Fully calibrated lanthanide atomic data for kilonova modeling

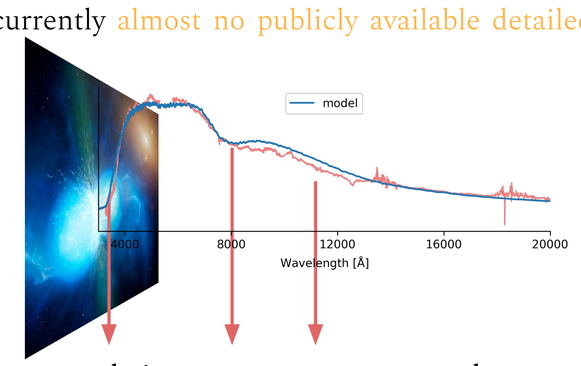
Andreas Flörs[1], R. Ferreira da Silva[2], L. J. Shingles[1], G. Martínez-Pinedo[1,3,4]

[1] *GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany*
[2] *Laboratório de Instrumentação e Física Experimental de Partículas (LIP) and Faculdade de Ciências, Universidade de Lisboa (FCUL), Portugal*
[3] *Institut für Kernphysik (Theoriezentrum), Fachbereich Physik, Technische Universität Darmstadt, Schlossgartenstraße 2, 64289 Darmstadt, Germany*
[4] *Helmholtz Forschungsakademie Hessen für FAIR, GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany*

Kilonovae and the r-process

Lanthanides and actinides in the universe originate from the r-process. In 2017, the electromagnetic counterpart to the gravitational wave detection of two merging neutron stars was observed. From the light curve alone it was possible to identify ejecta that contain lanthanides and possibly actinides, as they have a ~100 times higher opacity than iron-group material [1].

To identify specific elements, spectroscopic information is required. A great challenge for spectroscopic modelling of kilonovae is the almost non-existent atomic data currently available for lanthanides and actinides. While some progress has been made with regard to lanthanide atomic data recently [e.g. 2,3,4], there is currently almost no publicly available detailed atomic data for actinides.

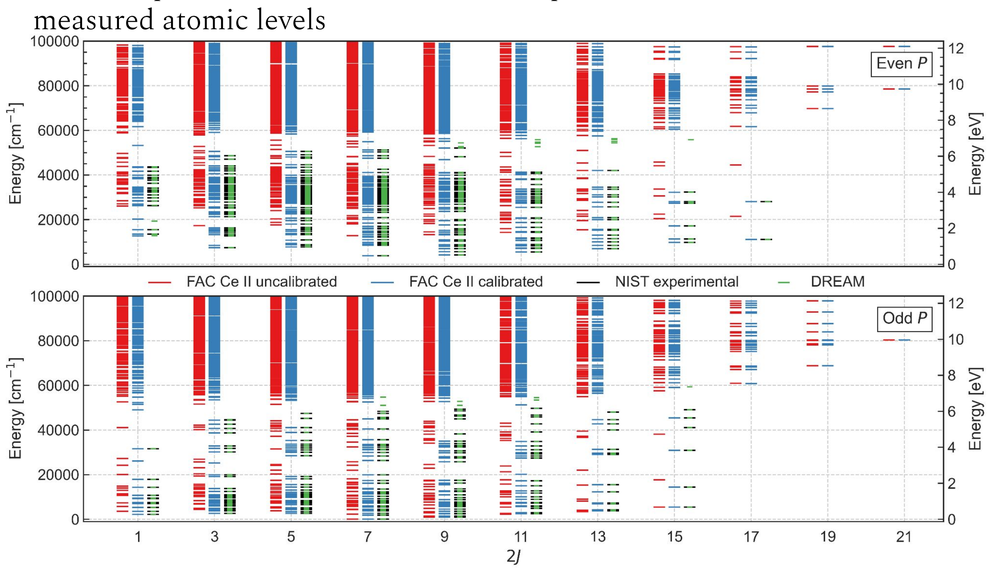


spectral signatures → r-process elements?

