{\xi_3}\ 6p^{\xi_4}\ \ldots$$

$$\alpha_{Ac} = [\mathrm{Rn}]\ 5f^{\xi_1}\ 6d^{\xi_2}\ 7s^{\xi_3}\ 7p^{\xi_4}\ \ldots$$

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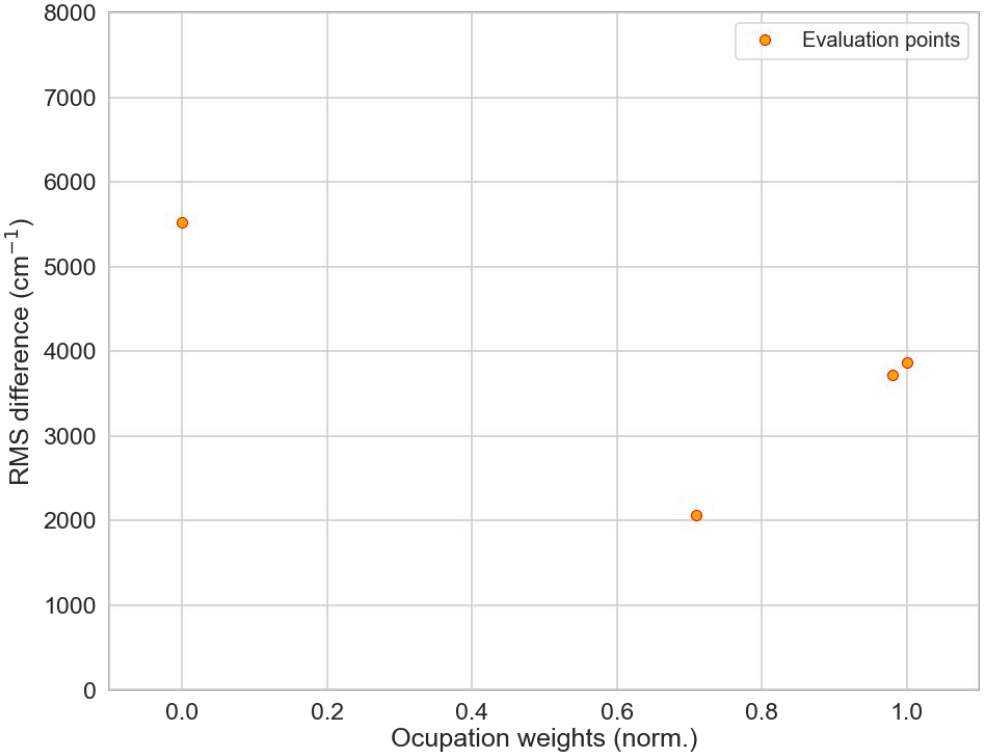
Find the set of ~~weights~~ that provide best match available experimental data
fractional occupation numbers

Optimization procedure

- Choice of fractional occupation numbers (weights) are usually done by hand
  - Choice on how to evaluate data - (weighted) RMS difference, (weighted) average deviation, level density, transition probabilities, convergence…

- After gathering a few points can we learn something?



Example optimization for 1 parameter (4f)
(5d, 6s, 6p) fixed at (0.357,0.0714,0.0714)

Optimization procedure

- Choice of fractional occupation numbers (weights) are usually done by hand
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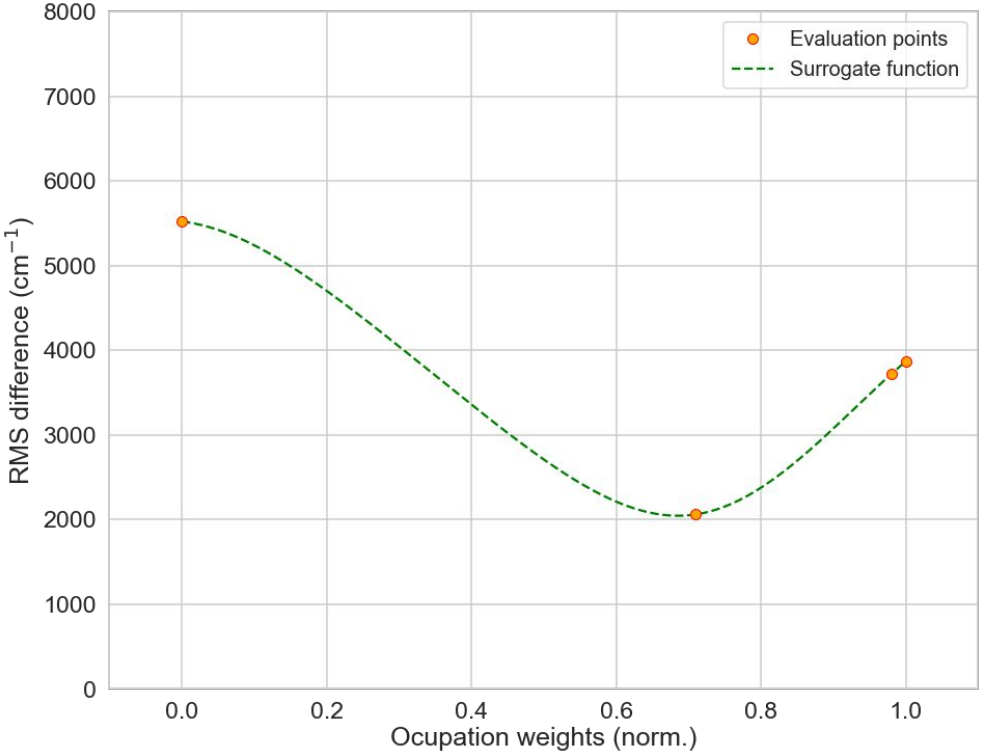
- After gathering a few points can we learn something?
  - Fit a model
    - Different models: Gaussian process, random forest…



