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Atomic Structure Calculations of Neodymium and Uranium for Kilonova Emission Modeling

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In 2017, the electromagnetic counterpart AT2017gfo to the binary neutron star merger GW170817 was observed by all major telescopes on Earth. While it was immediately clear that the transient following the merger event, is powered by the radioactive decay of r-process nuclei, only few tentative identifications of light r-process elements have been made so far. One of the major limitations for the identification of heavy nuclei based on light curves or spectral features is incomplete or missing atomic data which greatly affects the results of radiative transfer models. While progress has been made on lanthanide atomic data over the last few years, for actinides there has been less emphasis, with the first set of opacity data only recently published.

This talk will present converged large-scale atomic structure calculations of lanthanides (focusing on neodymium, ($Z = 60$)) as well as actinides (focusing on uranium, ($Z = 92$)). Using two different codes (FAC and HFR) for the calculation of the atomic data, we investigate the accuracy of the calculated data (energy levels and electric dipole transitions) and their effect on kilonova opacities. I will show a comparison of bound-bound opacities as a function of included electron configurations, for both ab-initio and experimentally calibrated atomic structure calculations. Finally, I will present how optimization of the local central potential model in atomic structure calculations increases the accuracy of the obtained level energies, and, as a result, the opacities.

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