Contribution ID: **61** Type: **Oral Contribution**

Atomic Data Requirements for Non-LTE Modeling of Kilonova

Monday 9 June 2025 12:10 (20 minutes)

The observation of kilonova AT2017gfo following the neutron star merger GW170817 [1] has provided compelling evidence for the production of r-process elements in these events. While recent spectral analyses have identified several elements in the ejecta [2,3,4], accurate abundance determinations remain challenging due to limitations in available atomic data, especially for modeling later epochs where non-LTE effects become crucial [5].
We present extended and improved calculations for lanthanides and actinides, including forbidden transitions, using both the Flexible Atomic Code [6] and AUTOSTRUCTURE [7], with atomic structure optimized using our recently developed sequential model-based optimization procedure [8]. Additionally, for selected elements, we benchmark electron-impact excitation cross sections and collision strengths calculated within the distorted wave approximation. We also present preliminary results extending these calculations to selected lanthanides, providing new atomic parameters necessary for non-LTE modeling of kilonova spectra.
This expanded atomic dataset, including forbidden transitions, improved energy levels, and electron-impact excitation rates, establishes the construction of a foundational atomic dataset that can be used for more reliable modeling of late-time kilonova spectra where non-LTE effects dominate the emission features.

[1] Abbott et al., Astrophys. J. 848, L13 (2017)
[2] Domoto et al., Astrophys. J. 939, 8 (2022)
[3] Gillanders et al., MNRAS stac1258 (2022)
[4] Vieira et al., Astrophys. J. 962, 33 (2024)
[5] Pognan et al., MNRAS 510, 3806 (2022)
[6] Gu et al., Can. J. Phys. 86, 675 (2008)
[7] Badnell, Astrophys. Source Code Libr. ascl:1612.014 (2016)
[8] Flörs et al., MNRAS 524, 3083 (2023)

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