Example optimization for 1 parameter (4f)
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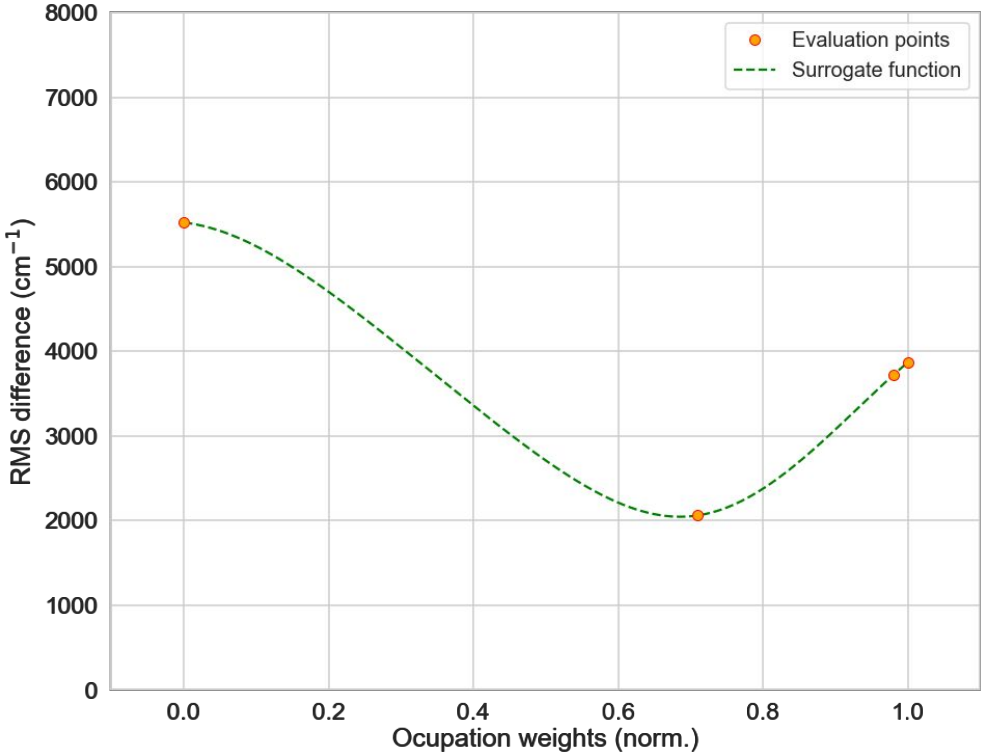
Optimization procedure

- Which point to evaluate next?



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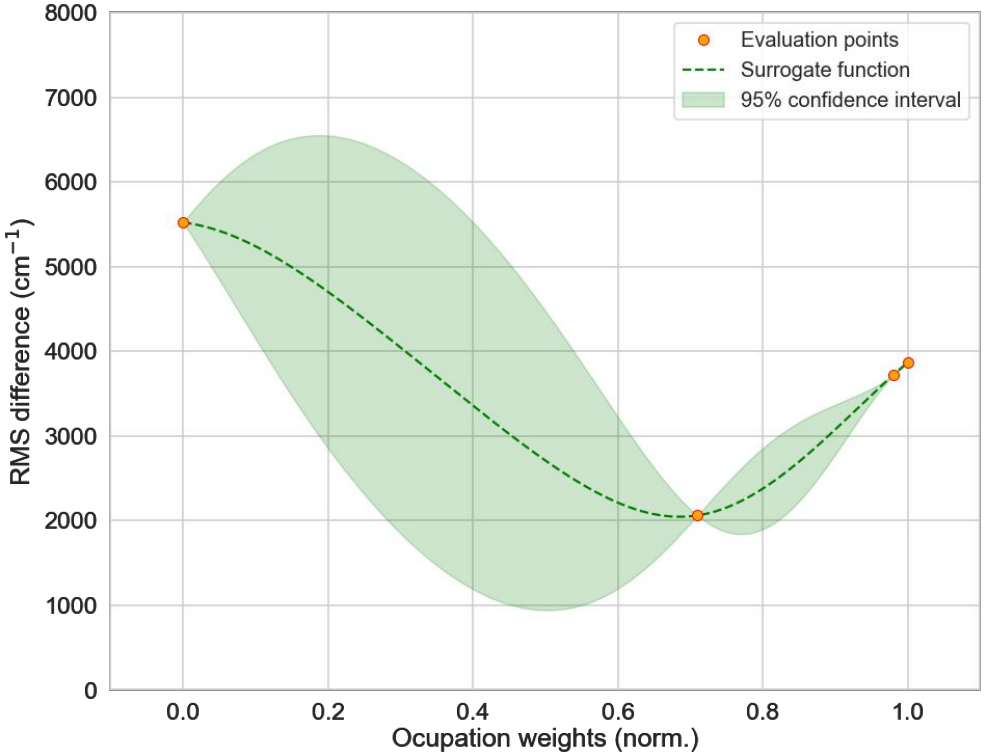

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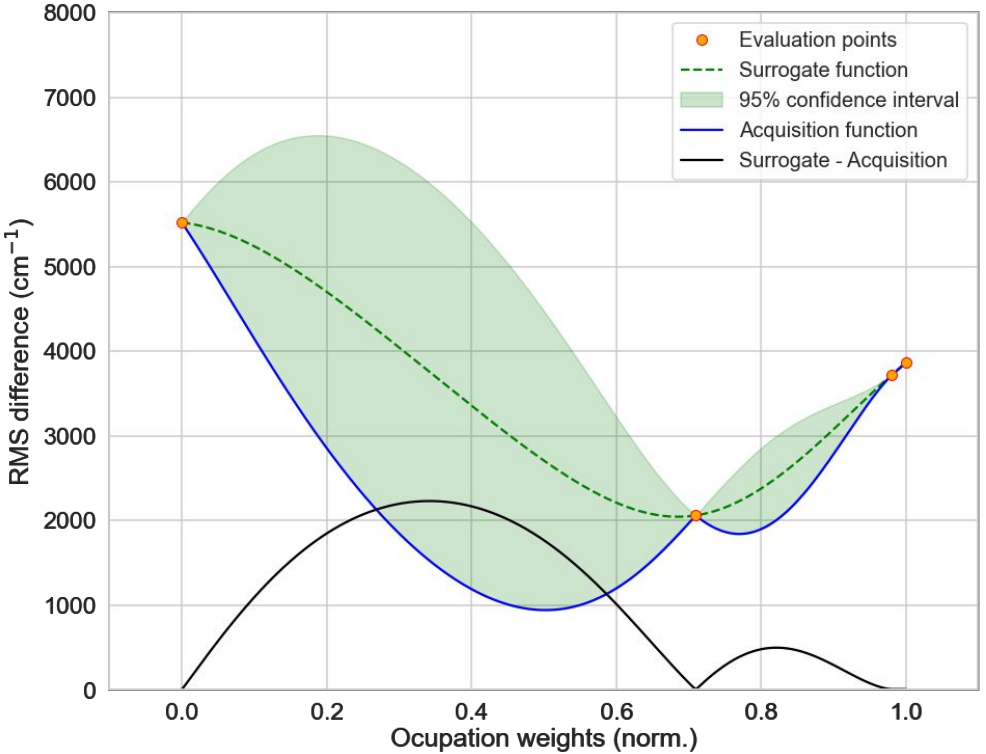
Optimization procedure

