12 March 2024

Dr. Michael C. McCarthy
Chair, Astronomy and Astrophysics Advisory Committee
Deputy Director, and Senior Research Scientist, Atomic and Molecular Physics Division
Center for Astrophysics | Harvard & Smithsonian

Dear Dr. McCarthy,

On behalf of the Laboratory Astrophysics Taskforce, I am pleased to submit to the Astronomy and Astrophysics Advisory Committee (AAAC), our report. This report was formally endorsed by unanimous consent at the February 23, 2024, public meeting of the AAAC.

This report is the culmination of extensive research, community engagement, and detailed analyses over the last nine months by a large, diverse, and dedicated group of scientists. The document provides an extensive overview of laboratory astrophysics and its importance in interpreting astronomical data, alongside current challenges and recommendations for future research directions. It covers topics such as the need for high-quality laboratory astrophysics data, the impact of underfunding in the field, the role of laboratory astrophysics in interpreting data from telescopes like ALMA and JWST. The report is structured around key findings and recommendations for programmatic support, workforce development, database management, facility access, and improving communication within the field.

Contributions to Astronomical Discovery and Analysis: The report details how laboratory astrophysics underpins the interpretation of data from many observational facilities, demonstrating its essential role in validating and expanding our understanding of cosmic phenomena.

Resource Evaluation and Support Needs: An assessment of the current resources available for laboratory astrophysics research is presented, alongside identified gaps. Recommendations for enhancing programmatic needs are provided to ensure sustained growth and innovation in the field.

Workforce Development and Database Enhancement: The importance of cultivating a skilled workforce dedicated to laboratory astrophysics is discussed, with suggestions for educational and training initiatives. Furthermore, the report addresses the need for comprehensive and accessible databases to facilitate research and collaboration.

Facility Resources and Collaborative Efforts: Our findings emphasize the critical need for high-quality facility resources and encourage the fostering of interdisciplinary collaborations to leverage diverse expertise in tackling complex scientific challenges.

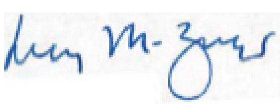
Recommendations for Strategic Advancement and Investment: The report concludes with a series of actionable recommendations aimed at strengthening the foundation of laboratory astrophysics. These include increased opportunities to participate in existing funding solicitations, enhancing community engagement, and investing in infrastructure and technology development.

This document is intended to serve as a resource for stakeholders, funding agencies, and the scientific community at large, by providing a data-driven analysis as to the current landscape of laboratory astrophysics and outlining clear, tangible, and cost-effective recommendations that can be undertaken to strengthen the field and in turn maximize the scientific return from current and proposed facilities and missions.

I look forward to the opportunity to discuss the contents of this report in greater detail should you have further questions and would welcome the opportunity to continue the dialogue on how to strengthen the connection between laboratory astrophysics and the astronomy community.

Thank you for considering our findings and recommendations. Your continued support and engagement are crucial in advancing the important work of laboratory astrophysics which serves as a cornerstone of the enabling foundation facilitating astronomical discovery.

With best regards,



Prof. Lucy Ziurys
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Enabling Cosmic Discoveries: The Vital Role of Laboratory Astrophysics

A report from the ad hoc Task Force on Laboratory Astrophysics

Prepared for:
The Astronomy and Astrophysics Advisory Committee (AAAC) at the request of NSF and NASA as part of an effort by the two agencies to address Astro2020's recommendation in this subject.

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12 March 2024

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Acronym List

AAAC: Astronomy and Astrophysics Advisory Committee
AAG: Astronomy and Astrophysics Research Grants
ADAP: Astrophysics Data Analysis Program
ALMA: Atacama Large Millimeter Array
APD: Astrophysics Division at NASA headquarters
APRA: Astrophysics Research and Analysis
ARC: NASA Ames Research Center
ASCEND: Ascending Postdoctoral Research Fellowships
AST: NSF's Division of Astronomical Sciences
ATLAS: Argonne Tandem Linac Accelerator System
DOE-FES: DOE's Fusion Energy Sciences
DOE: Department of Energy
EBIT: Electron Beam Ion Trap
FRIB: Facility for Rare Isotope Beams. Michigan State University operates this user facility on behalf of the DOE's Office of Science (DOE-SC)
GSFC: NASA's Goddard Space Flight Center
GRANTED: Growing Research Access for Nationally Transformative Equity and Diversity
HITRAN: High-Resolution Transmission Molecular Absorption Database
ISM: Interstellar Medium
JPL: Jet Propulsion Laboratory
JWST: James Webb Space Telescope
LANL: Los Alamos National Laboratory
LATF: Laboratory Astrophysics Task Force
LEAPS: Launching Early-Career Academic Pathways
LLNL: Lawrence Livermore National Laboratory
MPS: NSF's Directorate of Mathematical and Physical Sciences
NASA: National Aeronautics and Space Administration
NASEM: National Academies of Sciences, Engineering, and Medicine
NIST ASD: NIST's Atomic Spectra Database
NIST: National Institute of Standards and Technology
NSF: National Science Foundation
OCdb: Optical Constants Database
PAARE: Partnerships in Astronomy & Astrophysics Research and Education
PDART: Planetary Data Archiving, Restoration, and Tools
PSD: Planetary Science Division at NASA Headquarters
SETI: Search for Extraterrestrial Intelligence
SMD: Science Mission Directorate at NASA Headquarters
SNL: Sandia National Laboratories
SSW: Solar System Workings
XRP: Exoplanetary Research Program

1. Introduction and Context

Laboratory astrophysics plays a key role in astronomical and planetary sciences. This broadly defined field consists of a wide range of laboratory experiments (e.g., spectroscopy, kinetics, surface science), as well as theoretical calculations and modeling. It covers almost the entire electromagnetic spectrum, from radio to gamma-rays, and involves critical studies of atomic, molecular, nuclear, plasma, and solid-state systems. Such studies provide the fundamental basis for interpreting observations and drive new scientific advances in virtually every area of modern astrophysics. High-quality data are particularly needed now, as observatories such as the Atacama Large Millimeter Array (ALMA) and the James Webb Space Telescope (JWST) are in their prime science mission, generating an enormous volume of exquisite data that need interpretation. As highlighted in the most recent National Academies of Sciences, Engineering, and Medicine Decadal (NASEM) Survey report titled "Pathways to Discovery in Astronomy and Astrophysics for the 2020s" (Astro2020),[1] which was released in November 2021,

> "Laboratory astrophysics is a critical but often hidden and underappreciated cornerstone of the enabling research foundation. It has been chronically underfunded; concerns were raised in both the 2000 and 2010 decadal surveys, but the problem persists. Research in this area needs to be regarded as a high priority, and the existing approaches are not sufficiently advancing the field."

Examples illustrating the need for laboratory astrophysics data are shown in Figure 1. Here spectra from ALMA and JWST highlight the many unidentified features in the interstellar medium (ISM) and in exoplanets. Also shown are theoretical predictions of nuclear yields for neutron star/white dwarf merger, based on many reaction rates that are unknown. It is clear from these and other examples that a full and complete analysis of observational data is limited by the lack of laboratory measurements and theoretical calculations. It should be emphasized that many areas in astronomy and astrophysics require input from laboratory astrophysics, from the origin of the elements to searches for biosignatures in exoplanet atmospheres. A compilation of relevant problems in astronomy and planetary science, and the data from laboratory astrophysics needed to advance our understanding in these areas is given in Appendix A

In response to the multi-agency recommendation on laboratory astrophysics in Astro2020, recommendations highlighted in previous Decadal Surveys, and findings

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[1] https://www.nationalacademies.org/our-work/decadal-survey-on-astronomy-and-astrophysics-2020-astro2020

reiterated by the 2021-2022 Astronomy and Astrophysics Advisory Committee (AAAC), NSF and NASA requested in August 2022 that the AAAC establish an ad hoc task force as part of an effort by the two agencies to address Astro2020's recommendation in this subject. Specifically, the task force was asked to perform an assessment on behalf of the US community of the utility and priorities in laboratory astrophysics that would enable advances in astrophysics. The resulting analysis and

