White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	19 June 2015

Indicate the primary area this white paper addresses by placing "P" in right column.
Indicate secondary area or areas by placing "S" in right column

	"P", "S"
• Plasma Atomic physics and the interface with chemistry and biology	P
• Turbulence and transport	
• Interactions of plasmas and waves	
• Plasma self-organization	
• Statistical mechanics of plasmas	

Indicate type of presentation desired at Town Hall Meeting.

	"X"
Oral	X
Poster	
Either Oral or Poster	
Will not attend	

Title:	Evaluated Atomic Databases for Plasma Diagnostics
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- ***Describe the research frontier* and importance of the scientific challenge.**

A significant fraction of information on terrestrial plasmas and almost all data on space plasmas are obtained with spectroscopic observations in various parts of spectra. From dense laser-produced plasmas to EUV lithography to magnetic fusion devices to solar corona, the measured spectra are extensively used for diagnostics of the most important plasma parameters, e.g., particle temperature, density, and electric and magnetic field strengths. Such widely used techniques as intensity ratios of dielectronic satellites to resonance lines in He-like ions and motional Stark effect with neutral beams in tokamaks and stellarators have become true examples of versatility and capability of spectroscopic plasma diagnostics in science and industry.

Any meaningful analysis of plasma spectra necessarily involves identification of the measured spectral features. While modern theoretical methods in atomic physics show impressive advances, nonetheless for many atomic systems their accuracy is still insufficient for unambiguous assignment of spectral lines and development of reliable methods of their use in plasma diagnostics. The neutral atoms and low-charge ions of such important elements for plasma physics as Fe and W possess such rich and complex spectra that presently only high-precision measurements can provide the required level of accuracy in spectra identification. This situation calls for development and implementation of advanced methods for atomic spectra evaluation and expansion of atomic databases containing evaluated and recommended atomic data of interest for plasma physics research.

- ***Describe the approach to advancing the frontier and indicate if new research tools or capabilities are required.***

For many decades the Atomic Spectroscopy Group at the National Institute of Standards and Technology (NIST) has been involved in evaluation of atomic structure data and its dissemination via advanced online databases. The databases can be freely accessed through the NIST Physical Reference Data Program webpage at http://www.nist.gov/pml/data/. The most extensive Atomic Spectra Database (ASD) [1] responds to more than 2000 data requests per day. Presently ASD contains detailed evaluated information on more than 227,000 spectral lines and 107,000 energy levels for chemical elements from H (Z=1) to Ds (Z=110). However, as is clearly seen from Figure 1, much more data should be analyzed, evaluated and collected in databases in order to improve spectroscopic plasma diagnostics under various conditions.

The atomic data evaluation procedure developed at NIST has evolved over many decades and a few generations of researchers [2]. It involves accumulation of all available information from the literature, analysis of relevant uncertainties from original papers, examination of possible systematic effects on spectra, evaluation of data consistency, optimization of energy levels, derivation of ionization energy (if relevant), theoretical interpretation of energy levels, isoelectronic comparisons, check of various regularities and so on. This meticulous approach heavily relies upon experience of data compilers and evaluators which can only be developed over a significant period of time and/or under supervision of skilled researchers.

In addition to evaluation of emerging sets of atomic structure data, new modules are to be added to the existing databases and online codes. For instance, the online collisional-radiative code FLYCHK [3] is currently used by more than 750 researchers for calculation of ionization distributions, radiative power losses and spectra from very diverse plasmas (transient, non-Maxwellian, opaque, and so on). It would greatly benefit from a better interface to ASD which would allow significant improvement in spectra synthesis. Also new ASD modules containing calculated ratios of line intensities under various conditions should provide immediate and valuable contributions for diagnostics of astrophysical and other low-density plasmas.

- ***Describe the impact of this research on plasma science and related disciplines and any potential for societal benefit***.

Expanded atomic databases will be used not only in plasma physics research but also in atmospheric science, industrial applications and education of young researchers. The Grotrian diagram interface in ASD is actively used in US and other universities in atomic physics courses as an illustration of complex atomic structures.

References

1. A. Kramida, Yu. Ralchenko, J. Reader, J. and NIST ASD Team (2014). NIST Atomic Spectra Database (version 5.2), [Online]. Available: http://physics.nist.gov/asd. National Institute of Standards and Technology, Gaithersburg, MD.
2. A. Kramida, "Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities." Fusion Sci. Techn. **63**, 313 (2013).
3. H.-K. Chung, M.H. Chen, W.L. Morgan, Yu. Ralchenko and R.W. Lee, "FLYCHK: Generalized population kinetics and spectral model for rapid spectroscopic analysis for all elements", High Enrg. Dens. Phys. **1**, 3 (2005); available online at http://nlte.nist.gov/FLY.