- Which point to evaluate next?
  - Compute acquisition function
    - Choice between exploration and exploitation
    - Choice between different methods: Gaussian process LCB, Expected Improvement, Probability of Improvement…



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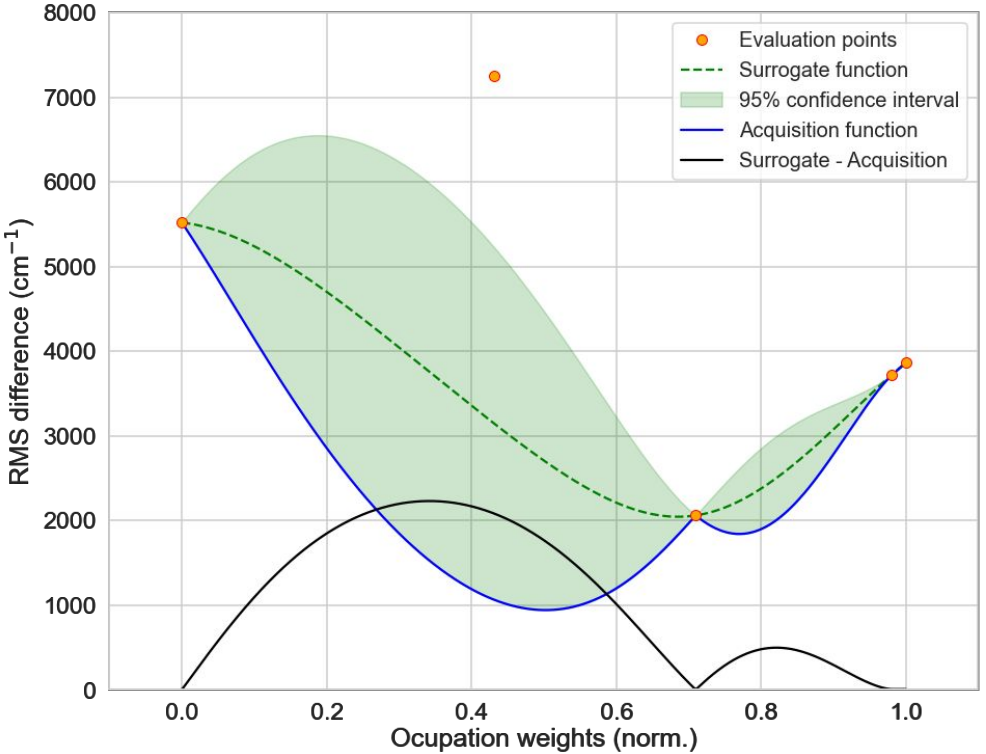

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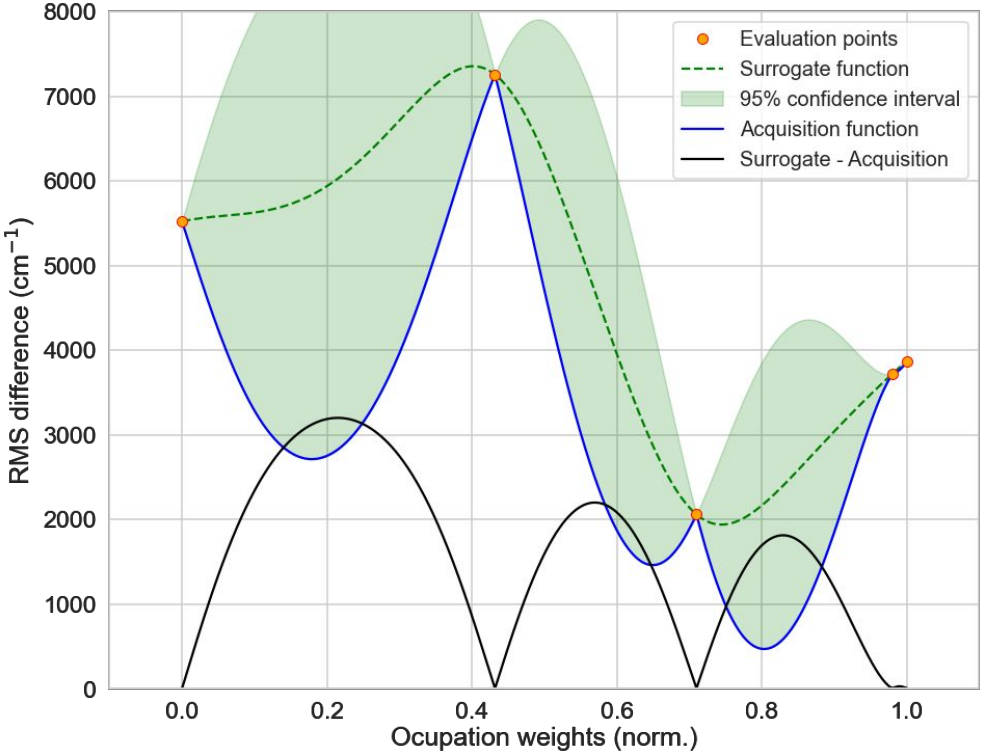

