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Improvement and benchmarking of atomic data for kilonova modeling

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Given the recent detection of multiple neutron-star merger events, in particular the AT2017gfo observation, in which the ejection of hot and radioactive matter, termed kilonovae, was detected as an electromagnetic signal. It is critical to combine a more comprehensive description of nuclear and atomic properties with advanced astrophysical simulations in order to produce accurate predictions of r-process nucleosynthesis yields and electromagnetic signals when compared with observational data.

Since the luminosity and spectra of the radiative emission depend significantly on the atomic opacities of the heavy elements ejected [1,2], in this work we provide results for large-scale calculations of data needed to compute those opacities for lanthanides and actinides. The atomic data was calculated utilizing the Flexible Atomic Code (FAC) [3], as it allows for structure, radiative and collisional data, needed for kilonova modeling. Structure calculations are carried out by FAC employing a configuration interaction approach and a central potential improved with existing experimental data utilizing machine learning methods. In this work we also performed benchmarking tests on our atomic data to investigate the implications of using this central potential model in our calculations.

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The Astrophysical Journal, vol. 939, no. 1, p. 8, Oct. 2022, doi:
10.3847/1538-4357/ac8c36.

[2] R. F. Silva, J. M. Sampaio, P. Amaro, A. Flörs, G. Martínez-Pinedo and J. P.
Marques, "Structure Calculations in Nd III and U III Relevant for Kilonovae Modelling,"Atoms, vol. 10, no. 1, p. 18, Mar. 2022, doi:
10.3390/atoms10010018.

[3] M. F. Gu, "The Flexible Atomic Code,"Canadian Journal of Physics, vol. 86,
no. 5, pp. 675–689, May 2008, doi: 10.1139/p07-197.

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