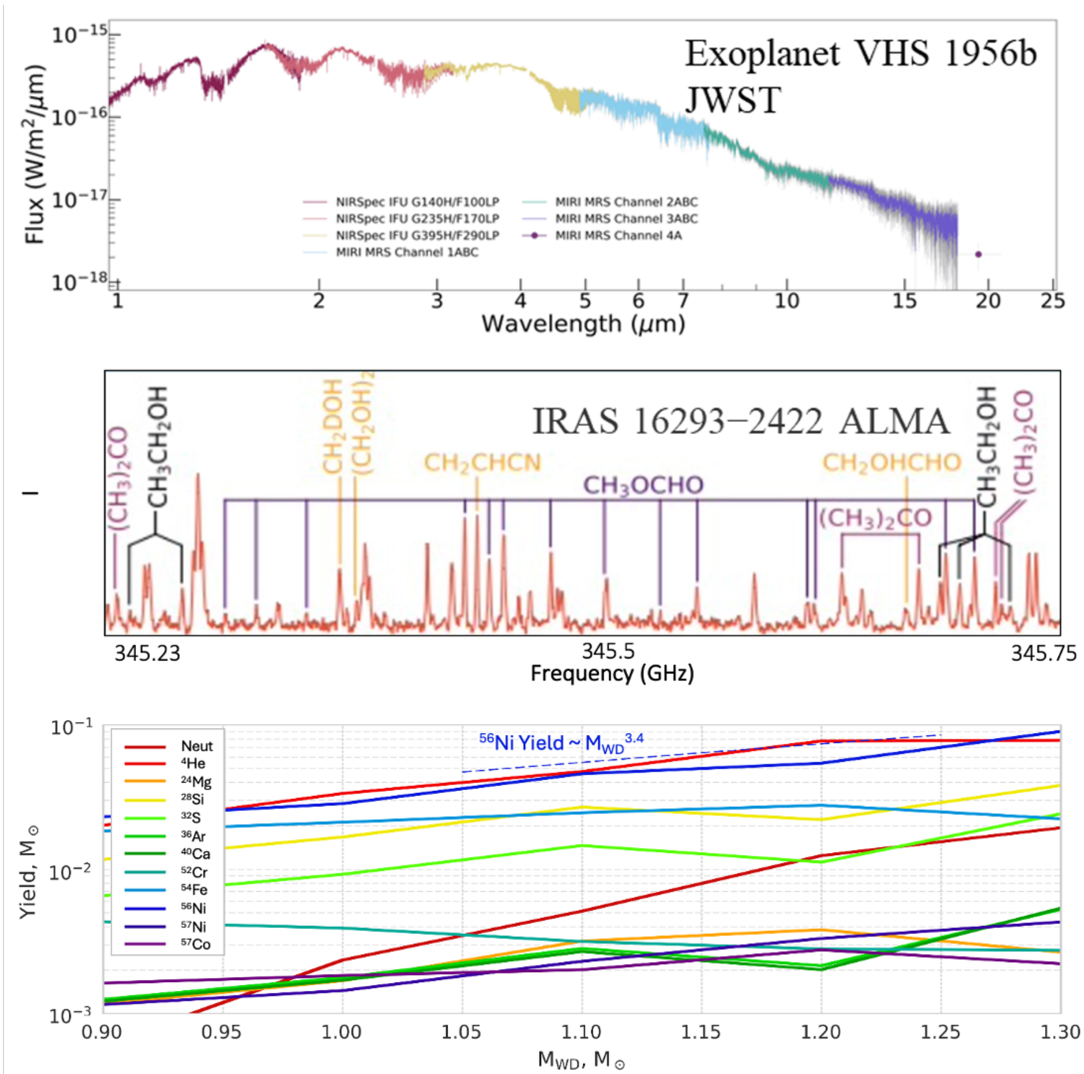

Figure 1: *UPPER: Spectrum of exoplanet VHS 1256b, with multiple molecular ro-vibrational transitions, most of which are identified (Miles et al. 2023). MIDDLE: ALMA spectrum at Band 7 showing a plethora of molecular lines in the binary protostellar IRAS 16293−2422, over half of which are unidentified (Jørgensen et al. 2016; see Fig. 2C of Appendix E) LOWER: Nuclear yields predicted for neutron star/white dwarf merger as a function of WD mass, based on many estimated nuclear rates (Bobrick et al. 2022).*

report aims to assist these agencies in developing a robust plan to effectively allocate available resources to enable and maximize astronomical discovery. The membership of the laboratory astrophysics taskforce (LATF) was large and diverse, including laboratory astrophysicists, theorists, and database curators, as well as observational astronomers and modelers who rely on laboratory astrophysics. The LATF was specifically asked to provide input on four key topics:

- Survey the current state of laboratory astrophysics, drawing from the wide range of available materials (e.g., Decadal Survey reports, white papers, community workshop reports, etc.)
- Identify the needs for supporting laboratory data to interpret results from observatories and missions
- Identify the national resources that can be brought to bear to satisfy those needs
- Consider new approaches or programs for building the requisite databases

The full Charter and Purpose of the ad hoc Task Force can be found in Appendix B; the committee membership is provided in Appendix C.
To effectively undertake this endeavor, the LATF was organized into three subgroups of roughly equal size, covering three broad topical areas:

1. Interstellar Medium (ISM): Chemistry/physics of molecular clouds, star/disk formation, the cycle of matter in the Galaxy.
2. Planets and Exoplanets (PlEx): Exoplanet atmospheres and interiors, habitability, protoplanetary disks, planet formation, solar system Objects.
3. Stellar, Nuclear, and Plasma Astrophysics (SNP): Stellar structure/ evolution, stellar populations, cosmic chemical evolution, plasmas in low-density nebulae through stellar interiors, very dense matter, and neutron stars.

To ensure the LATF had broad community engagement and input, a wide range of activities were carried out over a 9-month period, between March 2023 and January 2024. These included regular monthly meetings among the sub-groups and between the subgroups, as well as a 3-day hybrid meeting of the full task force in September 2023 that was hosted at the Center for Astrophysics | Harvard & Smithsonian in Cambridge, MA. These meetings centered on data collection, discussion of tasks, implementation, and ultimately findings and recommendations. In addition, several community town halls were held at national meetings, including the Summer 2023 American Astronomical Society meeting (June 2023), the annual International Symposium on Molecular Spectroscopy (June 2023), and the American

Chemical Society meeting (August 2023) to solicit community feedback and input. Two surveys were also conducted by email/listserv to the scientific community: one focusing on practitioners of laboratory astrophysics, the second for consumers of these data in astronomy and astrophysics/planetary science communities. These surveys helped identify the status and needs of the laboratory astrophysics practitioners and helped inform the needs for laboratory astrophysics research in astronomy and planetary science. In addition, subject-matter experts in laboratory astrophysics, as well as observational astronomy and planetary science were invited to LATF meetings to discuss the status and needs of their particular fields. Overall, community input from many scientific perspectives was substantial and helped frame the details of this report.

This document is a synthesis of reports by each of the three subgroups. The subgroup reports provide detailed information, research, and analyses in the three topical areas, and are the basis for many of the findings and recommendations provided here. These are appended to this summary.

Although there are many aspects of laboratory astrophysics that could be addressed in a report of this type, the Task Force identified five areas that are critical to laboratory astrophysics in support of astronomical discovery. These are:

- Programmatic support
- Workforce development
- Status of crucial databases
- Facilities and resources
- Interdisciplinary efforts, communication, and collaboration

A number of specific recommendations are put forth as a result of these findings.

2. Current Findings

A. *Programmatic support*

Programmatic support for laboratory astrophysics research pertinent to astrophysics is primarily from the NSF Astronomy and Astrophysics Research Grants (AAG) program, NSF Physics, DOE Office of Science, and the NASA Astrophysics Research and Analysis (APRA) and Astrophysics Data Analysis Program (ADAP) programs.

For ISM-related laboratory astrophysics research, based on a review of publicly available data from NSF and NASA, it is estimated that the NSF AAG program invested approximately $12 M into ISM-relevant laboratory astrophysics research over the 2014-2023 time period (9 years) and NASA APRA invested $12 M over 2016-2021 (5 years). These awards are primarily single-investigator grants for 3-4 years with a total value of $450-500 K(or about $150 K/year). On average, approximately $4 M per year has been directed to ISM-related laboratory astrophysics research across the US through competitive grant programs.

In the case of exoplanet research, which is cross-disciplinary, traditional NASA Astrophysics and Planetary Science programs that support Laboratory Astrophysics do not accept proposals for exoplanetary research, with the exception of the interdisciplinary Exoplanetary Research Program (XRP). XRP has a very broad scope and typically funds 1-2 laboratory astrophysics proposals annually. In the last decade, NSF has only had a small number of proposals funded for exoplanet research. Planetary-relevant laboratory studies (that can potentially be leveraged for exoplanet research) can be funded through other very competitive NASA programs that support research of the Solar System planets, including Planetary Data Archiving and Restoration Tools (PDART) and Solar System Workings (SSW).

Finding #1: The programs that provide dedicated support for laboratory astrophysics are small and are limited by the funding levels available to the agencies.

A lack of coordination with laboratory astrophysics limits the scientific potential and impact of next-generation facilities. Given that multi-billion-dollar missions are becoming increasingly routine, a very modest allocation of the total mission cost to laboratory astrophysics would provide a significant boost to laboratory astrophysics and maximize the discovery potential of missions and telescope facilities. Effective alignment of laboratory astrophysics with prime missions is critically needed and requires a closely coordinated effort between mission scientists, experimentalists, theorists, modelers, and database curators. Ideally, this effort would start during the planning stages of missions and telescopes, but it should also be undertaken as the scientific objectives evolve during active operations.

Finding #2: Although laboratory astrophysics is essential in maximizing the scientific potential and impact of astronomical missions and observatories, funding to support these efforts is not a formal part of mission or observatory planning and long-term mission or observatory support.

B. The laboratory astrophysics workforce

For laboratory astrophysics, university PIs are mostly mid-career and senior researchers, with some early-career faculty, and a mixture from national laboratories and universities. There is anecdotal data indicating current PIs and academic departments do not have the resources required to maintain a robust

workforce in laboratory astrophysics, and the loss of critical expertise is detrimental to astronomy. Attrition in the workforce is primarily because of insufficient resources to train and retain the next generation of practitioners. A substantial fraction of laboratory astrophysics funding and research takes place at NASA centers, and this is where a larger fraction of mid-career researchers remaining in the field reside. Nevertheless, these laboratories face challenges in providing training opportunities for undergraduate and graduate students. In general, there is reasonable support at universities for a limited number of undergraduate and graduate students. Only a small number of laboratory astrophysics grants request postdoctoral researchers, possibly due to an active effort by the PIs to keep their budget requests close to the average funding levels of grant programs. There have only been a small number of early career awards, and many laboratory astrophysics researchers holding permanent positions are required to divide their time between laboratory astrophysics research and research funded by other disciplines.
It is difficult to precisely determine the number of research groups actively engaged in laboratory astrophysics in the USA, however, a review of publicly available NSF and NASA funding awards suggests roughly 40-60 groups at universities and 10-15 groups in national laboratories. The funded PIs reside almost exclusively at doctoral research universities with a very high research activity (labeled as R1 institutions), while those from government laboratories reside mostly at NASA Goddard, NASA Ames, JPL, SETI Institute, and the Harvard-Smithsonian Center for Astrophysics.

In the case of laboratory ISM research, considering the responses received on our community survey, a representative (though not necessarily average) ISM research group at a university consists of approximately 3 graduate students, 5 undergraduate students, and 1 postdoctoral scholar over a 5-year period. Government laboratories represented in the survey consisted of an average of 2.5 undergraduate students, 2 graduate students, 4.5 postdoctoral scholars, and 5 staff scientists, over a 5-year period.