Atomic Structure Codes

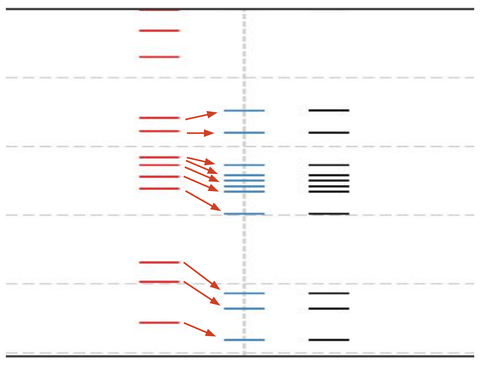
Lanthanide and actinide ions each have of order 10^6 relevant transitions
→ ~10 – 100 times more than iron-group ions
→ only a tiny fraction of all transitions has been measured for a few selected ions
Theoretical calculation of atomic data necessary!

Use Flexible Atomic Code (FAC) [5]
→ relativistic atomic structure code based on the diagonalization of the Dirac-Coulomb Hamiltonian
→ MCMC optimisation of the local central potential to reduce differences to measured atomic levels



Calibration of Energy Levels

We calibrated the atomic data using the `grasp/jj2lsj` module to compute spectroscopic terms and match levels with NIST for each P-J group.



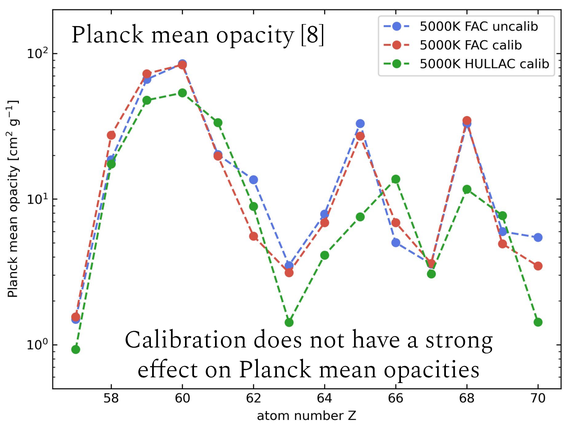
→ P, J & spectroscopic term known for FAC & some NIST levels
→ Match NIST levels with corresponding FAC levels
→ FAC levels without NIST data: use combination of mean correction from P-J group and mean correction from configuration

Importance of Calibrated Atomic Data

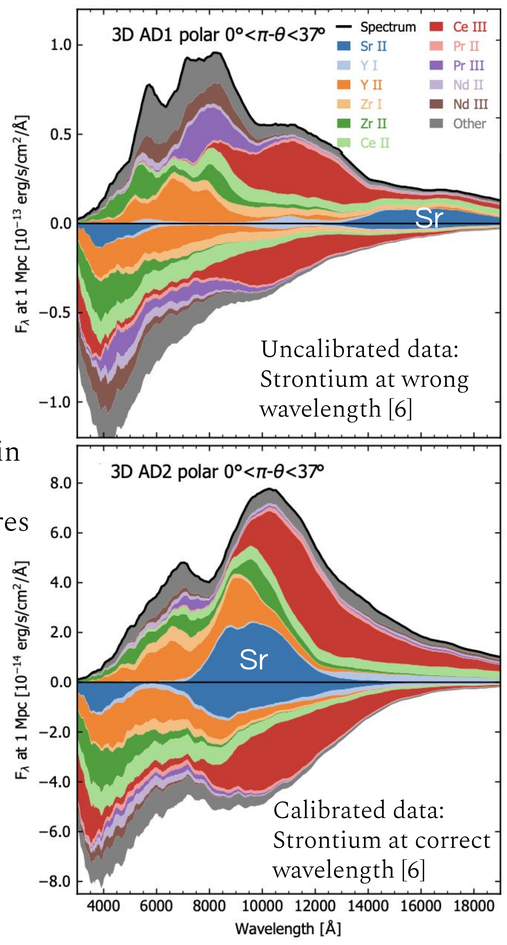
Kilonova light curve and spectral modeling relies significantly on the availability and completeness of atomic opacities:

Light curve modeling:
→ mostly sensitive to the total opacity (e.g. Planck mean opacity)
→ calibration not necessary to obtain accurate results

Spectral modeling:
→ transition wavelengths and total opacity extremely important for spectral modeling and line identification
→ uncalibrated data can lead to differences in transition wavelengths of several 1000 Å
→ risk of misidentification of spectral features



Comparison of radiative transfer results:

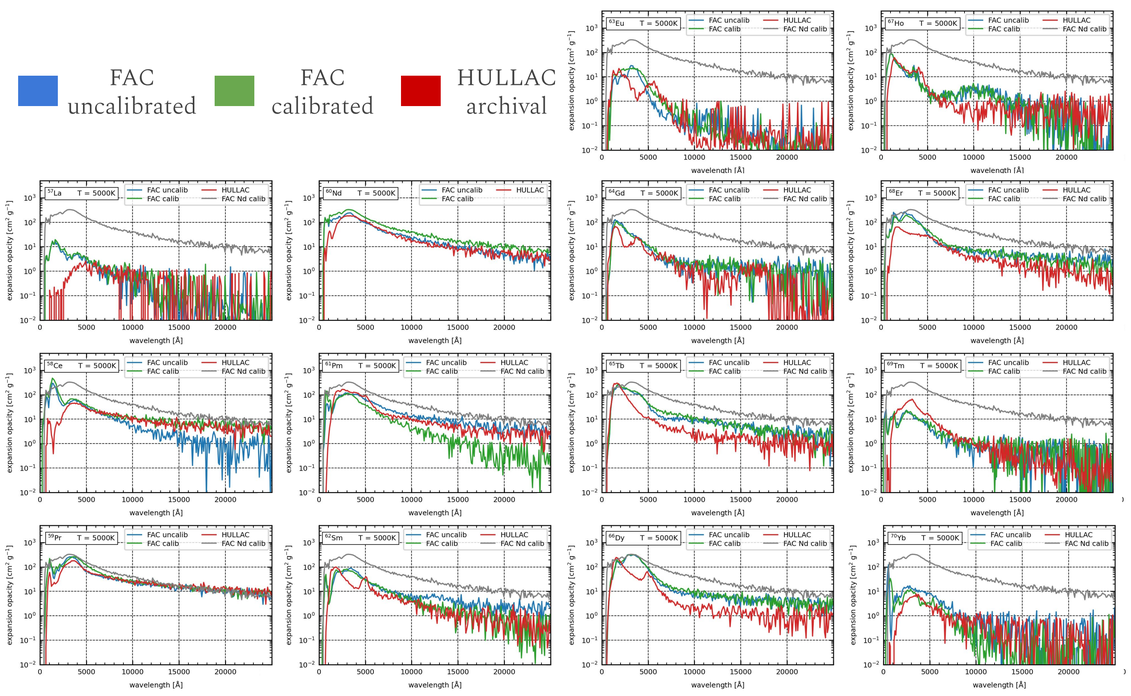


Complete Set of Lanthanide Atomic Opacities

Calculated opacities are ~50% higher than previously published atomic data
→ higher density of near-ground levels in the majority of investigated ions in agreement with experimental data
→ larger opacity at short wavelengths due to higher number of included electronic configurations

Negligible effect of inclusion of additional configurations on opacity
→ not the total number of lines important, only lines between near-ground levels
→ inclusion of additional configurations only increases opacity at wavelengths below ~2000Å

Our computed and calibrated atomic data will be made openly available after publication.
This will be the first complete set of converged lanthanide atomic structure calculations with accurate transition wavelengths [Silva in prep., 7, Flörs in prep., 8].



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References

[1] Kasen et al., Nature, 551, 80 (2017)
[2] Tanaka et al., MNRAS, 496, 1369 (2020)
[3] Silva et al., Atoms, 10, 18 (2022)
[4] Flörs et al., MNRAS, 524, 3083 (2023)
[5] Gu et al., Can. J. Phys., 86 (5), 675 (2008)
[6] Shingles et al., ApJL, 954, L41 (2023)
[7] Silva et al., in prep
[8] Flörs et al. in prep