The Ongoing Development and Support of Atomic Physics in Solar and Heliospheric Science

White paper for the Heliophysics 2050 workshop

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1. Motivation: This white paper outlines the necessity for the availability, accessibility, and expansion of atomic physics values and analysis tools for the meaningful interpretation of spectroscopic observations, and their connection to the heliosphere. Our models of the Sun, and all associated space weather phenomena, rely on the accuracy and availability of these atomic physics quantities. For instance, the calculation and interpretation of spectral radiance or irradiance, including both spectral line and continuum intensities and uncertainties, fully relies upon accurate atomic data. Derived spectroscopic diagnostics and a full understanding of measurements from EUV imagers (e.g. AIA on SDO) and spectrometers (e.g. EIS on Hinode) require a detailed understanding of the atomic physics of spectral line formation. In addition, simulations of charge states within the radially expanding solar wind, that connect remote to *in situ* ion observations, completely rely on the accuracy of the ionization and recombination rates in the calculations. It is fair to say that advances in almost every aspect of the physics of the solar atmosphere, including coronal heating, solar wind, and solar activity, are dependent on the atomic data and transition rates used to interpret solar emission. Because of this, ***there are severe limitations on the scientific return of solar and heliospheric missions which rely on the availability and accuracy of atomic data and modeling codes for physical interpretation.*** Therefore, it is critical for technological advances to be coupled with the improvement and development of atomic physics repositories and analysis tools through explicit funding to these projects and ongoing community level collaboration in the upcoming decades.

2. State of atomic databases: Presently, there are several independent atomic databases used by the solar and astrophysics community, for example AtomDB[1], ADAS[2], CHIANTI[3], Cloudy[4] and NIST[5]. These databases were initially created for the purpose of analyzing spectra from specific instruments or developed for different scientific focuses, e.g. solar physics, astrophysical phenomena, and fusion. Since their initial development, each has expanded to include more physical processes and spectral ranges to broaden the range of plasmas that can be modeled. However, the databases contain different data, which can be relevant across various fields, and contain their own analysis software. Therefore, this requires each user to assemble and familiarize themselves with several software packages to analyze data across many resources, which is a time consuming task that often inhibits meaningful scientific progress. Furthermore, since atomic databases are developed with different needs in mind, they are built under specific assumptions driven by the target plasma's temperature and density environment. One of the major differences is the inclusion, or exclusion, of specific processes that are considered when calculating atomic level populations, or ion fractional abundances in the plasma, that become relevant depending on the region of the Sun or specific phenomena. For instance, CHIANTI assumes that all emission is optically thin, neglects charge exchange

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[1] http://www.atomdb.org/
[2] https://open.adas.ac.uk/
[3] https://www.chiantidatabase.org/
[4] https://www.nublado.org/wiki/DataBase
[5] https://www.nist.gov/

processes at low temperature, and assumes that free electrons follow a thermal velocity distribution. However, ***to accurately model the solar wind between its release at the photosphere, acceleration through the corona, and into the solar wind, it is critical to quantify and model departures from these assumptions to properly interpret the increasing sensitivity of measurements from future solar observatories.***

3. Short term goals: The Continued Improvement and Expansion of Current Databases. As we move towards observing the Sun at higher spatiotemporal resolutions, and near-continuously at a range of wavelengths, it becomes critical to develop the appropriate atomic data and physics tools to facilitate scientific progress (*see Smith et al. J. Phys. B: At. Mol. Opt. Phys. 2020; Del Zanna and Young Atoms 2020,* for in depth discussion).

For example, to support the development of optically-thick/radiative transfer models of cool, dense plasma such as the photosphere/chromosphere regions of the Sun, as well as filament/prominence environments, it is necessary to expand current atomic databases to include: 1) detailed models of atoms, 2) atomic data for neutral/low ionized atoms, and 3) charge exchange and photoionization processes. These atomic quantities and processes are critical to properly model these regions of the Sun. However, this information is largely lacking in current databases. Moreover, current radiative transfer solvers (e.g. *RH, Uitenbroek ApJ 2001*) do not interface directly with databases to gather information; rather, they rely on user-generated standalone *atom files* for a single ion, and often use outdated atomic data from different resources. This is an example in which duplicate efforts, and potential errors, can be minimized through the accessibility of the necessary atomic data from repositories to easily build these files, or working towards interfacing solvers directly with databases.

