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Advancing solar and heliospheric science through the ongoing development and support of atomic and laboratory plasma physics

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This paper outlines the necessity for the availability, accessibility, and expansion of atomic physics data and analysis tools for the meaningful interpretation of spectroscopic and polarimetric observations. As we move towards observing the Sun at higher spatio-temporal 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. We recommend the continued improvement and expansion of current databases to support the development of optically-thick/radiative transfer models, evaluate non-thermal and non-equilibrium ionization effects, and quantify uncertainties in atomic and molecular values. A critical long-term goal will require extending and strengthening collaborations across the atomic, solar/heliospheric, and laboratory plasma physics communities through the participation and training of early career scientists. We also recommend establishing funding for a centralized atomic physics resource made up of a comprehensive and user-oriented atomic database and modeling framework.

KEYWORDS
atomic physics, laboratory physics, heliophysics, solar physics, spectroscopy

1 Scientific motivation and background

This paper outlines the necessity for the availability, accessibility, and expansion of atomic physics data and analysis tools for the meaningful interpretation of spectroscopic and polarimetric observations that can reveal key processes driving solar and heliospheric dynamics. Our models of the Sun, planetary ionospheres, magnetospheres, and our prediction of space weather phenomena, rely on the accuracy and availability of these atomic and molecular physics quantities. For instance, the calculation and interpretation of spectral radiance or irradiance, including both spectral line and continuum intensities and their uncertainties, fully relies upon accurate atomic data. Derived spectroscopic diagnostics and a full understanding of measurements from broadband 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 their emission. Despite decades-long efforts at calculating, measuring, and distributing accurate atomic data and transition rates, there are still significant limitations on the scientific return of solar and heliospheric missions and ground observatories 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 and molecular 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 atomic databases used by the solar and astrophysics community, for example AtomDB[1], ADAS[2], CHIANTI[3], Cloudy[4], HITRAN[5], XSTAR, and NIST[6]. These databases were initially created for the purpose of analyzing spectra from specific instruments or developed for different scientific focuses, e.g. solar physics, atmospheric physics, astrophysical phenomena, and fusion energy. The long-term storage of atomic data is a serious problem, as in most cases new versions replace the previous ones. Over time, each database 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 which can often overlap and result in duplicate efforts to produce the same basic functionality. Beyond that, 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. Furthermore, since atomic databases are developed with different needs in mind, they are built under specific assumptions driven by the target plasma's properties. One of the major differences is the inclusion, or exclusion, of specific processes 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. However, *it is critical to quantify and model departures from these assumptions to properly interpret the increasing sensitivity of measurements from future solar observatories.*

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.hitran.org.
6 https://www.nist.gov/.

3 Short-term goals

3.1 The continued improvement and expansion of current databases

As we move towards observing the Sun at higher spatio-temporal 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 2001; Del Zanna and Young Atoms 2020, for in depth discussion). As most of the atomic and molecular physics databases used to analyze spectra are predominantly created and supported by theoretical and experimental atomic and molecular physicists, it is critical for solar and heliophysicists to work towards fully engaging with those communities.

3.2 Radiative transfer

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) atomic data and transition rates for neutral/low ionized atoms, 2) charge exchange and photoionization/recombination processes, and 3) density-dependent ionization/recombination rates and time-dependent ionization. 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 and statistical equilibrium solvers (e.g. RH, Uitenbroek 2001; CLE; Judge and Casini 2001; HAOS-DIPER; Judge 2007) do not interface directly with databases to gather information; rather, they rely on user-generated standalone *atom files* for a single ion, and sometimes 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*

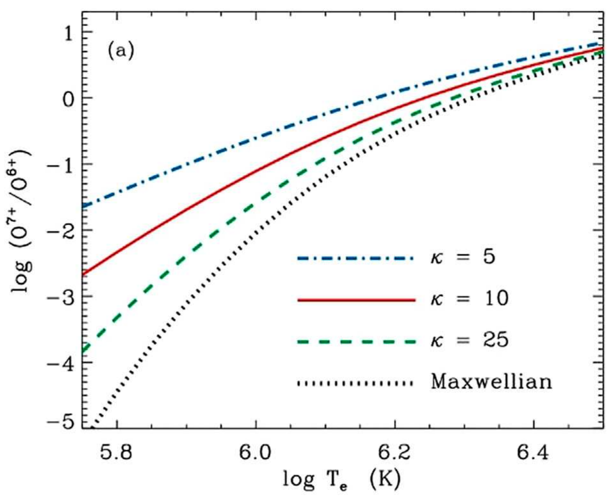

FIGURE 1
O^{7+}/O^{6+} ratio with increasing electron temperature for a Maxwellian and several kappa distributions adapted from Cranmer et al (2014).