Example optimization for 1 parameter (4f)
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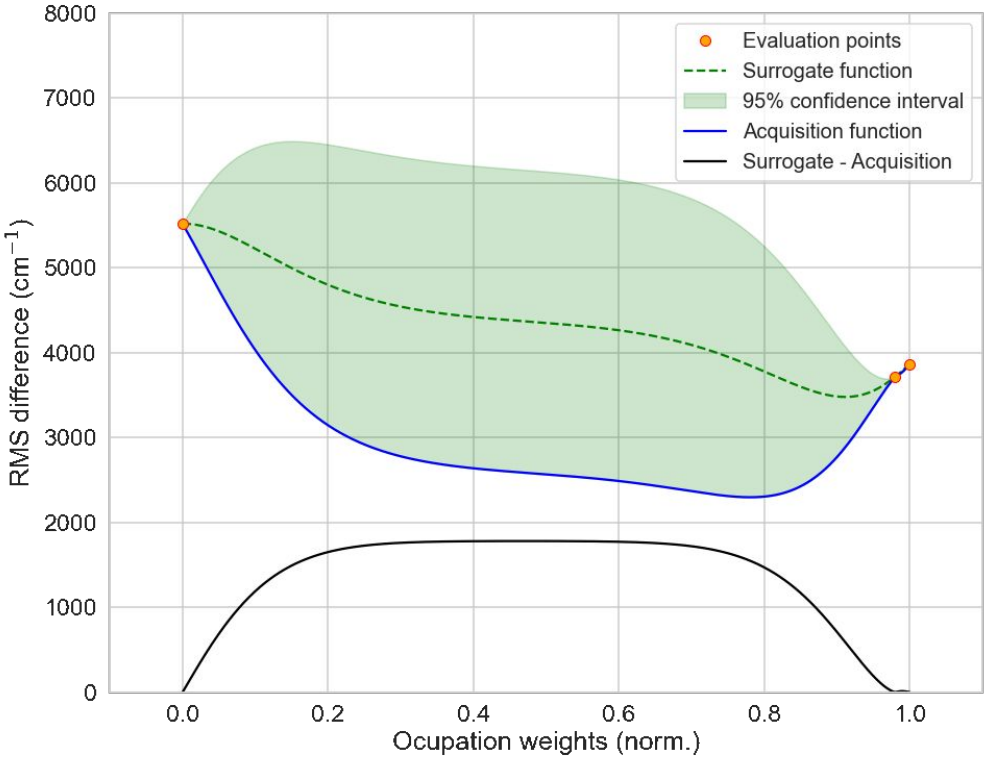
Optimization procedure

1. Get a set of initial points
2. **Fit** a surrogate model for a specific loss function
3. Compute **acquisition function** - dynamically chosen between EI, PI and GP-UCB
4. Evaluate new point
5. Repeat 2. - 4. until convergence of loss function evaluation (exploitation) or chosen number of iterations (exploration)
6. **Make recommendation**

Sequential Model-Based Optimization (SMBO)