In the case of laboratory nuclear astrophysics, our survey has shown that a significant number of graduate students are attracted to this field. Though available data are likely incomplete, it is estimated that there are 80-90 graduate students, the majority (~60) supported by NSF with the largest known groups at Michigan State University, University of Notre Dame, and Florida State University. This finding reflects the important role that laboratory nuclear astrophysics plays in attracting students into low-energy nuclear physics and thus establishing a clear pathway for developing the Nation's nuclear workforce. University laboratories, large national user facilities such as Facility for Rare Isotope Beams (FRIB), and the smaller university-based accelerator programs therefore play an important workforce development role. In addition, about 25 postdocs are supported annually, with support roughly equally divided between NSF, DOE nuclear physics awards, and DOE national laboratories.

Finding #3: To maintain competitiveness at the international level in the STEM fields, the United States must develop a workforce with critical-thinking skills, deep scientific understanding, and experience in hands-on laboratory methods and data science. Training in laboratory astrophysics is an ideal vehicle for developing these critical skills, which are readily transferable to industrial settings, strengthening the overall workforce in the nation.

Supporting the workforce in laboratory astrophysics presents a significant challenge, primarily due to the prevailing academic and funding climate that often prioritizes "transformative" research over what is perceived as "enabling" research. This distinction impacts the allocation of resources, funding, and institutional support, creating a complex landscape for practitioners in the field to navigate. Enabling research is crucial for the advancement of science, but it is often undervalued because its outcomes are seen as incremental rather than revolutionary. However, laboratory astrophysics studies provide the essential foundation upon which transformative discoveries are built.

Another significant hurdle in hiring university faculty in experimental laboratory astrophysics is the large startup costs which are currently in the range of $1M to $2M. Start-up funds have now become a major factor in making new hires, and one that adversely impacts the health of laboratory astrophysics specifically. Setting up and maintenance of equipment in a new laboratory by an early-career faculty member needs substantial investment, which Physics or Chemistry departments at many universities (both R1 and R2, i.e., doctoral research universities with very high and high research activities) are not able to provide. In contrast, many national laboratory facilities have world-class equipment, but need early career staff to maintain and advance their research programs.

In terms of grant funding, the average award size ($150-175 K/year) for laboratory astrophysics has remained approximately constant at both NSF and NASA even as core inflation has increased by 30% over the last 10 years. Barring an increase in award size, PIs increasingly must operate with smaller teams and restrict the scope of projects. In addition, the short timeframe (3 years) of a typical research grant and the low funding rate (<20%) present other major challenges. One of the most consequential outcomes of decreased funding is the limitations it can place on undergraduate research experiences and graduate student training opportunities, which is vital to developing a strong pipeline of practitioners, and likely contributes to challenges around the critical mass required to maintain expertise in many specialized areas within the broad umbrella of laboratory astrophysics.

Finding #4: An increase in funding levels and duration of laboratory astrophysics awards is needed for continued and sustained laboratory astrophysics research.

NSF provides a variety of workforce development grant programs (e.g., ASCEND, GRANTED, PAARE, LEAPS, etc.) at the AST Division, MPS, and NSF-wide levels, many targeting institutions with few resources and limited research activities. However, it appears that few practitioners in laboratory astrophysics have pursued these funding opportunities to leverage their research capacity.

Finding #5: Greater communication and outreach are needed to increase the community's awareness of existing funding opportunities.

C. Status of crucial databases

There are many available Laboratory Astrophysics databases (>75) that provide data, tools, and models relevant to atomic, molecular, nuclear, and solid-state research– see Appendix D and Figure 2. The provided data represent a significant effort involving careful measurements and calculations, from molecular and atomic transition frequencies to nuclear cross sections, to optical constants. Furthermore, the databases represent considerably more than the simple archiving of tables of numbers that have been measured or calculated. To create a meaningful database, specialized knowledge is required in the rigorous evaluation, validation, and curation of the data, as well as modeling and visualization tools. Users certainly benefit from well-developed formats and formalisms of the databases, including consistent units and uncertainties. In addition, user interaction with the database provider is critical. For instance, managers of the HITRAN database get about three questions per day (there are over 30,000 users). There is a strong case for more communication between the user communities and those generating the data. It is also important that such databases provide the original sources for reference. However, many databases are compendiums of un-evaluated data, lacking internal and inter-database consistency, and there is no contact person for help. Comparing data from multiple sources often does not occur but should be encouraged and supported.

The existence of a large number of databases also creates problems. The need for a publicly accessible "Database of Databases" and "Database of Facilities" have been identified as useful tools, but they currently do not exist.

The wide extent of available databases also does not imply that any of them are complete. While much information has been archived, many data sets have limited coverage in parameter space, such as temperature or frequency ranges, or are simply missing data, for example, transitions for a certain ionized state of atomic iron. These features have led to the creation of specialized databases, which target these deficiencies. For example, Kelly's line list database at Harvard (see Appendix D) is for Z=1-30 and wavelengths covering X-ray to UV. It has not been updated since 2009 and has no personnel or funding to support it. Another example is the ACTINIDES database, which covers energies and spectra for only the actinides. There are thus needs for the generation of missing data – particularly on the molecular side – and for updating the existing data. There is also a significant backlog of evaluating nuclear data. This backlog is due to the lack of funding for a sustained and coordinated effort by a sufficiently large workforce with longer term career perspectives and expertise in both experimental and theoretical physics.

In addition, there is a need for including uncertainties with archived data. Among the listed atomic and molecular databases, only NIST ASD and HITRAN contain critically quantified uncertainties on the evaluated and recommended data. Similarly, only one nuclear astrophysics database (STARLIB) includes uncertainties. The optical constants database (OCdb) for solid samples includes uncertainties when they are published with the data. Efforts are underway for the development of methods to assign uncertainties on theory data in atomic, molecular, and nuclear physics. It should become the normal practice that uncertainties are provided with any experimental or theoretical data archived in the databases; however, a significant increase in effort and support is required.

It should also be noted that while significant portions of the databases are from data that were calculated or measured as part of non-astrophysics funding (e.g., DOE-FES, Chemistry programs), this situation is becoming rare. As a result, it is becoming even more important that astrophysical funding be made available for database support.

Databases ensure the legacy value of laboratory astrophysics data. Presently, none of the databases outside of national laboratories have guaranteed support.

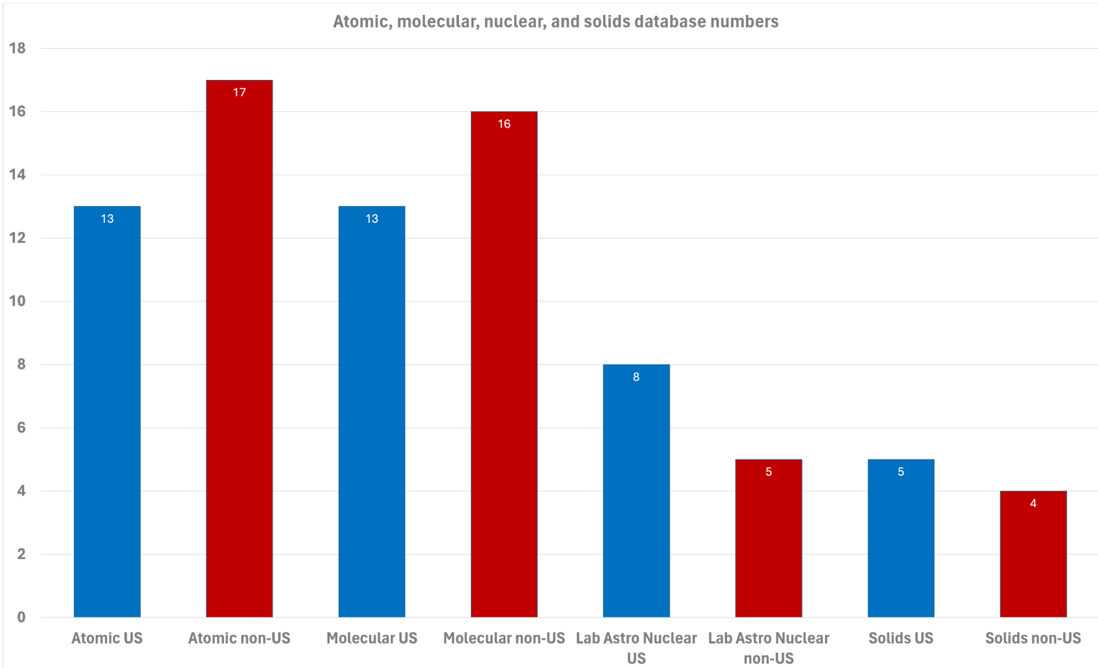

Figure 2: *The number of existing databases per laboratory astrophysics subject area at US (in red) and non-US institutions* ***(****in blue****).***

Finding #6: Databases are becoming increasingly important in all areas of astronomy and astrophysics, and they must be curated and validated for maximum utility, requiring modest yet sustained investment by the astronomical community.

D. Facilities support and resources

Research relevant for much of laboratory astrophysics is undertaken primarily at large government laboratories, such as NASA Ames Research Center (ARC), NASA Goddard Space Flight Center (GSFC), NASA Jet Propulsion Laboratory (JPL), NIST, LLNL, LANL, and SNL, and at a number of universities across the United States. Some national labs have DOE Office of Science-supported national user facilities (e.g. FRIB and ATLAS). It is often the case that the instruments at national labs and universities were built up from funding outside of laboratory astrophysics, such as from chemistry or the nuclear programs. This combined set of facilities form a network that represents a history of infrastructure development that has led to experienced researchers, instruments, and theoretical/computational tools.

