Triumphs, Twilight and Resurgence of the NIST Atomic Spectroscopy Group

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For about 120 years, the Atomic Spectroscopy Group at the National Institute of Standards and Technology (NIST) was one of the world leaders in experimental and theoretical atomic and plasma spectroscopy, production of standard reference data for atomic parameters, and development of atomic databases. Nonetheless, in early 2025 the group was abruptly terminated due to the apparent change of priorities for NIST research. Fortunately, the whole ASG scientific and engineering team was soon adopted by NASA Goddard Space Flight Center and the University of Maryland College Park which allowed us to preserve its rich legacy and offer new opportunities. We will briefly describe the achievements and status of the group at this pivotal moment of its history as well as its research plans for the near future.

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1. Introduction

There currently exist only a handful of research groups whose primary efforts are directed toward measurement, analysis, and dissemination of precision spectra from atoms and ions of chemical elements across the whole Periodic Table. For about 120 years, the Atomic Spectroscopy Group (ASG) at the National Institute of Standards and Technology (NIST) was the leading research organization in this field. It is quite symbolic that the very first scientific paper from NIST back in 1904 was on atomic spectra [1]. Over decades, ASG researchers, among them William Meggers and Charlotte Moore Citterly, William Martin and Joseph Reader, Wolfgang Wiese and Jack Sugar, Charlotte Froese Fischer and Yong-Ki Kim, published hundreds of highest-quality scientific papers on experimental and theoretical atomic and plasma spectroscopy, spectral line broadening, critical evaluation of atomic data, spectroscopy of highly-charged ions and so on. They were honored by numerous awards from NIST, US Government, and numerous US and international organizations.

Regretfully, the allegedly changing priorities for the federal research policies resulted in termination of the group in the Spring of 2025. This news shocked the whole international atomic and plasma physics community that extensively relies upon highest quality data from ASG for diverse scientific programs, from atomic clocks to search for exoplanets to diagnostics of multi-million-degree fusion plasmas. Immediately a petition was initiated to oppose the layoff of NIST ASG [2], numerous articles and broadcasts reporting ASG dissolution appeared in the US and international media (*e.g.*, [3–6]), hundreds of e-mails of enthusiastic support and offers to save the online databases and our collection of photographic spectral plates were received. The reputation of the group and the highest quality of its research were certainly the primary reasons why by early Summer 2025 its scientific and engineering staff found a new home at the University of Maryland College Park (UMCP) through the CRESST II collaboration [7] with the NASA Goddard Space Flight Center (GSFC). It is fair to say that this auspicious development has in fact saved one of the most prominent scientific programs in atomic and plasma spectroscopy.

In this paper, we will briefly describe the main achievements of the NIST Atomic Spectroscopy Group, its present status, and immediate plans for continuation and expansion of its research activities.

2. Recent ASG Research

The recent ASG research program could be roughly split into five fields, namely:

- High Resolution Classical Spectroscopy
- Spectroscopy of Highly Charged Ions
- Critical Evaluation of Atomic Data
- Development of Atomic and Plasma Databases
- Theoretical Atomic and Plasma Spectroscopy

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All these components interact with each other in a very fruitful, synergetic manner. For instance, the standard reference atomic databases are in part based on the locally generated critical evaluated data while precise collisional-radiative calculations provide indispensable information for analysis of newly measured spectra from highly charged ions. Below each of the five fields is briefly presented.

2.1 High resolution classical spectroscopy

The experimental program on high resolution measurements of atomic spectra goes back many decades. Over the years, the group accommodated probably the world's best collection of precise spectroscopic instruments operating from the extreme ultraviolet (~ 1 nm) to the infrared (~ 5,500 nm) parts of electromagnetic spectrum. The instruments comprise a 10.7-m Normal Incidence Vacuum Spectrograph (Fig. 1), a 10.7-m Grazing Incidence Spectrograph, a Czerny-Turner spectrometer, a 2-m path difference Fourier Transform (FT) spectrometer, a vacuum ultraviolet (VUV) FT spectrometer and several others. The laboratory infrastructure includes specifically designed isolated floors and heavy multi-ton slabs of granite to prevent even tiniest vibrations. With the resolving power from tens of thousands to several millions (for FTS), these spectrometers allow extremely precise measurements of various spectral characteristics including, for instance, hyperfine structure of radiative transition probabilities [8] or accurate reference data for search of variations of the fine structure constant [9]. Some of these instruments, for instance, were utilized to analyze the calibration lamps of the Space Telescope Imaging Spectrograph (STIS) that were returned from the Hubble Space Telescope during one of the service space missions—and this work received a special NASA Public Service Group Achievement Award.

