Atomic calculations in moderately charged lanthanide ions (from La to Pm) relevant for plasma opacity studies in the context of kilonovae

H. Carvajal Gallego[1], J. Berengut[2], P. Palmeri[1], P. Quinet[1,3]

[1] *Physique Atomique et Astrophysique, Université de Mons, 7000 Mons, Belgium*

[2] *School of Physics, University of New South Wales, Sydney NSW 2052, Australia*

[3] *IPNAS, Université de Liège, 4000 Liège, Belgium*

On August 17, 2017, the LIGO-VIRGO collaboration observed gravitational waves from a neutron star merger for the first time [1]. In this coalescence, hot and radioactive matter is ejected causing a very luminous explosion called kilonova. In this latter, they are nuclear reactions forming heavy elements such as lanthanides (Z = 57 – 71). They play an important role because, given their rich spectra, they contribute intensely to the opacity affecting radiation emission [2]. To interpret the spectrum of a kilonova, it is crucial to precisely know the atomic data characterizing these elements. Some studies determined these parameters but only for the first degrees of ionisation (up to 3+). Unfortunately, there is almost no data available for ions higher than 3+. Therefore, our project aims to make a significant contribution in this field as it consists of a detailed study of the radiative processes characterizing moderately charged lanthanide ions (from 4+ to 9+) and to deduce the corresponding astrophysical opacities. Our calculations are based on a multi-platform approach involving different independent theoretical methods, namely the pseudo-relativistic Hartree-Fock (HFR) [3,4], the fully relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) [5-8] and Configuration Interaction Many-Body Perturbation Theory (CI+MBPT) [9,10] methods. In the absence of sufficient experimental data, this approach is the only way to estimate the accuracy of the results obtained through systematic comparisons between distinct computational procedures. In the present contribution, we report the results obtained as regards the atomic structures and radiative parameters in moderately lanthanide ions (La to Pm) and the corresponding monochromatic opacities for application to early phases of kilonovae emission spectra observed following neutron star mergers.

1. B. Abbott et al., Phys. Rev. Lett. 119, 161101 (2017).
2. D. Kasen, B. Metzger, J. Barnes, E. Quataert and E. Ramirez-Ruiz, Nature 551, 80 (2017).
3. R.D. Cowan, The Theory of Atomic Structure and Spectra (U. of California Press, Berkeley, 1981).
4. P. Quinet et al., Mon. Not. Roy. Astron. Soc. 307, 934 (1999).
5. I.P. Grant, Relativistic Quantum Theory of Atoms and Molecules (Springer-Verlag, Berlin, 2007).
6. P. Jönsson, G. Gaigalas, J. Biéron, C. Froese Fischer and I.P. Grant, Comput. Phys. Commun. 184, 2197 (2013).
7. C. Froese Fischer et al., J. Phys. B : At. Mol. Opt. Phys. 49, 182004 (2016).
8. C. Froese Fischer, G. Gaigalas, P. Jönsson and J. Bi´eron, Comput. Phys. Commun. 237, 184 (2019).
9. V.A. Dzuba, V.V. Flambaum and M.G. Kozlov, Phys. Rev. A 54, 3948 (1996).
10. E.V. Kahl and J.C. Berengut, Comput. Phys. Commun. 238, 232 (2019).