Support for laboratory astrophysics research at universities is provided by faculty hires who are normally given one-time start-up funds that can vary substantially. Astronomy departments typically have smaller start-ups than chemistry or physics and have less funding for equipment purchases. At government laboratories, dedicated funding equivalent to faculty start-up packages is far less common; new workforce capabilities are instead developed primarily by attrition when existing researchers move on to mission/institutional work and/or retirement. Additionally, once start-up is spent, it is often challenging for PIs to purchase new equipment except through extremely competitive federal funding programs (e.g., NSF MRI).

An example of the complexity and breadth required in laboratory astrophysics infrastructure development is that created in the last four decades to study the chemistry in (exo)planetary atmospheres. IR Fourier transform and laser-based spectrometers have been fabricated/purchased for measurements of the gas-phase, UV-IR high-resolution spectral signatures of molecules at different thermodynamic (P, T) conditions. The majority of existing laboratories can obtain spectra only at room temperature, while measurements at very low to very high pressures and temperatures require specialized instrumentation and facilities that are not readily available in most laboratories. These experiments allow for building semi-empirical line lists and determining optical constants of aerosol and cloud particle analogs needed for the interpretation and modeling of exoplanet spectra. Furthermore, mass spectrometry experiments can be used to investigate chemical pathways leading to the formation of larger molecules and solid particles in gas mixtures representative of exoplanet atmospheres.

Multibillion-dollar DOE facilities such as EBIT plasma experiments or synchrotron light sources are not easily accessible to laboratory astrophysicists. Devoting a small fraction of available user time, plus modest resources to ensure access to floor space could efficiently leverage these state-of-the-art facilities for laboratory astrophysics measurements with little to no additional cost.

Finding #7: The astronomical community has historically benefited from studies and data produced in related fields, primarily Chemistry, Earth Sciences, and Physics, which has been supported by these disciplines. With the shifting priorities in these core disciplines, this level of support has diminished over time. Increasingly, the astronomical community will need to fund these activities to better understand observations from ground-based observatories and space-based missions.

In the solid state, it is important to characterize haze/cloud particles pertinent to planetary atmospheres. Laboratory analogs produced in the laboratory are studied using, for example, mass spectrometry, UV-FIR spectroscopy, scanning electron microscopy, X-ray photoelectron spectroscopy, and X-ray absorption near-edge structure spectroscopy; vapor pressure measurements are also carried out of relevant molecular species. Producing and characterizing solids require specialized experimental facilities that are not traditionally found in astronomy departments but may be found in atmospheric chemistry labs. Despite the wide range of studies currently ongoing, there are many experimental measurements still needed to support astronomical observations (Fortney et al., 2019) including: (1) optical constants of atmospheric ice, aerosol, and surface analogs from 5 K-300K; (2) laboratory simulations of planetary surface chemistry (ice, grains); and (3) laboratory degradation studies of biotic biomarkers and abiotic organic compounds.

In addition to experiments, there is an important theory and modeling component to the study of such atmospheres, including theoretical gas-phase simulations with haze/cloud particles as well as exoplanet surface composition and processing, and planetary interiors. Global circulation models for Exoplanets, Mars, Venus, Gas Giant planets, etc. are also needed. To carry out such simulations, quantum chemical calculations of rovibrational line lists for characterizing exoplanet atmospheres and spectroscopic constants for molecular species are needed, as well as corresponding atomic and molecular opacities, and rate constants, branching ratios, and other reaction parameters crucial for molecular dynamics to explore formation and destruction pathways of complex organic molecules and ices. Quantum chemical calculations of IR spectral properties of aerosol and cloud particle analogs are also required and advanced theoretical simulations of the light scattering and absorption properties of porous, heterogeneous aggregates. Finally, theoretical calculations are required to simulate magma-atmosphere interfaces and interiors in exoplanets.

During the past several decades, over 50 modeling codes have been developed for planetary atmospheres (MacDonald &R.J., Batalha 2023). The most commonly-used US-developed codes include PandExo (community tool for transiting exoplanet science with the JWST & HST), PICASO (Planetary Intensity Code for Atmospheric Scattering Observations), Virga (cloud model for exoplanets and brown dwarfs), and Planetary Spectrum Generator (PSG, radiative transfer and observational simulator).

Experimental facilities, models, and theoretical expertise as discussed here for one aspect of laboratory astrophysics cannot be turned on and off as missions come and go. The infrastructure is unique and has a complex network of interconnecting parts, each of which cannot advance significantly without the others. Therefore, sustained investment in a diverse portfolio of experimental and theoretical capabilities is essential. This situation is typical for laboratory astrophysics work in all three sub-areas investigated. Furthermore, the existing infrastructure provides the foundation for new experimental and theoretical developments.

Finding #8: Laboratory astrophysics is a diverse, interdisciplinary field, ranging from fundamental investigations of phenomena to more applied studies. It includes experimental, theoretical, and modeling components. Furthermore, the infrastructure that supports laboratory astrophysics is a complex network of interconnecting parts, each of which often cannot advance significantly without the others.

E. Interdisciplinary efforts, communication, and collaboration

A general lack of communication has been identified between observational astrophysicists and astronomers, and laboratory astrophysicists, including experimental physical chemists and physicists, and theorists. The latter group often produces relevant data for astronomy, but channels of communication are limited. This communication gap often becomes very pronounced during ongoing missions like JWST. A concrete example is the recent discovery of many unidentified features in the JWST spectra of various exoplanets, comets, and protoplanetary disks, where crucial spectroscopic data are currently lacking.

One of the reasons for the "communication gap" is the dearth of interdisciplinary grants and observing proposals, as there are often no clear channels for collaboration. Additionally, there is often a lack of awareness about the potential contributions that scientists from different disciplines can offer to advance astronomical research objectives.

The problem is certainly recognized among astronomers. In the "user" survey done by the LATF, it was found that only 32.1% of users of laboratory astrophysics data, both experiment and theory, has satisfactory interactions with those producing the data. Another 35.7% has interactions, but not sufficient, while 32.1% has no interactions whatsoever (see Figure 3).

Finding #9: A lack of effective and meaningful communication between practitioners of laboratory astrophysics and the wider astronomical community has been identified.

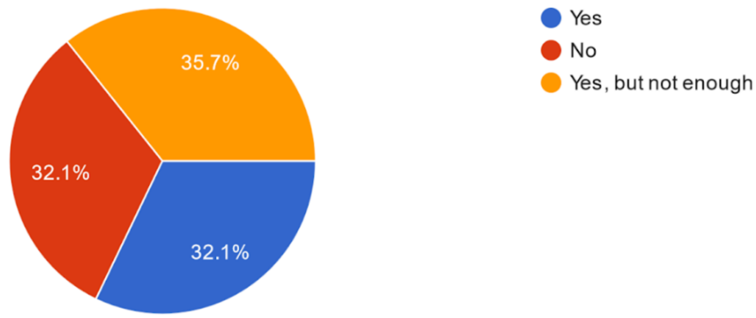

Figure 3: *Response to the laboratory astrophysics User survey, evaluating the degree of interactions with producers of laboratory astrophysics data, including experiment and theory. A total of 31 responses were received.*

3. Recommendations

A. Programmatic support

Recommendation #1: The agencies should increase access to funding opportunities for individual investigators and larger collaborative teams by developing joint programs and, where necessary, expanding the scope of current proposal calls to explicitly include laboratory astrophysics efforts.

NASA and NSF should explore joint and collaborative programs to meet common needs in the community, and as needed, pursue separate laboratory astrophysics funding lines to ensure sustained support for the critical enabling efforts of laboratory astrophysics. NSF should continue to pursue robust collaborative funding initiatives across Divisions within the Directorate for Mathematical and Physical Sciences (MPS), as well as other Directorates, prioritizing cross-cutting endeavors, a domain where laboratory astrophysics excels. Opportunities for collaboration with DOE should also be explored. The NSF/DOE Partnership in Basic Plasma Science and Engineering program which ran for over two decades might serve as a model for a joint program in laboratory astrophysics.

The LATF calls particular attention to support laboratory research for exoplanetary science in NASA's call for proposals. This opportunity could be offered on a biannual rather than annual basis, but nevertheless it is essential to enable further progress in this field.

Recommendation #2: Laboratory astrophysics should be explicitly incorporated in all phases of an observatory or mission from planning to extended operations.

Appropriate resources should be devoted for laboratory astrophysics in support of large NSF and NASA-funded observatories and missions, so as to ensure maximum scientific output and impact over the lifecycle of the project (e.g., expanding the scope of the ALMA Development Fund to explicitly include laboratory astrophysics projects, increasing the allocation of funds for Laboratory Astrophysics in JWST GO programs, and including laboratory astrophysics in the life cycle of a mission early on in its development).

Recommendation #3: The agencies should consider expanding certain programs that are beyond the scope of individual PIs to create and support modest-sized instrumentation or facility centers that provide professional and centralized services to the laboratory astrophysics community.

Examples include NSF-sponsored user facilities and NASA's Planetary Science Enabling Facilities (PSEF). The NSF-UCLA Secondary Ion Mass Spectrometry (SIMS) (https://uclasims.epss.ucla.edu/) facility is an efficient and inclusive model that might be expanded upon.

B. Laboratory astrophysics workforce development

Recommendation #4: The agencies should continue to prioritize and promote workforce initiatives spanning the career progression from the undergraduate to the early-career level, and beyond.

Many such programs exist, particularly at NSF, but there appears to be a need for greater awareness of these opportunities. Efforts to effectively promote and exploit these opportunities are essential to bolster the laboratory astrophysics research enterprise and help stem the loss of critical expertise from the field. Proposal solicitations should emphasize the importance of hands-on laboratory skills and data science training to promote the development of a competitive workforce with critical-thinking abilities and deep scientific understanding. Opportunities to develop partnerships between research-intensive universities and smaller resource-limited institutions are one of several promising avenues to increase access and exposure to laboratory astrophysics research.

C. Databases

Recommendation #5: Approaches for long-term support for the curation and further development of existing and future databases with emphasis on critical data evaluation and uncertainty quantification should be pursued.