2.2 Spectroscopy of highly charged ions

The Electron Beam Ion Trap (EBIT) at ASG was the second EBIT in operation, and its first spectra were recorded in 1993. With the maximal beam energy of 30 keV, it is capable of producing heavy ions with charges above 70+ in a controlled environment. A number of excellent spectroscopic instruments including a state-of-the-art transition-edge-sensor microcalorimeter (TES) (energy range E = 500–13,000 eV) [10] and an extreme ultraviolet (EUV) grazing-incidence spectrometer (wavelength range λ = 1.5–40 nm) [11] were utilized over the last 30 years to measure and analyze hundreds of unknown spectra of importance for multi-million-degree plasmas of astrophysics, magnetic and inertial confinement fusion, EUV lithography, etc. In addition to generating new precise spectroscopic data for our standard reference databases, the EBIT research program also discovered very fine relativistic and quantum electrodynamic effects in spectra of highly-charged ions [12], contributed to development of novel powerful diagnostic techniques [13], and helped analyze highly forbidden electric-octupole transitions in Ag-like ions [14]. For some of the measurements the experimental precision was so high that in combination with accurate theoretical calculations it even allowed us to pinpoint the effects of finite nuclear sizes on atomic spectra and thus determine the charge radii of heavy nuclei [15].

Fig. 1. A 10.7-m Normal Incidence Vacuum Spectrograph providing resolving power $\lambda/\delta\lambda \sim 300{,}000$ in the spectral range between 30 and 500 nm.

2.3 Critical evaluation of atomic data

As the official mission of the NIST ASG was "to measure, calculate, critically compile, and disseminate *reference data* on atomic properties and fundamental constants in support of basic research, commercial development, and national priorities", critical evaluation of atomic spectroscopic data rapidly became the cornerstone of the ASG scientific program. Since Charlotte Moore's classical publications in late 1940s [16], production and dissemination of critically evaluated data has been firmly associated with the ASG activities. Since then, dozens of monographs and data compilations (*e.g.*, [17–19]) were published that offered true spectroscopic benchmarks for spectroscopists, plasma physicists, astronomers and astrophysicists.

In the course of this work, the ASG scientists developed advanced detailed procedures for analysis of experimental and theoretical spectroscopic data and their uncertainties (see, *e.g.*, [20]). This procedure involves elaborate statistical methods that allow to significantly improve the estimates of intrinsic uncertainties in the reported data. The newly generated critical data compilations are regularly added to the NIST atomic databases, yet the rate of their production is far from satisfactory. The challenging and, more often than not, time-consuming process of data evaluation requires superior knowledge of both experimental and theoretical methods for spectroscopic data production, and this expertise is becoming less available in the community. Additionally, the number of research publications on atomic spectroscopy is ostensibly diminishing over the last decades in spite of its importance for various fields of physics. These issues may seriously jeopardize the availability of spectroscopic benchmarks for future research unless the involved stakeholders and funding agencies address them soon.

2.4 Atomic and plasma databases and tools

For the wide physics community, NIST atomic and plasma databases [21] have always been the most visible and valuable contribution to scientific research. Since mid-1990s, when world wide web became the medium for fast and reliable data exchange, the critically evaluated data originating from the ASG became available through a number of atomic databases. The largest and most important of them, the Atomic Spectra Database (ASD), now contains more than 300,000 spectral lines, 129,000 radiative transition probabilities, and 120,000 energy levels from approximately 1,100 different atoms and ions. Figure 2 presents the availability of ASD data on spectral lines for different chemical elements. The absolute majority of data are given for natural abundances although for several isotopes (*e.g.*, D, T, and ^{198}Hg) lines and energy levels are available as well. ASD also holds more than 6,000 ionization potentials for all elements and their ions from Hydrogen (Z = 1) to Darmstadtium (Z = 110). In addition to the "standard" tabular output, the database offers various graphical options, *e.g.*, dynamically generated Grotrian diagrams and colorful visible spectral images that are particularly useful for educational purposes. Other online databases and calculational tools include the interface for calculation of local thermodynamic equilibrium (LTE) spectra for laser-induced breakdown spectroscopy (LIBS) diagnostics, the lanthanide-actinide opacity database for kilonova studies developed in collaboration with Los Alamos National Laboratory (LANL), and the time-dependent collisional-radiative code FLYCHK for very fast calculations of population kinetics and light emission from various plasmas. The highest importance of the NIST atomic and plasma databases is exemplified by the exceptionally high citation rates—*e.g.*, ASD is currently cited, on the average, twice a day, and the annual number of ASD queries is close to 1,000,000.

2.5 Theoretical atomic and plasma spectroscopy

The experimental program at ASG was always actively supported by world-class theorists who developed sophisticated approaches to calculation of atomic structure, collisional characteristics, and plasma emission. From the multi-configuration Dirac-Hartree-Fock approach to relativistic model potential method, from simple LTE models to large-scale collisional-radiative (CR) simulations, ASG theorists provided crucial assistance for analysis and interpretation of the measured spectra, both at NIST and at many other laboratories around the world.

