A community platform for just atomic computations

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Electronic structure calculations of atoms and ions have a long tradition in physics with applications in basic research and spectroscopy. With the Jena Atomic Calculator (JAC), I here present a new implementation of a (relativistic) electronic structure code for the computation of atomic amplitudes, properties as well as a large number of excitation and decay processes for open-shell atoms and ions across the periodic table. JAC [1] is based on Julia, a new programming language for scientific computing, and provides an easy-to-use but powerful platform to extent atomic theory towards new applications.

A primary guiding philosophy in designing JAC was to develop a general and easy-to-use toolbox for the atomic physics community, including an interface that is equally accessible for working spectroscopists, theoreticians and code developers. In addition, I also wish to provide a modern code design, a reasonable detailed documentation of the code and features for integrated testing [2].

References

[1] S. Fritzsche, Comp. Phys. Commun. 240, 1 (2019); https://github.com/OpenJAC/JAC.jl
[2] Fritzsche, User Guide & Compendium to JAC (unpublished, 2019).