This support should cover specialized database workforce as well as resources to connect and search the databases. It is recommended that a "Database of Databases" and "Database of Facilities" be created to bring awareness to what is available in the scientific communities and enable collaborations.

D. Facility support and infrastructure coordination

Recommendation #6: Because laboratory astrophysics is a highly interdisciplinary enterprise, the agencies should explore opportunities for interagency coordination to streamline existing resources.

For example, NASA and NSF-funded projects could effectively leverage resources that exist at DOE facilities (e.g., EBIT plasma experiments, synchrotron light sources).

E. Communication and Collaboration

Recommendation #7*:* The agencies should consider facilitating community meetings that highlight the interplay of laboratory astrophysics with forefront astronomical problems and promote meaningful interactions between astronomers who rely on laboratory astrophysics data and the researchers who generate and curate those data. Because laboratory astrophysics is uniquely positioned to bridge the gap between astronomy and numerous key subfields of chemistry and physics, the meetings should also highlight interdisciplinary efforts, synergies, as well as cross-disciplinary and interagency funding opportunities that could be leveraged to address critical data needs of current and proposed astronomical missions.

Topical meetings and workshops at professional society conferences could provide an ideal forum to inform and promote collaborative efforts. For example, the European community is sponsoring a conference in Italy in July 2024 titled, "European Laboratory Astrophysics in the JWST Era" to enhance scientific coordination between laboratory astrophysics and the broader astronomy community. Equivalent efforts should be undertaken within the US community.

***Recommendation #8**: Given the importance that Astro2020 placed on laboratory astrophysics as a cornerstone of the enabling research foundation, and the explicit finding by Astro2020 that existing approaches are not advancing the field sufficiently, the LATF recommends that the agencies provide an assessment of their progress toward addressing support for laboratory astrophysics prior to the mid-decadal NASEM Survey. This review is especially timely as the science drivers for planned flagship missions and observatories are defined in the next several years, and the needs of existing ones continue to evolve.*

4. Concluding Remarks and Outlook

As specified by its Charter, the present report of the LATF addresses various aspects of laboratory astrophysics, including the current state and challenges related to funding, workforce development, database management, facility access, the need for improved communication and collaboration within the field, as well as interagency coordination. On the basis of a detailed analysis of publicly available data and substantive community input, this report provides a number of findings and recommendations in each of these areas. However, it is not a comprehensive summary of all activities in this dynamic and multifaceted field. Furthermore, specific strategies for implementing recommended actions, detailed examples of successful initiatives, analysis of the economic impact of enhancing laboratory astrophysics, and considerations for international cooperation and competition are areas that require future assessment.

A vibrant community of experienced and highly capable researchers currently exists who perform high-quality and specialized laboratory astrophysics research that is critical to the field of astronomy. Although the present report highlights areas of concern, the future of laboratory astrophysics remains bright. Effective integration of laboratory astrophysics with astronomy and a robust interplay between the two promises to enable new and exciting avenues for research and discovery. With careful planning, execution, and interagency coordination there is no fundamental obstacle to achieving this outcome, and one that will ultimately benefit astronomy.

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Appendix A

Relevant Science Questions Requiring Laboratory Astrophysics

Themes (and Associated *Telescopes/Missions)*	*Science Questions*	*Application to Laboratory Astrophysics*
Diffuse ISM *(HST, JWST, ALMA, US ELTs, NOIR Lab telescopes)*	What sets the density, temperature, and magnetic structure of the diffuse ISM, enabling the formation of molecular clouds? How do molecular clouds form from diffuse clouds ? How does injection of energy, momentum, and metals from stars ("stellar feedback") drive the circulation of matter between phases of the ISM and CGM?	Measurement of optical properties of dust from x-ray to mm wavelengths Rate coefficients and branching ratios for gas-phase and heterogeneous reactions Photoabsorption and photoionization cross sections and branching ratios for small molecules Electronic, vibrational and/or rotational spectroscopy of cations, radicals and PAHs, PAH cations, fullerenes, and related species

Molecular Clouds *(ALMA, JWST)*	What processes are responsible for the observed velocity fields in molecular clouds? What is the origin and prevalence of high-density structures in molecular clouds, and what role do they play in star formation? What generates the observed chemical complexity of molecular gas?	Optical properties of dust and astrophysical ices at multiple wavelengths Rate coefficients and branching ratios for low-temperature gas phase reactions involving radicals and ions Chemical reaction rates, energetics, and nonthermal desorption processes on astrophysical ices Rotational spectroscopy of isotopologues and vibrationally excited states of stable complex organic molecules and exotic isomers and of complex organic radicals and cations
Stellar, Nuclear, and Plasma Astrophysics **Multi-messenger astronomy** (*JWST, HST, LIGO, VIRGO, FERMI, SWIFT, BlackGEM, DECam, GOTO, the Vera C. Rubin Observatory's LSST, ULTRASAT, VISTA, and WINTER*)	Determining the origin and evolution of heavy elements in the Universe. What are the dynamics of Neutron star mergers?	For heavy elements: - Lab measurements of nuclear reaction rates - Atomic opacity calculations and oscillator strengths - Electron-impact collision calculations and measurements for excitation, ionization, and recombination

Sources of X-rays and UV emission (*XRISM, CHANDRA, XMM-NEWTON, ATHENA*)	What is the source of high energy radiation in accreting black holes? What are the conditions and dynamics in supernova explosions?	Inner-shell photo- and electron-impact ionization of K- and L-shell electrons High accuracy atomic structure measurements and calculations for satellite lines in atomic systems.
Photoionized plasmas (*JWST, HST*)	What is the mechanism for the abundance discrepancy factors in planetary nebulae and H II regions? What are the abundances of complex atoms in photoionized plasmas?	Photo-absorption data for gas-phase molecules containing O and Fe. Improvements in the accuracy of low temperature dielectronic recombination rate coefficients
Stellar interiors	What is the nature of stellar structure, stellar evolution, and stellar populations?	Improved electron-impact data for Fe-peak elements Nuclear reaction rate coefficients and opacities for astrophysically abundant elements
The solar wind interaction with atmospheres of comets and planets (*JWST, XRISM, XMM-NEWTON, CHANDRA*)	What is the role of the interaction of the solar wind with atmospheres?	Charge-exchange data for the range of solar wind velocities of H and He on the atoms and molecules present in cometary and planetary atmospheres. High resolution measurements of molecular spectra for species in

		cometary and planetary atmospheres
Accreting neutron stars *(XRISM, XMM-NEWTON, CHANDRA, ATHENA)*	What is the compactness of neutron stars? What is the contribution of explosive nucleosynthesis to the origin of the elements?	Nuclear reaction rates on unstable neutron deficient isotopes
Stellar explosions including Novae and Supernovae *(COSI, INTEGRAL, NuSTAR, Kepler, XRISM, CHANDRA, XMM-NEWTON, ATHENA)*	How do supernovae explode?	Nuclear reaction rates on stable and unstable nuclei, including weak interaction rates Improved Fe-peak element electron-impact data for non-equilibrium ionization balance conditions
Exoplanetary Atmospheres (*HST, JWST, ALMA, Ariel, Pandora, US ELTs, NOIR Labs telescopes, HWO)*	What are exoplanetary atmospheres, clouds, and haze particles composed of? What are the atmospheric circulation and radiative properties that regulate exoplanetary atmospheres and their climate? What is the photochemistry generated by radiation from the parent star in exoplanet atmospheric layers?	Measurement of chemical reaction rates under non-terrestrial conditions of gases and surface/gas interactions Measurement of energies, oscillator strengths, collisional cross sections for determining gas opacities over a large temperature range Modeling of haze and cloud formation, surface/atmosphere interactions

		Optical spectra and scattering properties of relevant gases and particles
Habitability *(JWST, HWO)*	How do habitable environments arise and evolve within the context of their planetary systems? How can signs of habitable life be identified and interpreted in the context of their planetary environments? What are the "false positives" for potential biosignature gases?	Accurate line lists for biosignature molecules and contaminating species at near-terrestrial temperatures Optical spectra, oscillator strengths of atmospheric gases Scattering properties of haze Theoretical modeling of planetary atmosphere chemistry and evolution to interpret biosignature gases
Exoplanet interiors	How do bulk planetary properties and formation/thermal histories affect planetary interior and magnetic fields? How do structure and composition of planetary interiors connect to its surface and atmosphere?	Measurement of solid/liquid phase diagrams under high pressure and temperature Mineral behavior under high pressure and temperature conditions Energy transport in liquid/solid materials

Protoplanetary Disks and Planet Formation (*ALMA, JWST, NOIR Labs Telescopes, HWO)*	What is the composition of protoplanetary disks? How are volatiles distributed during and after planet formation? How do dense molecular cloud cores collapse to form protostars and their disks?	Characterization of volatiles and organics through spectral line catalogs Input to the catalogs from millimeter-wave/ Far IR spectroscopy of gases and dust analogs Determination of optical properties of dust Measurement/calculations of reaction rates for relevant gases, ices, and solids Studies of surface chemistry and grain/ice interactions
Solar System objects *(JWST, ALMA)*	What are the atmospheric properties of planets and satellites (Earth, Venus, Titan, Pluto, Jupiter, Saturn) and how can they help better model and understand exoplanet atmospheres composition, dynamics and evolution?	Experimental/Theoretical Modeling of gas-phase/solid state chemistry under specific planetary conditions General Circulation Models (GCM) to interpret observations of Venus, Mars, Earth, Titan as applied to exoplanets

Appendix B: Charge to the AAAC

Dr. Kyle Dawson
The University of Utah
115 S 1400 E Rm. 201
Salt Lake City, UT 84112

Dear Dr. Dawson,

The National Science Foundation (NSF) and the National Aeronautics and Space Administration (NASA) request that the Astronomy and Astrophysics Advisory Committee (AAAC) establish an ad hoc taskforce as part of an effort by the agencies to address the 2020 Decadal Survey on Astronomy and Astrophysics (Astro2020) Recommendation on laboratory astrophysics. [1]

Background

Recognizing that laboratory astrophysics is essential "*for enabling science across astrophysics*" and "*to realize the full potential of recent and imminent major observatories,*" the Astro2020 Report concludes that supporting research in laboratory astrophysics "be regarded as a high priority," and that "the existing approaches are not sufficiently advancing the field." Accordingly, the Report made the following multi-pronged Recommendation:[2]

NASA and the National Science Foundation should (1) convene a broad panel of experts to identify the needs for supporting laboratory data to interpret the results from the new generation of astronomical observatories, (2) identify the national resources that can be brought to bear to satisfy those needs, and (3) consider new approaches or programs for building the requisite databases. This panel should include experts in laboratory astrophysics as well as representative users of the data, who can best identify the highest-priority applications.