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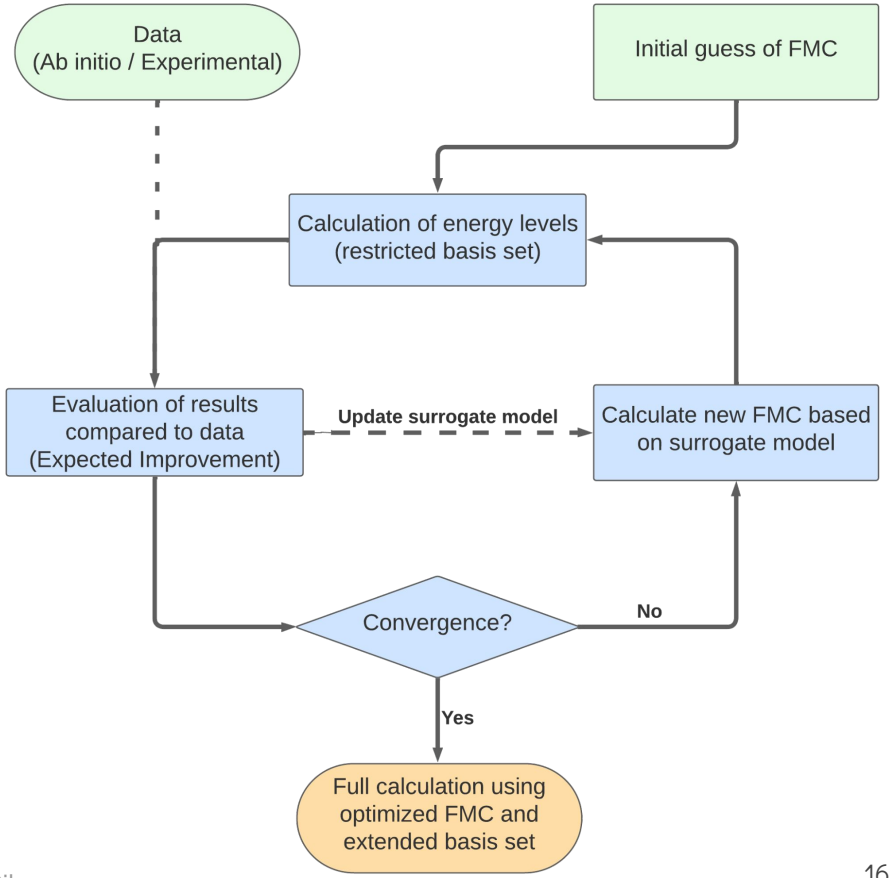
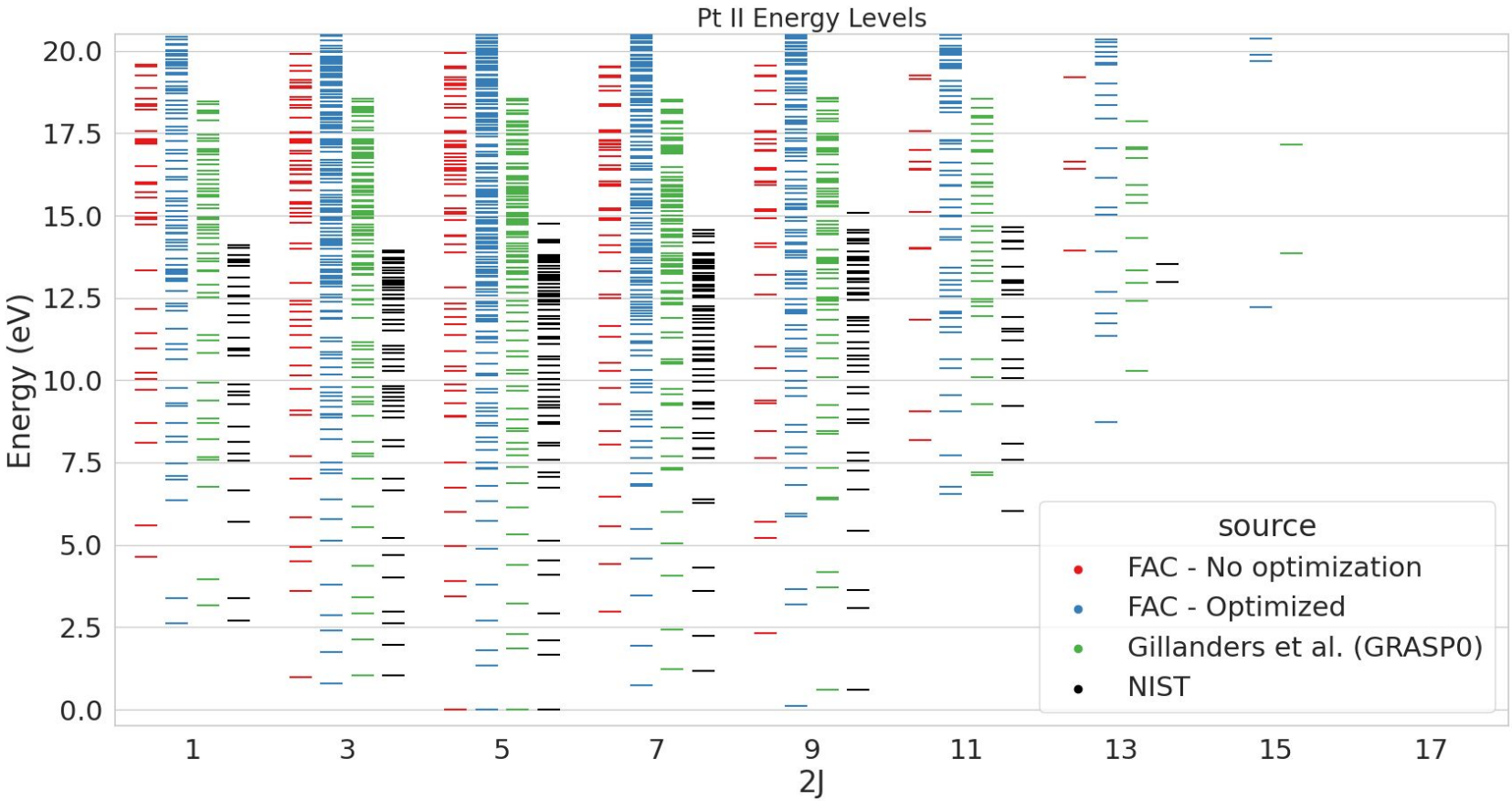
FAC – Potential Optimization

- **General** optimization that can be applied to other codes and/or structure methods
- **Flexible** loss function - can be adapted to optimized for different needs
- **Systematic** improvement possible with the use experimental data or *ab initio* calculations of few low lying levels
- **Sensitivity** of atomic data predicted with (optimized) mean local potential can be estimated