Figures

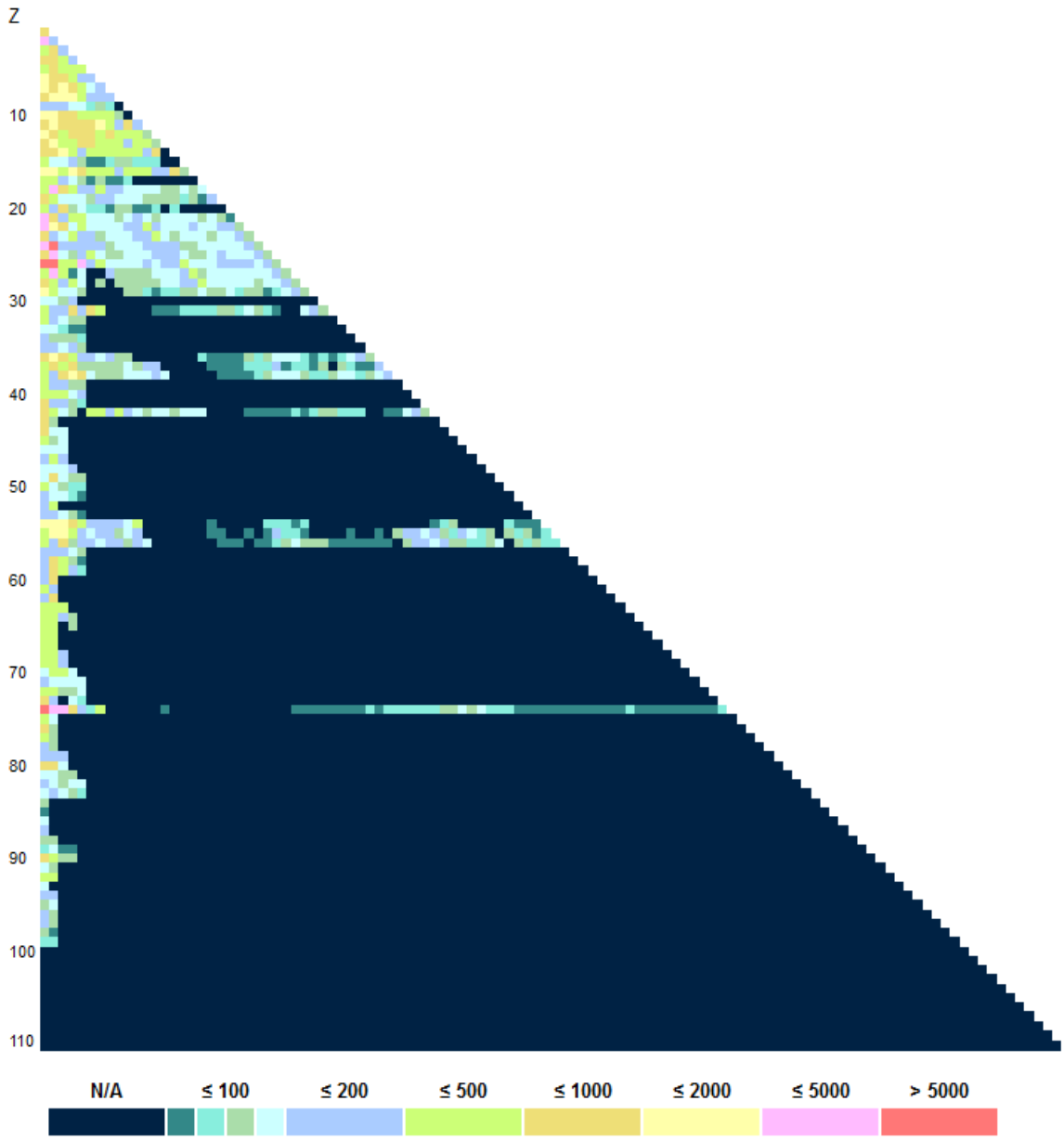

Figure 1 – The coverage of atomic data on spectral lines in the NIST Atomic Spectra Database v. 5.2 (as of June 2015). The *y*-axis is the nuclear charge, the *x*-axis is the ion charge (0,1…).