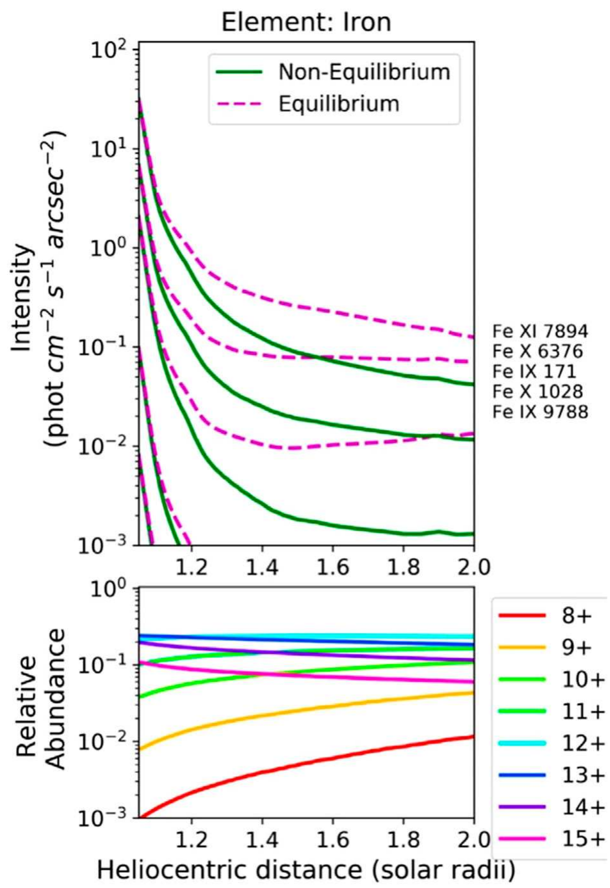

FIGURE 2
Simulated emission under equilibrium and non-equilibrium conditions (top) associated relative abundances (bottom) with increasing heliocentric distance adapted from Rivera et al 2019.

necessary atomic data from repositories to easily build these files, or working towards interfacing solvers directly with databases.

3.3 Evaluating non-thermal and NEI effects

It is necessary to consider non-thermal velocity distributions, and non-equilibrium ionization (NEI) to properly interpret emission in the low corona (Landi et al 2012; Cranmer et al 2014). At the solar transition region, there is a sharp drop in density and large increase in temperature, both of which decrease Coulomb collisions in the plasma. Atomic quantities, such as reaction rate coefficients, are computed under the assumption that electrons remain in a Maxwellian velocity distribution. However, it may become less and less valid higher in the corona and in the solar wind or during eruptive events, where electrons can become more influenced by non-thermal effects, such as wave-particle interactions and turbulence. For instance, the non-thermal features can be significantly reflected in the ionization stage outflowing plasma as is indicated by a study showing the changes in the O^{7+}/O^{6+} ratio with increasing electron temperature for several kappa electron distributions in Figure 1, adapted from Cranmer et al (2014). The O^{7+}/O^{6+} ratio is routinely used as a distinguishing characteristic in the solar wind, making it a key marker of solar wind origin and formation that provides an important link between the Sun and heliosphere phenomena, as detailed in Rivera et al 2022.

Solar flares are another instance where the plasma can depart significantly from Maxwellian assumptions. The acceleration of particles in flares is well known (e.g. Holman et al 2011), producing non-thermal particle distributions that are characterized by power law spectra. These non-thermal particles not only transport energy efficiently, they can directly ionize plasma in the chromosphere and transition region, and radically alter the ionization stages (e.g. Ricchiazzi & Canfield 1983; Allred et al 2005). Additionally, there is evidence that the ambient plasma in flares strongly departs from Maxwellian, being better characterized by kappa distributions due to the impact of the electron beams on the lower atmosphere (Dzifčáková & Dudík 2018; Dzifčáková et al 2018). The assumption of Maxwellian plasma therefore may lead to large errors in the interpretation of spectral line profiles and derived quantities in flares. *A possible solution is for databases to store cross-sections, which are independent of the electron distribution, rather than or in addition to effective collision strengths that would allow for the flexibility of analyzing spectra under non-thermal scenarios.*