Results – Pt and Au



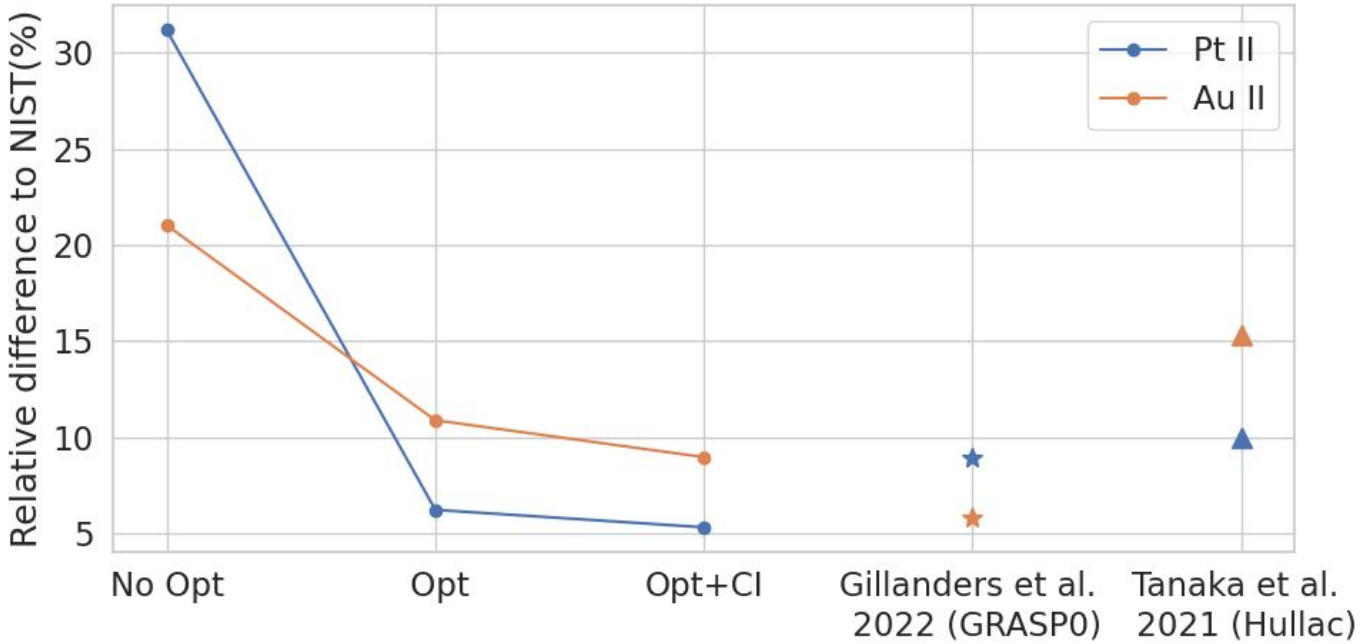
Results

Sample of transition rates for Au II

Transition	A-value (s^{-1})				
levels	**Configuration**	GRASP0*	FAC2*	**Rosberg & Wyart**	This Work (FAC - Optimized)
1 → 18	5d10 $^1S_0$→ 5d9 6p $^3P_1$	8.96E+07	1.07E+08	3.59E+08	9.71E+07
1 → 21	5d10 $^1S_0$→ 5d9 6p $^3D_1$	2.12E+08	5.18E+08	3.70E+09	3.41E+08
1 → 24	5d10 $^1S_0$→ 5d9 6p $^1P_1$	1.65E+09	1.00E+09	2.14E+09	8.46E+08
2 → 13	5d9 $^3D_3$→ 5d9 6p $^3P_2$	4.08E+08	1.37E+08	2.27E+09	5.26E+08
2 → 16	5d9 $^3D_3$→ 5d9 6p $^3F_4$	7.27E+08	6.13E+08	7.81E+09	4.34E+08
2 → 17	5d9 $^3D_3$→ 5d9 6p $^1D_2$	1.05E+07	1.22E+07	2.31E+08	1.30E+07

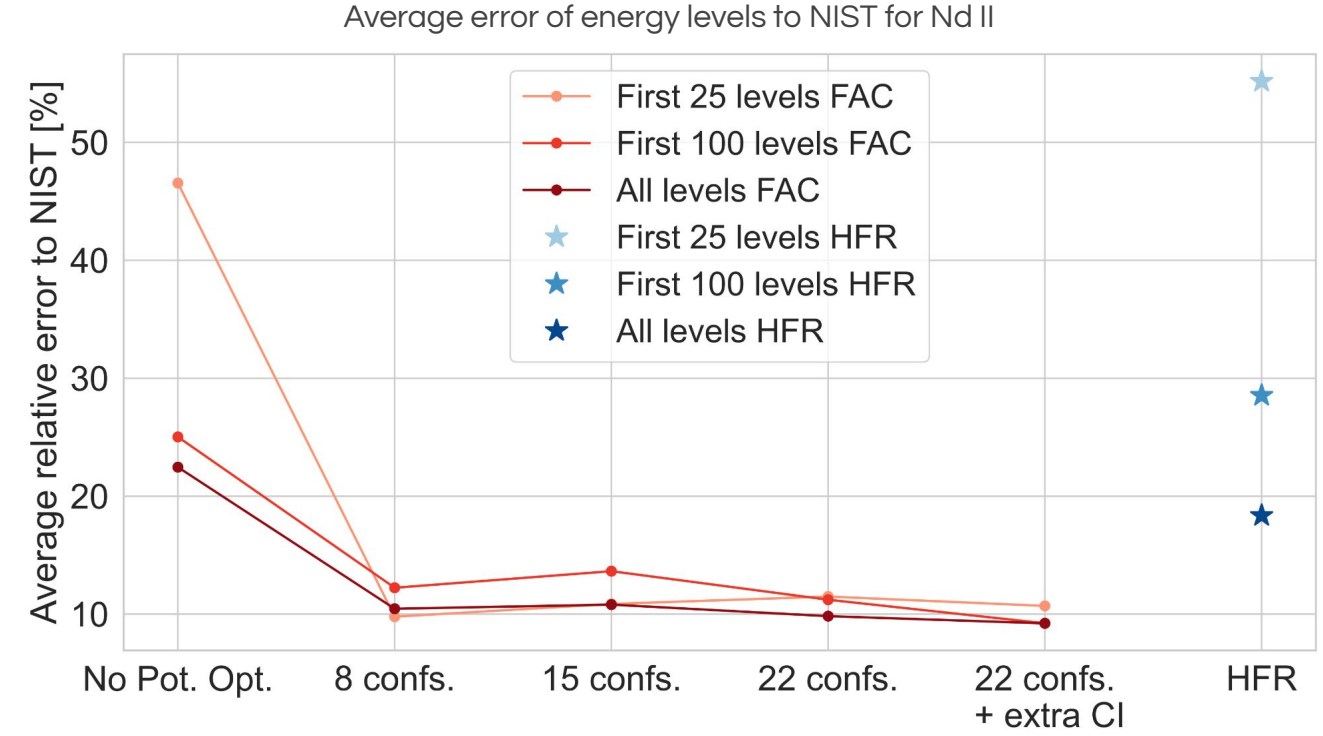
*As from McCann et al. 2022, https://doi.org/10.1093/mnras/stab3285