The 2021-2022 AAAC report[3] reiterated the Astro2020 Recommendation, adding:

"Although all three agencies have laboratory astrophysics programs, their strategic alignment with national priorities and the community that they serve must be assessed. To this end, the AAAC recommends that an advisory group to NASA, NSF, and DOE be established to identify strategic and community needs, and to set priorities in laboratory astrophysics."

While the Astro2020 report includes suggestions on actions that can be taken to strengthen laboratory astrophysics, what is needed is a robust assessment of the field with focused input from observational, theoretical, and laboratory astrophysics communities. This will allow the

[1]https://www.nationalacademies.org/our-work/decadal-survey-on-astronomy-and-astrophysics-2020-astro2020
[2]See chapter 4.5.5 of the Astro2020 report
[3]https://www.nsf.gov/mps/ast/aaac/reports/annual/aaac_2022_report.pdf

agencies to identify the most impactful ways to enhance the scientific return of observatories and missions by supporting the laboratory astrophysics community.

Charge and Purpose

The ad hoc Taskforce is asked to develop an assessment of the scientific utility and priorities in laboratory astrophysics for the US community that will enable the greatest advances in astrophysics. The purpose is to allow the agencies to devise a robust plan to make the most effective use of available resources to enable discovery science by supporting the community.

Comprised of laboratory astrophysicists, theorists, and database curators, as well as observational astronomers and modelers who rely on laboratory astrophysics, the ad hoc Taskforce is asked to:

- **Survey the current state of laboratory astrophysics, drawing from the wide range of available materials (e.g., Decadal Survey reports, white papers, community workshop reports, etc.)**
  - Assess resources that currently support laboratory astrophysics, including grant programs, databases, facilities, and infrastructure.
- **Identify the needs for supporting laboratory data to interpret results from observatories and missions**
  - Identify and prioritize the needs for interpretation of data from current and future observatories and missions.
  - Identify the corresponding requirements for laboratory and theoretical research to support those needs.
  - Identify workforce and infrastructure needs.
- **Identify the national resources that can be brought to bear to satisfy those needs**
  - Identify national resources and interagency synergies (e.g., DOE, DOD, NIST, …) that are not being exploited at present.
  - Identify ways in which existing resources can be used more efficiently.
  - Identify the specific areas that might benefit from targeted additional investments.
  - Consider how resources for laboratory astrophysics should be integrated into the planning and operation phases of observatories and missions.
- **Consider new approaches or programs for building the requisite databases**
  - Identify the database gaps, both nationally and internationally.
  - Define database requirements that would enhance interpretation of astronomical observations.
  - Identify new modalities of support (e.g., "Centers" for laboratory astrophysics and databases).

The Taskforce is requested to report its initial findings to the AAAC in mid-2023, with a final report to be delivered by early 2024. In accordance with Federal Advisory Committee (FACA) rules, the report will be discussed and approved by the AAAC at a public meeting before formal transmittal to the agencies.

We appreciate your effort in establishing this taskforce. Its deliberations and findings will inform the agencies on the strategic needs for federal support of laboratory astrophysics and contribute to the agencies' planning activities. The formation of the ad hoc taskforce does not imply any commitment by the agencies to provide specific funding for laboratory astrophysics.

We look forward to working with you in this important endeavor. The points of contact for each agency are listed below.

Sincerely,

Debra Fischer

MARK CLAMPIN Digitally signed by MARK CLAMPIN Date: 2022.08.23 16:29:04 -04'00'

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Director, Division of Astronomical Sciences
Directorate for Mathematical and Physical Sciences
NSF

Mark Clampin
Director, Astrophysics Division
Science Mission Directorate
NASA Headquarters

23 August, 2022

Date

Date

Appendix C
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Appendix D

Summary of Current Databases

There are a large number of atomic, molecular, nuclear, and solid-state databases available for Laboratory Astrophysics. We list them here, separating them into databases hosted in the USA and those hosted in other countries. It should be noted that this list is likely not comprehensive, but reflects the majority of the databases in each category. The following list could be used to assemble a 'database of databases' for the community.

As well as the databases mentioned below, there are a number of databases that search other database sources. These include:

VAMDC: https://vamdc.org/
The National Institute for Fusion Sciences (NIFS): https://dbshino.nifs.ac.jp/

a) Atomic:

For the atomic databases, the following acronyms are used for conciseness.
DR – dielectronic recombination
CX – charge exchange (cross sections)
EIE – electron-impact excitation
EII – electron-impact ionization
EIR – electron-impact recombination
PE – photoexcitation
PI - photoionization
RR – radiative recombination

i) USA:

NIST ASD: Energies, wavelengths, *A*-values, spectral modeling (Saha-Boltzmann plasma emissivities); Z = 1-110, λ = X-ray to radio; ≈300,000 lines (≈43% with *A*-values)

NIST HBASD: Energies, wavelengths, *A*-values; Z = 1-99, λ = EUV to FIR; 12,012 lines

NIST-LANL Opacity DB: Opacities, Z = 57-70, 89-102; λ = X-ray to radio

Los Alamos OPLIB database: LTE Opacities, Z=1-30, λ = X-ray to radio

NIST FLYCHK collisional-radiative code: online modeling of NLTE plasma emission spectra (Z = 1-79)

ATOMDB: Focused on X-ray astrophysics; wavelengths, *A*-values, simple modeling of emissivities; Z = 1-30, λ = X-ray to FIR; 99,510,189 transitions with *A*-values

NASA XSTAR: Energies, wavelengths, *A*-values, PI, DR, spectral modeling (emissivities, opacities); Z = 1-30, λ = X-ray to radio; 736,256 transitions with *A*-values

NASA uaDB: Focused on X-ray astrophysics; energies, wavelengths, *A*-values, PI, EII, EIE, EIR, RR, DR, PE; Z = 1-30, λ = X-ray to radio; millions of lines/transitions

CHIANTI: Energies, wavelengths, *A*-values, EII, EIR, EIE, spectral modeling of emissivities; Z = 1-30, λ = X-ray to FIR; 1,954,916 transitions with *A*-values; collisional-radiative modeling of photon emissivity

Kurucz's Atoms (Harvard): Energies, wavelengths, *A*-values; Z = 1-53, λ = X-ray to FIR; 2.3×10^6 transitions

Kelly's Line List (Harvard): Z = 1-30, λ = X-ray to UV; ≈100,000 lines, has not been updated since 2009. No personnel or funding

KRONOS (UGA): Charge exchange cross sections

ALL database (University of Kentucky) This is a compilation of approximately 1.76 million allowed, intercombination, and forbidden atomic transitions with wavelengths in the range from 0.6 Å to 1000 µm, is current and is updated regularly

ii) Other countries:

OPEN-ADAS: EII, EIR, EIE, RR, DR, AI, PI, CX, collisional-radiative modeling of photon emissivity; Z = 1-30, λ = X-ray to radio (Europe)

Spectr-W3: Z = 1-102, λ = X-ray to FIR; 371,906 lines, many with *A*-values (Russia)

ISESA Grotrian: Z = 1-102, λ = X-ray to FIR; ≈200,000 lines (≈30% with *A*-values) (Russia)

CAMDB: Z = 1-95, λ = X-ray to FIR; $>2\times10^6$ transitions, most with *A*-values; EIE, EII, DR, AI, PI, heavy particle collision data, opacities (China)

TOPBASE/TIPBASE: Z = 1-26, λ = X-ray to radio; 1,715,706 transitions with *f*-values; opacities (France)

ACTINIDES: Z = 89-99, λ = VUV to FIR; 3600 lines; energy levels (France)

STARK-B: Stark broadening and shift parameters for atoms and atomic ions, Z = 2-88 (France)

VALD3: Z = 1-92, λ = X-ray to FIR; 1,175,829 transitions with *f*-values (Sweden)

van Hoof's Atomic Line List: Z = 1-36, λ = X-ray to FIR; 1,720,000 transitions (many with *A*-values) (Belgium)

DREAM: Z = 57-71, λ = VUV to FIR; 72,707 transitions with *A*-values (Belgium)

DESIRE: Z = 73-77, λ = VUV to NIR; 11,624 transitions with *A*-values (Belgium)

BRASS: Z = 1-92, λ = UV-VIS; 82,337 lines with log(gf)-values (Belgium)
SPEX: Focused on X-ray astrophysics (Netherlands)
IAEA ALADDIN database (EII, EIR, EIE, DR, CX) (Austria)
IAEA CollisionDB (EII, EIR, EIE, DR, CX, and molecular) (Austria)
Database of Convergent Close Coupling data (EII, EIE) (Australia)
LXCat, the plasma data exchange project (electron and ion scattering processes) (international)
Scobeltsyn Institute of Nuclear Physics charge exchange data (CX) (Russia)

b) Molecular:

i) USA:

HIgh-resolution TRANsmission (HITRAN) and HIgh TEMPerature (HITEMP) databases of molecular spectral parameters. The database includes the line-by-line spectroscopic parameters required for high-resolution radiative-transfer codes, experimental infrared absorption cross-sections (for molecules where it is not yet feasible for representation in a line-by-line form), collision-induced absorption data, aerosol indices of refraction, water vapor continuum and general tables (including partition sums) that apply globally to the data. 80% of funding comes from the NASA grant, which needs to be renewed/reviewed every 3 years. 20% come from applications for different competitive grants that address planetary atmospheres. HITEMP is only funded as a portion of planetary grants.
Splatalogue (Remijan et al. 2020): 5,800,000 molecular lines, VIS to radio
NIST Molecular Spectroscopic Data has not been updated for a while now, but still a very useful resource.
Millimeter and Submillimeter Molecular Spectroscopy Catalog, Jet Propulsion Laboratory
Ames Molecular Spectroscopic Data For Astrophysical And Atmospheric Studies, NASA Ames. Funding sporadic, from small NASA grants from different calls that fund calculations of particular molecules.
MolList, semi-empirical line-lists and measured cross-sections for a number of molecules (https://bernath.uwaterloo.ca/molecularlists.php) (several NASA grants (PDART, Outer planets).
Raman Spectral Database, Raman spectra developed and maintained at NASA Ames Research Center. Funded by APD/PSD.

