Gateways 2021, October 19-21, 2021

Portal for High-Precision Atomic Data and Computation

udel.edu/atom

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1. ABSTRACT

In many applications, ranging from studies of fundamental physics to the development of future technologies, accurate atomic theory is indispensable to the design and interpretation of experiments. Direct experimental measurement of relevant parameters is often infeasible if not impossible.

This paper reports the release of Version 1 of an online atomic portal for high-precision atomic data and computation that provides such information to a wide community of users. Version 1 of the portal provides transition matrix elements, transition rates, radiative lifetimes, branching ratios, hyperfine constants, quadrupole moments, and scalar and dynamic polarizabilities for atoms and ions. Version 1 includes data for the elements and ions Li, Be+, Na, Mg+, K, Ca+, Rb, Sr+, Cs, Ba+, Fr, and Ra+. The atomic properties are calculated using a high-precision, linearized coupled-cluster method.

All values include estimated uncertainties. Where available, experimental values are included, with references to their sources. Data for more elements and properties will be added in the future, with alkaline earth metal atoms planned for the next release. Future updates will also include releases of user-friendly, atomic computational codes. Community input is sought to improve the portal and guide the next stages of the project. The portal includes the requisite user feedback functions for guiding future releases. A site tour and help functions allow new users to orient themselves quickly.

The current portal version shows pre-computed information through an interactive interface, providing instant access to the requested data, equipped with common print and download functionality. Future versions will also allow users to request properties and elements that are rarely needed and information that has not yet been computed. Such requests will invoke the needed computations on-demand and notify the user when complete. For some requests, the response time may be a few seconds, while more advanced calculations require minutes to hours.

The current implementation of the portal uses a static page design, with the data directly embedded in HTML. The pages, written in HTML, CSS, and JavaScript, are created automatically, via python scripts, from the original CSV-formatted physics data. One challenge was the representation of the denominations for electron states, such as $5f6p^2\ ^2F^0_{5/2}$, for which LaTeX inserts are generated. Graphs for such properties as polarizabilities make use of the Bokeh visualization package.

The computational codes are written in Fortran 77/90 and have been parallelized using OpenMP for efficient execution on multicore nodes. The code runs consume significant resources, making use of concurrent runs on many nodes of the computational clusters at the University of Delaware, for the computation of properties of multiple elements simultaneously.

The team includes both physicists and computer scientists, driving the design of the portal from both the physics and the software engineering angle, applying best practices for collaboration and software design.

Keywords—transition matrix elements; transition rates; radiative lifetimes; branching ratios; hyperfine constants; quadrupole moments; scalar polarizabilities; dynamic polarizabilities.

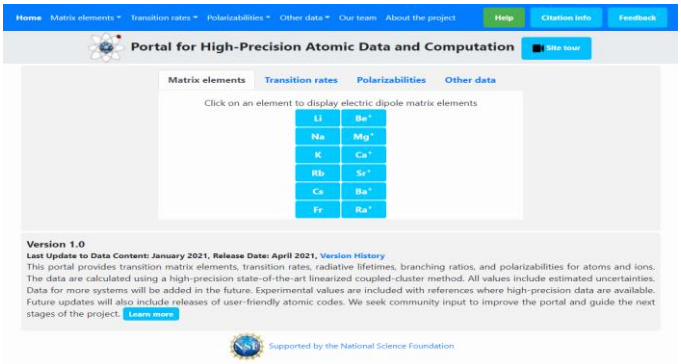

Figure 1: Home page of Atom portal at udel.edu/atom