Along with non-thermal particle distributions, large gradients in temperature, density, and outflow speed can lead to NEI conditions which affect the interpretation of the plasma properties inferred from their emission (Landi et al 2012; Gilly & Cranmer 2020). NEI develops for conditions where the thermodynamic state of plasma changes rapidly such that the ionization and recombination processes that establish ion abundances become unbalanced and lead to ion quantities that do not reflect the immediate plasma state (Shen et al 2017; Szente et al 2022). Figure 2, adapted from Rivera et al 2019, shows a comparison of synthetic intensities in select spectral lines of outflowing solar material for equilibrium (dashed magenta) and NEI (solid green) conditions indicating that a rapid deviation from the ionization equilibrium assumption can occur low in the corona. *In these cases, the general assumption of ionization equilibrium fails and, if unaccounted for, can lead to potentially incorrect assumptions about the characteristic quantities and dynamics of coronal structures and the outflowing solar wind necessary to understand their evolution.*

3.4 Quantify uncertainties in atomic and molecular values

Lastly, it is of critical importance to quantify uncertainties of atomic and molecular 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 (Loch et al 2013; Del Zanna et al 2019; Schiffmann et al 2021; Gu et al 2022). Including these values in atomic physics databases can improve community awareness of assumptions and limitations to their calculations (Yu et al 2018). Similarly, molecular processes are important to understanding lower temperature environments such as the solar photosphere/temperature minimum region and planetary ionospheres (Huestis et al 2008). 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 at the Sun and heliosphere.*

4 Long-term goals

4.1 Collaborations across the atomic, solar/heliospheric, and laboratory plasma physics communities

It is necessary to extend and strengthen collaborations across the atomic, solar/heliospheric, and laboratory plasma physics communities through the participation and training of early career scientists (also see Lichko et al 2020 and Lichko et al, Enabling Discoveries in Heliospheric Science through Laboratory Plasma Experiments white paper submitted to the 2024 Solar and Space Physics Decadal Survey). Atomic databases benefit from new calculations of transition rates and experiments to measure cross-sections carried out with improved atomic codes 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. This is particularly important for polarimetrically sensitive lines (e.g. the IR Fe XIII pair), where just radiative excitation without including anisotropy and alignment effects will lead to unrealistic intensity calculations. 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 and spectro-polarimetric 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.*

4.1 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 fully-funded site hosting atomic data and software tools for the use of the scientific community. The tools could pertain to a range of software, from basic spectral line fitting to more sophisticated radiative transfer solvers. The site could resemble the Community Coordinated Modeling Center (CCMC) that develops, hosts, and carries out simulation services for 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 Barnes et al 2020) that are organized and maintained in a coherent manner. 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.

It is important that funding agencies introduce dedicated programs for funding the full range of laboratory astrophysics within Heliophysics, including atomic data calculation, and database maintenance and development. A component dedicated to the funding of early career scientists will also encourage and support the participation in this field. *Training the next-generation of scientists is presently of critical importance as the expertise in atomic physics and spectroscopy in our community is declining and in need of young researchers.*

5 Summary and action points

The current atomic databases rely on assumptions that limit their applicability and lack a comprehensive assessment of uncertainties in its atomic values. To address this issue it is necessary to, 1) include atomic data to support optically-thick/radiative transfer calculations, 2) consider non-thermal and NEI effects, and 3) quantify errors in atomic quantities. This will ultimately lead to atomic databases that include all levels, transitions and other information needed to enable a comprehensive analysis of the photosphere, corona, and its connection to the solar wind, and transients.

In addition, atomic databases receive insufficient support for the long-term maintenance and improvement of atomic databases by the community. To mitigate these issues, it is critical to provide research funding dedicated to expanding the atomic, solar/heliospheric, laboratory physics community by training new graduate students and supporting postdocs in this topic. Dedicated funding opportunities will be essential to support the next-generation of scientists to produce the atomic and molecular data needed for progress in solar and heliophysics.

Lastly, the present state atomic information exists scattered across several databases which can be relevant in different fields. It is necessary to establish standardized definitions and data structures across databases that unify these values. Congruent to this goal, it is critical to establish dedicated funding for the development and maintenance of a centralized atomic database and software framework. Through this, the overall objective is to build a comprehensive, centralized, open framework of atomic and molecular data and analysis tools that is freely available to the community.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

The manuscript was compiled by YR with content and editorial contributions from all co-authors.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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