Polycyclic Aromatic Hydrocarbon Infrared Spectral database (PAHdb), developed in the last 10+ years and maintained at NASA Ames. Sporadic funding from small NASA grants from different calls, then from larger directed grants funded by APD and in a small part by PSD, and recently from an Internal Scientist Funding Model (ISFM) direct work package funded by APD.

Kurucz's Molecules (Harvard-Smithsonian CfA): Energies, wavelengths, *A*-values; Z = 1-53, λ = X-ray to FIR; 2.3×10^6 transitions

MAESTRO: Exoplanet Opacities Community Tool molecular and atomic opacity database, provides molecular opacities for Temperature=75.0-4000.0 Kelvin, Pressures=10^{-6}-3000 bar, Wavenumbers=30-30000 cm^{-1}.

ShockGas-IR Spectral Database: a database of gas-phase infrared absorption spectra measured at elevated temperatures and pressures. The measurements are performed in the Hanson Research Group shock tube facilities using rapid-tuning, broad-scan lasers to collect quantitative, spectrally-resolved absorption cross-section data over a wide wavelength range. Air Force funded.

Fundamental Kinetics Database Utilizing Shock Tube Measurements: Database summarizes the published shock tube experimental work performed in Hanson's lab at Stanford University. The database is divided into three types of data: ignition delay times, species time-history measurements, and reaction rate measurements.

Molecular spectroscopy at JPL

ii) Other countries:

The Cologne Database for Molecular Spectroscopy (CDMS) (Germany)

GEISA Spectroscopic Database, similar to HITRAN, targets terrestrial and planetary atmospheres (France)

ExoMol, *Molecular line lists for exoplanet and cool star atmospheres* (UK)

Spectroscopy and Molecular Properties of Ozone (France and Russia)

Spectroscopy of atmospheric gases (SPECTRA) (Russia)

TheoReTs, *Internet accessible information system "Theoretical Reims–Tomsk Spectral data* (France and Russia)

Leiden Atomic and Molecular Database (LAMDa), (Netherlands and Sweden)

Calculated spectroscopic databases in Dijon, - MeCaSDa for CH_4,- TFMeCaSDa for CF_4,- TFSiCaSDa for SiH_4, - GeCaSDa for GeH_4, - RuCaSDa for RuO_4, - SHeCaSDa for SF_6, - UHeCaSDa for UF_6, - ECaSDa for C_2H_4 (France)

BASECOL is devoted to the collisional ro-vibrational excitation of molecules by colliders such as atoms, ions, molecules, or electrons (France and Chile)

IDEADB, This database contains information about dissociative electron attachment upon interaction of low-energy electrons with molecules (Austria)

MPI-Mainz UV/VIS Spectral Atlas, Database of molecular UV cross-sections, Germany

KIDA is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies (France)

SESAM provides a molecular spectroscopy database dedicated to the electronic spectra of diatomic molecules (France)

NIFS, Atomic and Molecular Research Center: Atomic and Molecular Numerical databases for various collisional processes (Japan)

MCCC database for H2 electron and positron collision processes (Australia)

Diatomic Molecular Spectroscopy Database (Germany)

c) Nuclear:

i) USA:

NUBASE2020 Evaluation of nuclear properties (IAEA, collaboration between Argonne National Laboratory and Institute for Modern Physics (China))

ENSDF *Some relevant evaluated nuclear structure data, most not directly applicable to astrophysics* (National Nuclear Data Center)

AME Atomic Mass Evaluation *evaluated atomic masses* Collaboration between Argonne National Laboratory and the Institute for Modern Physics (China)

STARLIB *Evaluated nuclear reaction rates for astrophysics with uncertainties*, University of North Carolina at Chapel Hill

JINA REACLIB *Evaluated nuclear reaction rates for astrophysics* Joint Institute for Nuclear Astrophysics JINA-CEE

Maxwellian averaged cross sections and astrophysical reaction rates, NNDC

Weak Rate Library Theoretical weak interaction data for astrophysics, JINA-CEE and NSCL, Michigan State University.

Nucastrodata.org Website for access to various nuclear astrophysics data resources *ii) Other Countries:*

BRUSLIB Broad range of theoretical and experimental data for astrophysics (Belgium)

KADONIS *Evaluated Maxwellian averaged neutron capture and proton capture reactions for astrophysics* (Germany)

Reference Database for Beta-Delayed Neutron Emission, IAEA (Austria)

Portal for nuclear processes, IAEA (Austria)

ASTRAL Astrophysical Rate and Raw Data Library (Germany)

d) Solids

i) USA:

The Optical Constants database (OCdb) provides refractive indices of ices, ice mixtures, and solid organic refractory materials produced in the laboratory from ice chemistry (ice tholins) and gas chemistry (gas tholins) from several laboratories. OCdb is currently funded by NASA PSD and APD.

NASA Goddard Cosmic Ice Laboratory provides infrared spectra and optical constants of ices and ice mixtures. Funded by NASA PSD.

RefractiveIndex.info is a compilation of data from publicly available sources such as scientific journal articles and material datasheets published by manufacturers

Interstellar Dust Analogs Spectral Database provides mid- and far infrared spectra of minerals thought to be part of the condensation sequence, or identified in meteorites, and various simple chemical compounds.

Material Property Database of Organic Liquids, Ices, and Hazes on Titan summarizes a range of material properties for possible simple and complex organics on Titan.

ii) Other countries:

Jena - StPetersburg - Database of Optical Constants (JPDOC) provides optical constants of amorphous and crystalline silicates, ices, oxides, sulfides, carbides, carbonaceous species from amorphous carbon to graphite and diamonds and some other materials of astrophysical and terrestrial atmosphere interests (Germany)

Heidelberg - Jena - St.Petersburg - Database of Optical Constants (HJPDOC) provides 1150 references to papers, books, dissertations where the refractive index, reflectance, transmittance, mass absorption coefficient, etc were derived (Germany)

Leiden Ice Database for Astrochemistry provides infrared spectra and optical constants of ices and ices mixtures produced at the Leiden Laboratory for Astrophysics (Netherlands)

Solid Spectroscopy Hosting Architecture of Databases and Expertise (SSHADE) provides spectroscopic data of ices, snow, molecular solids, minerals, rocks, organic solids, carbonaceous materials (France)

e) Software

i) Nuclear:

BRICK R-Matrix Nuclear Reaction Analysis Code

AZURE II R-Matrix Nuclear Reaction Analysis Code

CINA Computational Infrastructure for Nuclear Astrophysics

ii) Atomic

The R-matrix codes for photo- and electron–impact processes [UK APAP]

Los Alamos Distorted-Wave codes [Cowan, GIPPER, ….]

The Flexible Atomic Code (for atomic structure, EIE, EII, RR, DR)

AUTOSTRUCTURE (for atomic structure, EIE, DR, RR, PI, PE)

The General-purpose Relativistic Atomic Structure package: GRASP

Cowan's atomic structure package (for atomic structure, radiative rates, Auger rates, DR)

pyAtomDB (for collisional-radiative modeling of astrophysical spectra)

XSPEC is an X-Ray Spectral Fitting Package

iii) Molecular

Quantemol molecular R-matrix codes

UK Molecular R-matrix codes

XSTAR is a computer program for calculating the physical conditions and emission spectra of photoionized gases.

Sherpa is a modeling and fitting application for X-ray observations.

Cloudy is an *ab initio* spectral synthesis code designed to model a wide range of interstellar "clouds", from H II regions and planetary nebulae, to Active

Galactic Nuclei, and the hot intracluster medium that permeates galaxy clusters.

PyPAHdb is a Python package to fit and decompose isolated astronomical PAH emission spectra into contributing PAH subclasses, i.e., charge and size

The Planetary Intensity Code for Atmospheric Spectroscopy Observations (PICASO).

VIRGA: a cloud model for Exoplanets and Brown Dwarfs

PandExo: A Community Tool for Transiting Exoplanet Science with the JWST & HST

iv) Plasma kinetics of atomic species

NIST FLYCHK Collisional-Radiative Code

CRUMPET: Collisional-radiative UEDGE modeler

Yakora Collisional-radiative model for H, H_2, and He

v) Solids

NASA Goddard Cosmic Ice Laboratory software tools for optical constant determination, and interference fringes fitting

Appendix E
Report from the Interstellar Medium (ISM) sub-group

Edwin Bergin (University of Michigan), Jennifer Bergner (University of California, Berkeley) Paola Caselli (Max Planck Institute for Extraterrestrial Physics, Garching, Germany), Kyle Crabtree, (Chair, University of California, Davis), Brian J Drouin (Jet Propulsion Laboratory), Lise Dubernet (Observatoire de Paris, Paris, France) Michael McCarthy (Center for Astrophysics | Harvard & Smithsonian)

Overview

Astronomy is a remote-sensing science. Our ability to interpret astronomical observations is fundamentally linked to and driven by laboratory measurements, theoretical calculations, and models that are derived from the combination of the two. This situation is highly relevant for studies of the interstellar medium (ISM) — the space between stars — because the primary information collected from many ground-based facilities and space-based missions must be directly linked to atomic and molecular data. To derive the maximum scientific impact from current and new observatories a strong foundation based on high-quality laboratory astrophysics data is therefore essential.