Results



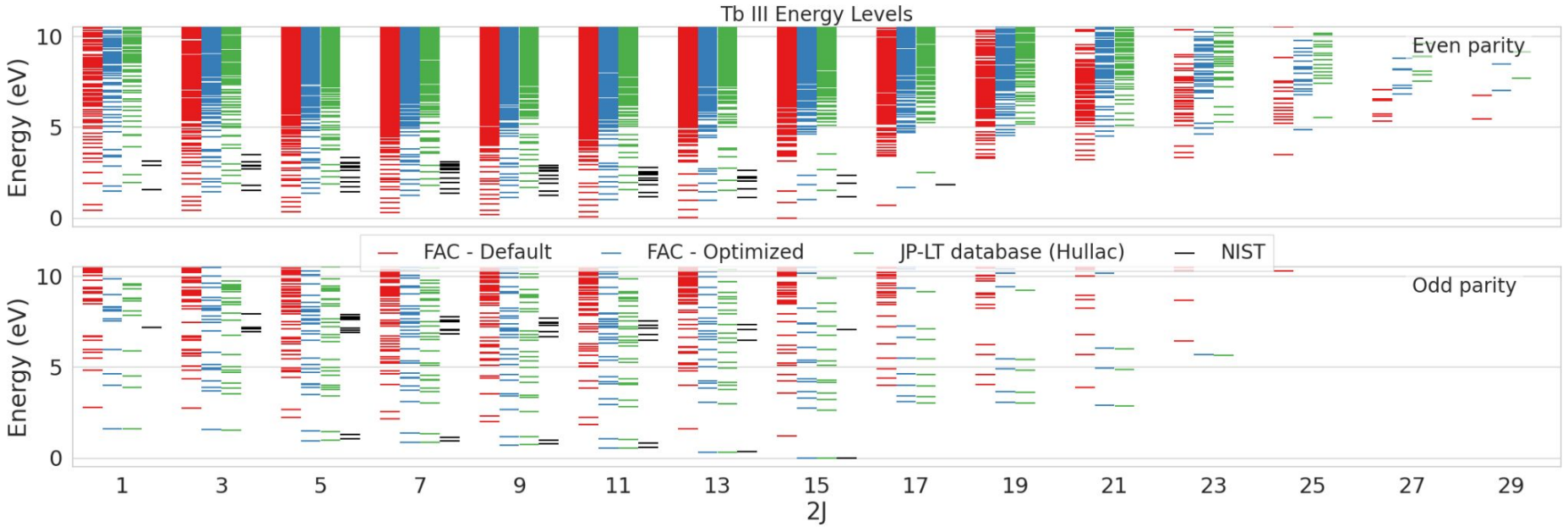
- Optimization has the biggest impact on the energy levels

Results



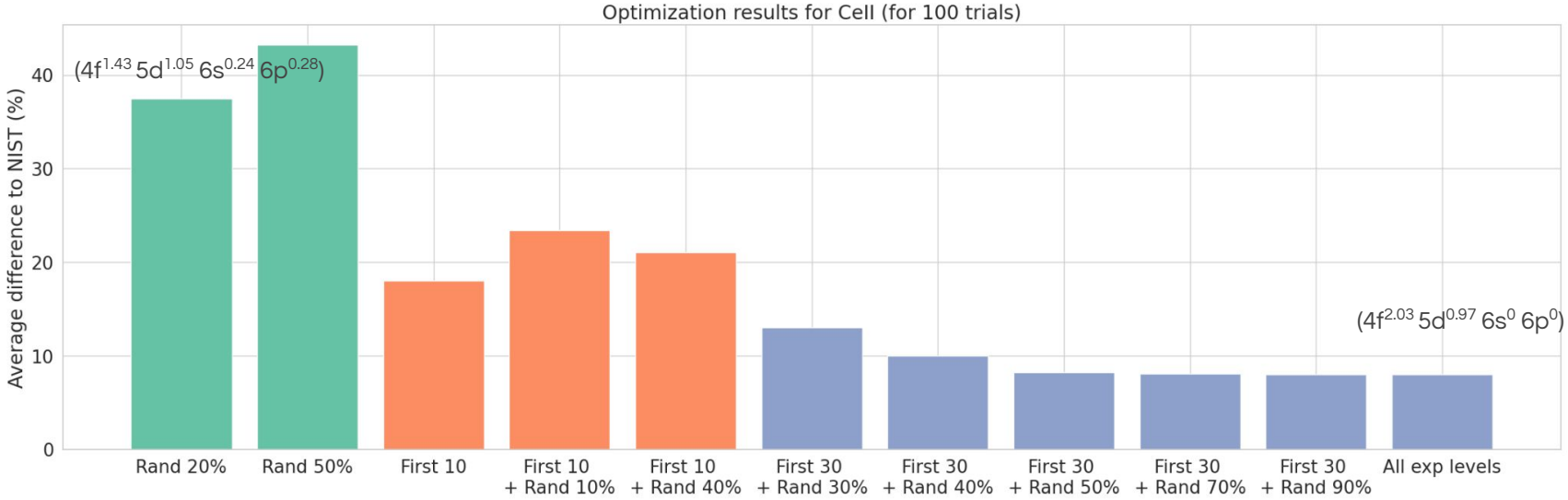
[A.Flörs+2023]

Results



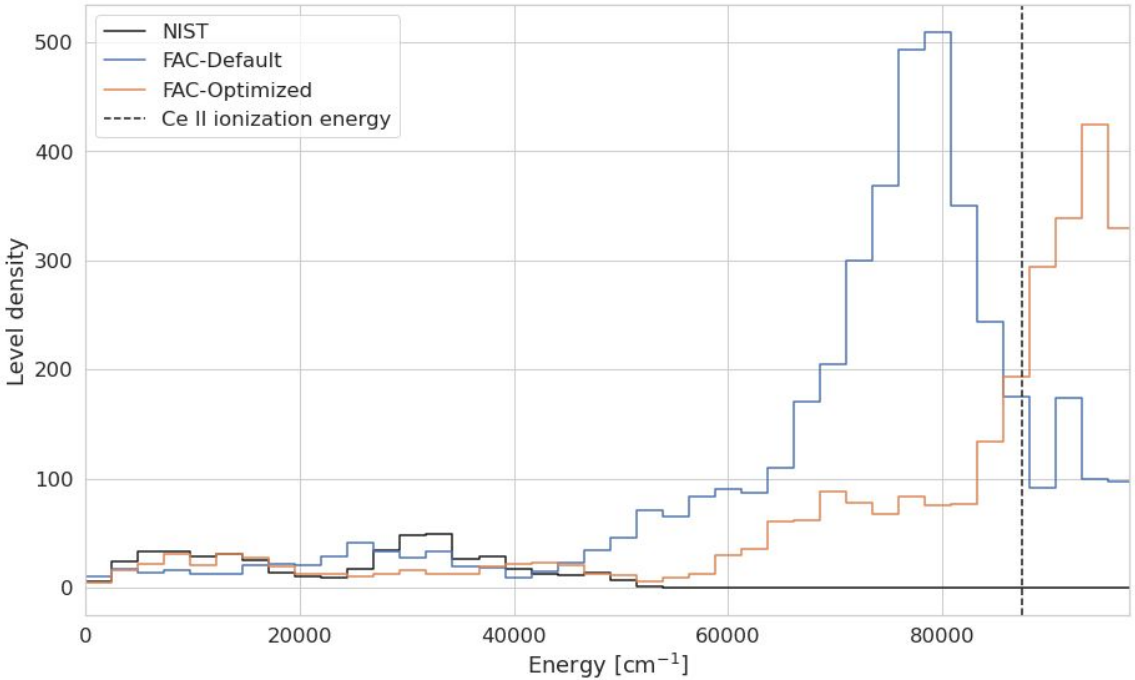
- Level identification (mainly) done by using level J^{π} position
  - Wavefunction composition can be studied for high lying levels
- Used reference set may be tweaked to avoid parity bias
  - Ignoring high lying or unreliably identified levels