Much effort was put into development of new plasma diagnostic techniques. The in-house developed CR models are used for analyses of astrophysical and terrestrial plasmas including those in magnetic fusion devices, laser-produced plasmas, non-Maxwellian plasmas of EBITs and solar flares. For several decades ASG physicists lead the international program on validation and verification of sophisticated CR codes [22]. An example of calculated plasma parameters submitted by more than a dozen groups for detailed analyses at one of the recent non-LTE Code Comparison Workshops is presented in Fig. 3.

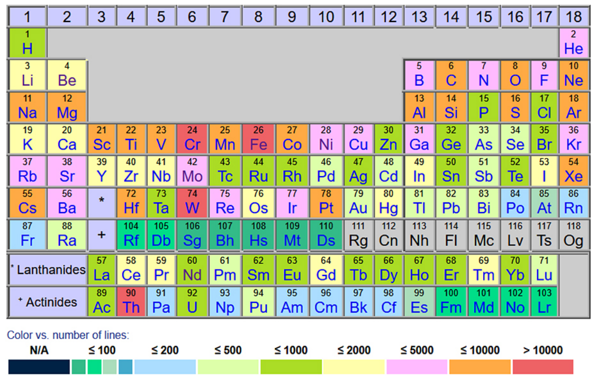

Fig. 2. Current availability of spectral lines in the NIST Atomic Spectra Database. The color palette at the bottom shows the number of lines for each element.

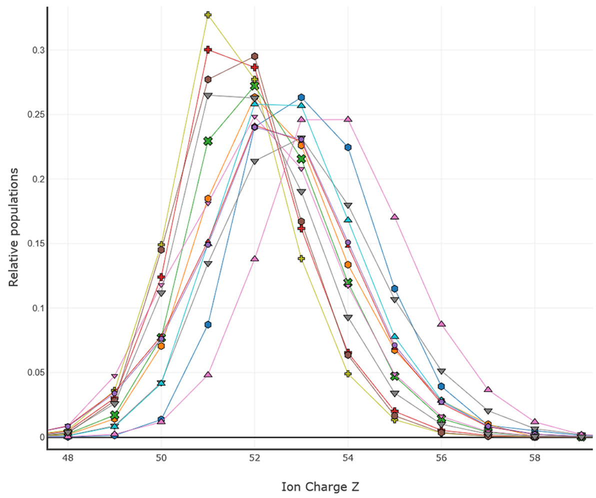

Fig. 3. Calculated ion distributions for Au at electron density $n_e = 10^{22}$ cm^{-3} and electron temperature T_e = 4,000 eV submitted for inter-code comparisons at the NLTE-12 Code Comparison Workshop (2023).

3. Future Plans

As noted above, the ASG scientific and engineering staff are now affiliated with UMCP and NASA GSFC (Greenbelt, Maryland) through the CRESST II collaboration. While our primary research focus is still with the production and evaluation of atomic data, the relocation has necessarily prompted adjustments to our scientific program. Thus, the atoms and ions of highest importance for astronomy and astrophysics will be prioritized in upcoming compilations of critically evaluated data. In particular, spectroscopic data for C III and IV will be updated, new recommendations for the electron-impact collisional data for He I will be released, and the NIST-LANL opacity database for kilonova studies will be expanded with newly generated data. We intend to relocate all atomic and plasma databases and tools to GSFC to ensure the community continues to have an uninterrupted access to the best available data. As for the experimental program, we plan to measure VUV, UV, and visible spectra as well as transition probabilities (oscillator strengths) for iron group elements and their low ions using the VUV FT spectrometer that has already been moved to its new home and will become fully operational within the next few months. The substantially larger EBIT experimental installation with all of its components and spectrometers including the recently acquired He liquefier system will arrive at GSFC during 2026 and will be immediately utilized for measurement of X-ray and EUV spectra of astrophysical interest. Unfortunately, the future of the remaining unique spectroscopic instruments at NIST is uncertain and they risk being lost to the community.

In spite of the relocation and ensuing shift in research priorities, we will nonetheless maintain active cooperation within the long-established collaborations. In particular, our group will remain an active member of the Data Center Network maintained by the International Atomic Energy Agency (IAEA), and we will continue to participate in the IAEA Cooperative Research Projects to the best of our abilities.

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I am very grateful to the APiP Organizing Committee for their generous support of my participation in the conference. I would like also to sincerely thank my ASG friends and colleagues Rodrigo Ibacache, Alexander Kramida, Karen Olsen, Joseph Tan, and Jacob Ward for being the most faithful team members during good and bad times. It is just impossible to list all Atomic Spectroscopy Group collaborators whose friendship and solidarity were always felt during the recent times, but we are profoundly thankful to all of you.

It was soon after the APiP conference that we lost the oldest member of our group, Joseph Reader, at the age of 90. He was an extraordinary scientist and incredible human being whose whole life was connected with the group. Joe's remarkable contributions to atomic spectroscopy will guide us for many years to come. This manuscript is dedicated to his memory.

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