In addition, it is critical to consider non-thermal velocity distributions, and nonequilibrium ionization (NEI) to properly interpret emission in the low corona (*Landi et al ApJ 2012; Cranmer et al ApJL 2014*). As plasma travels through the solar transition region, it experiences a sharp drop in density and large increase in temperature, both of which decrease Coulomb collisions in the plasma, $\nu \sim n_e/T_e^{3/2}$. Atomic quantities, such as reaction rate coefficients, are computed under the assumption that electrons remain in a Maxwellian velocity distribution. However, this becomes less and less valid beyond the transition region where electrons are more influenced by non-thermal effects, such as wave-particle interactions and turbulence. Non-thermal velocity distribution functions, along with large gradients in temperature and density, can lead to NEI conditions which affect the interpretation of the density, temperature, and velocity of the plasma inferred from their emission. These effects also impact simulations of ion densities used to interpret the thermodynamic evolution of plasma from charge states measured in the heliosphere. Therefore, it is critical to include these effects in our models to understand the dynamics of the emerging plasma into the corona and the solar wind.

Lastly, it is critical to quantify uncertainties of atomic physics quantities, such as cross-sections or rate coefficients, to determine the accuracy and limitations of such calculations. At present, uncertainty due to atomic parameters is almost completely absent in spectral fitting in the solar community, which could potentially cause misleading conclusions. Including these values in atomic physics databases can improve community awareness of assumptions and limitations to their calculations (*Yu et al ApJ 2018*). AtomDB is actively working to introduce some errors in atomic calculations, however this effort needs to be significantly extended to improve our understanding of the fundamental processes of the heliosphere.

4. Long term goals

Expanding and strengthening collaboration across the atomic, solar/heliospheric, and laboratory plasma physics communities through the participation and training of early career scientists (also see white paper by *Lichko et al*). Atomic databases benefit from new calculations for atomic data and transition rates carried out with improved atomic models which allow the use of more complex and complete atomic models. This means that these databases need to be continuously updated. Furthermore, the quality of intensity predictions and plasma diagnostics need to be tested against observations from solar, astrophysical and laboratory plasmas. These activities require strong collaboration across these communities and dedicated scientists to carry out the necessary updates and database benchmarking. This makes it imperative to ensure the active support and contribution to these projects by the upcoming generation of scientists in these fields. Given that the primary focus of the solar community is the application of spectroscopic methods as analysis tools to plasmas, and because these activities require detailed knowledge of several fields, it has fallen on the shoulders of a small number to expand and maintain these repositories for the use of our community. However, to ensure the continued knowledge and expertise in these topics, it is critical to prioritize research funding to strengthen and expand collaboration between atomic, solar/heliospheric, and laboratory plasma physics communities.

Establish funding for a comprehensive and user-oriented atomic database and modeling framework. To ensure the long term improvement and expansion to atomic datasets, our community should shift the duty of maintaining important atomic data from individual research groups, which are often not funded to do so, to formally funding a unified atomic physics resource. We suggest a central location where the community can access and contribute to an atomic repository, such as through the development of a NASA-funded site hosting atomic data and software tools[6] for the use of the scientific community. We envision a central database formed initially by unifying data from current major databases that would allow the ongoing contribution of atomic results and modeling codes from the community. The idea is to form a standardized library that is well-documented, multi-version accessible, and contains explicitly-funded software tools (see white paper by *Barnes et al*) that are organized and maintained by a single entity. Accessibility to such a framework would provide systematic atomic values to effectively compare different modeling methodologies, will facilitate the reproducibility of scientific results, and provide the capability to compare results under different assumptions.

Current State	Short/Long term goals	Goal for 2050
Current atomic databases focus on coronal physics in the optically thin regime. Also, no assessment of uncertainties to current atomic values are available	*Short:* 1) include atomic data to support optically-thick/radiative transfer calculations, 2) include non-thermal and NEI effects, 3) quantify errors in atomic physics quantities	Extending and improving atomic databases to enable a comprehensive analysis of the photosphere, corona, and its connection to the solar wind, and transients
Insufficient support for the long term maintenance and improvement of atomic databases by the community	*Long:* Provide research funding dedicated to expanding the atomic, solar/heliospheric, laboratory physics community by training new graduate students and supporting postdocs in this topic	Supporting the training and education of atomic, solar/heliospheric, and lab physics in the next generation of scientists
Scattered atomic information across several databases that are relevant across different fields	*Short:* Establish standardized definitions and data structures across databases *Long:* Establish funding for the development and maintenance of a centralized atomic database and software framework	Host a centralized, comprehensive, community accessible framework of atomic data and analysis tools

[6] This could pertain to a range of software, from basic spectral line fitting to more sophisticated radiative transfer solvers