Results – Sensitivity of the Optimization



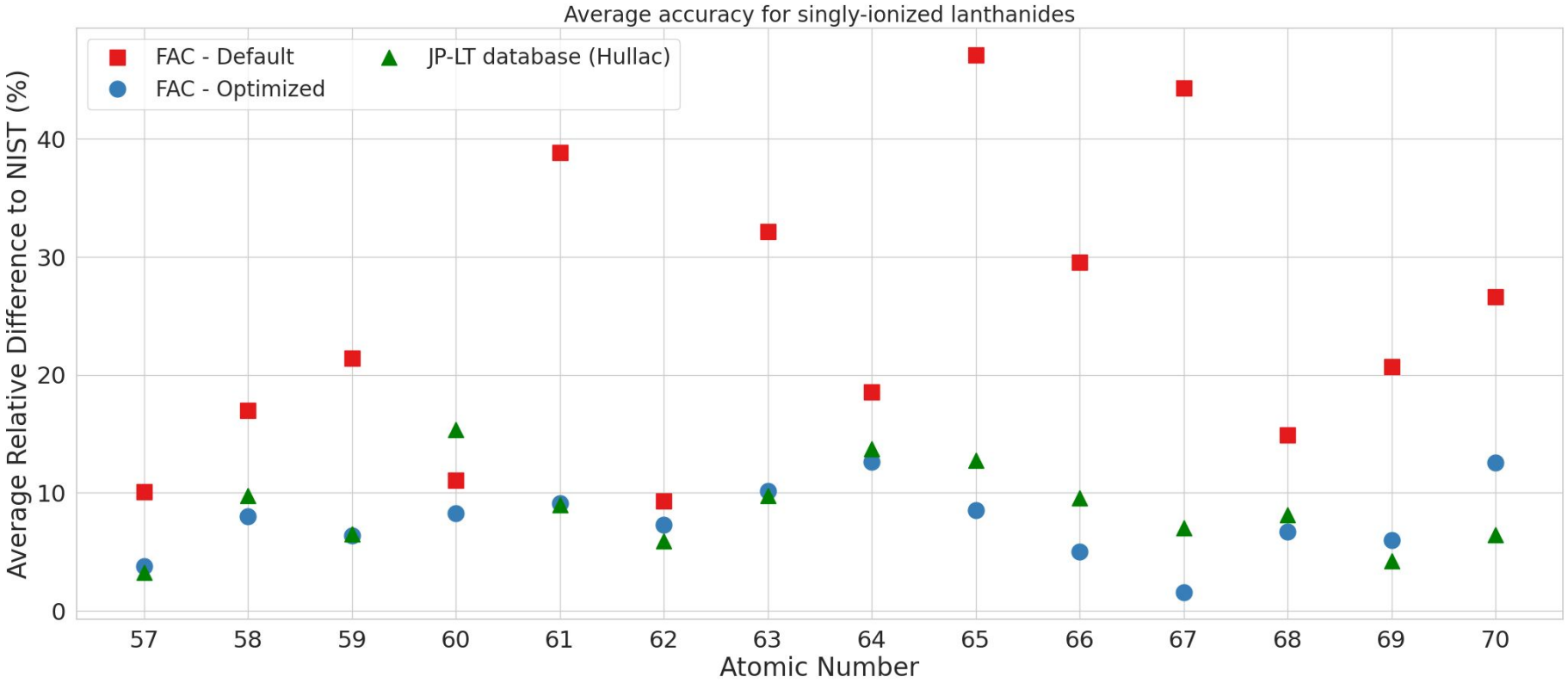
- Only very small changes to FMC after including more than 50% of the available data for Ce II - maintaining a relative accuracy of ~8%
- Close to ground state levels have the most impact (~10-30 levels)
- Provides confidence on it's predictive value for non-measured levels and robust to low amounts of data

Results - Effects on level density



- Contrary to calibration of individual levels optimization of the central potential impacts the full spectrum
- Optimized levels typically closer to exponential expected behavior (up to ionization energy)

Results – Energy Levels



Summary and future work

- A combination of high accuracy codes (benchmarking) with less computationally demanding ones (systematic calculations) is needed for reliable atomic data

- Our goal is to provide a complete set of atomic data to be used in the characterization of kilonova light curves and spectra
  - → Benchmarking of *ab-initio* for when no experimental data is available - FAC-MBPT, MCDFGME, GRASP
  - → We will make our data publicly available after publication (Zenodo)

- Optimisation of the mean local potential leads to very good agreement with NIST data and other structure codes (e.g. GRASP)
  - → Calibration still necessary -> next talk

- Radiative transfer calculations to test the impact of different atomic datasets - next talk
  - → Calculation of electron-ion cross sections, photoionization cross sections, recombination coefficients required for non-LTE modelling (Nebular evolution)

COLLABORATION

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Thank you for your attention!