Research relevant to the ISM is undertaken primarily at large government laboratories, most notably at JPL, NASA Ames, NASA Goddard, and at a number of Universities across the United States. Roughly 50% of university-based research takes place in Chemistry Departments, with the remaining 50% in Physics and/or Astronomy Departments (noting that some Universities do not have separate Departments). Support for ISM-related research at universities is provided in the form of faculty hires who are normally provided one-time start-up funds that can vary by an order of magnitude. At government laboratories, dedicated funding equivalent to faculty start-up packages is far less common; new workforce capabilities are instead developed primarily by attrition when existing researchers move on to mission/institutional work and/or retirement.

Programmatic support for laboratory astrophysics research pertinent to the ISM is primarily from NSF AAG (Astronomy and Astrophysics Grants) and the NASA APRA (Astrophysics Research and Analysis). Funding from DOE, DOC (NIST), other programs within NSF and NASA, and private foundations may contribute incidentally when specific projects are aligned with these initiatives or priorities. Generally, no program supports ISM research as a primary objective, nor is there a requirement to provide significant or regular funding for ISM-specific efforts.

Based on a review of publicly-available data from NSF and NASA, it is estimated that the NSF AAG program invested approximately $12 M into ISM-relevant laboratory astrophysics research over the 2014-2023 time period, (9 years) and NASA APRA invested $12 M over 2016-2021 (5 years). These awards are primarily single-investigator grants for 3-4 years with a total value of $450-500k (or about $150k/year). On average, approximately $4 M per year has been directed to ISM-related research across the US through competitive grant programs.
The remainder of this document is divided into three sections: (i) State of the Field, (ii) Databases, and (iii) Financial, Infrastructure, and Workforce Development. Specific findings and recommendations relevant to these topics are provided in each section.

State of the Field - Science Frontiers and Data Needs

The 2020 Decadal Survey identified three Science Questions and Discovery Areas relevant to the Interstellar Medium for which laboratory studies pertinent to atomic and molecular astrophysics need to be supported to exploit and interpret astronomical data from existing or new facilities. Current large facilities include ALMA and JWST, while next-generation facilities include the Extremely Large Telescopes (ELTs), the Habitable World Observatory, and the ngVLA, all of which will provide greatly improved observational capabilities and in turn will require further advances in laboratory, theory, and modeling, particularly since each will possess at least modest resolution spectroscopic capabilities.

Table 1: Science questions identified in 2020 Decadal Survey and associated laboratory astrophysics data needs.

Regime	Science Questions	Laboratory Astrophysics Needs
Diffuse ISM	a) What sets the density, temperature, and magnetic structure of the diffuse ISM, enabling the formation of molecular clouds? b) How do molecular clouds form from, and interact with, their environment?	- Optical properties of dust from x-ray to mm wavelengths - Rate coefficients and branching ratios for gas-phase and heterogeneous reactions relevant to dust formation and growth - Photoabsorption and photoionization cross sections and branching ratios for

	c) How does injection of energy, momentum, and metals from stars ("stellar feedback") drive the circulation of matter between phases of the ISM and CGM?	small molecules - Electronic/vibronic transition frequencies of cations and refractory large molecules - Vibrational spectroscopy of PAHs, PAH cations, fullerenes, and related species - Rotational spectroscopy of small cations and radicals
Molecular Clouds	a) What processes are responsible for the observed velocity fields in molecular clouds? b) What is the origin and prevalence of high-density structures in molecular clouds, and what role do they play in star formation? c) What generates the observed chemical complexity of molecular gas?	- Optical properties of dust at mm wavelengths - Rate coefficients and branching ratios for low-temperature gas phase reactions involving radicals and ions - Optical properties and morphologies of astrophysical ices - Chemical reaction rates, energetics, and nonthermal desorption processes in astrophysical ices - Rotational spectroscopy of isotopologues and vibrationally excited states of stable complex organic molecules and exotic isomers - Rotational spectroscopy of complex organic radicals and cations
Protostars/Disks	a) How do dense molecular cloud cores collapse to form protostars and their disks? b) How do protostars accrete from envelopes and disks, and what does this imply for protoplanetary disk transport and structure? c) Is the stellar mass function universal?	- Optical properties of dust at mm wavelengths - Rate coefficients and branching ratios for low-temperature gas phase reactions involving radicals and ions - Optical properties and morphologies of astrophysical ices - Chemical reaction rates, energetics, and nonthermal desorption processes in astrophysical ices - Rotational spectroscopy of isotopologues and vibrationally excited states of stable complex organic molecules and exotic isomers - Inelastic scattering/energy transfer cross sections for gas-phase molecules

The scientific method generally used in astrophysics is cyclical (Figure 1). Laboratory astrophysics research can be motivated by interpreting data from existing/planned missions; however, to view laboratory astrophysics research as an effort that exists only to serve the needs of missions understates its importance and intellectual breadth. This field also serves to develop and test the core astrophysical hypotheses at the center of the field and to define the measurement requirements for next-generation observatories. Thus, in addition to efforts responsive to the needs of current/upcoming missions, a significant portion of laboratory astrophysics research efforts needs to be more fundamental and broader in focus, helping to define what astronomical questions are asked in the first place.

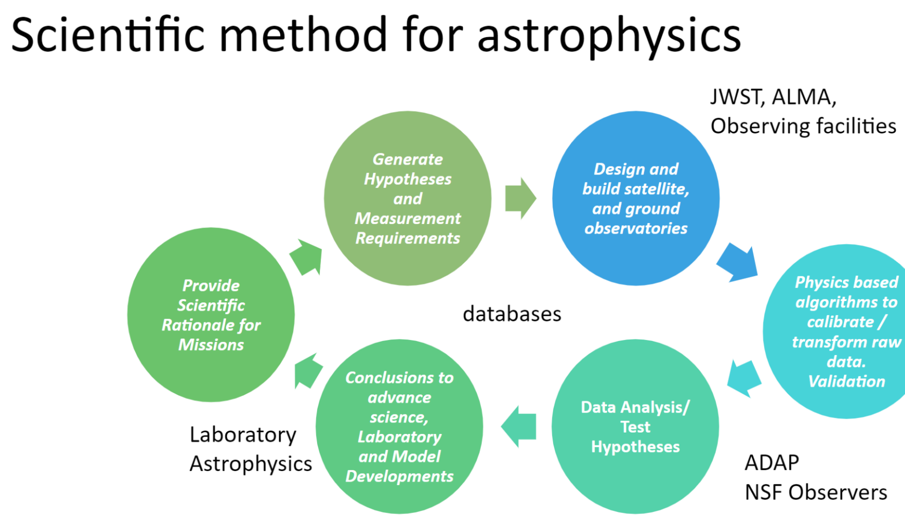

Figure 1: The integral role that laboratory astrophysics plays in both interpreting data from missions and guiding future directions in astrophysics.

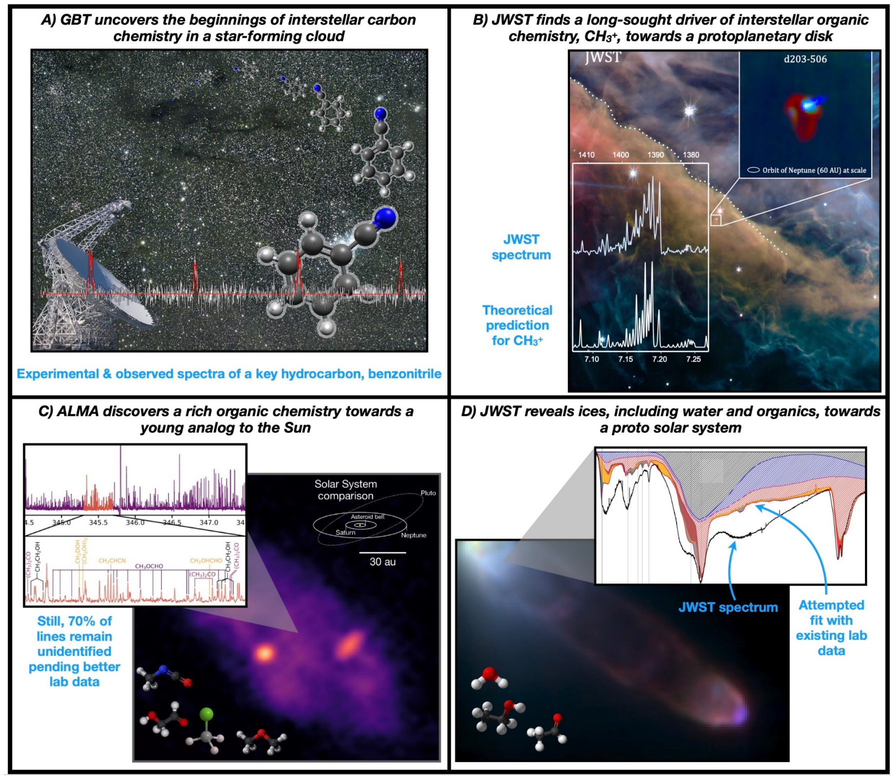

Figure 2: Recent ISM discoveries enabled by laboratory astrophysics data. *Image credits: McGuire+2018 Science, Berne+2023 Nature, Jorgensen+2016 Astronomy & Astrophysics, Maureira+2020 The Astrophysical Journal, Yang+2023 The Astrophysical Journal Letters, B. McGuire, MPE, Y. Yang*

Figure 2 showcases a sample of the complex landscape where laboratory astrophysics has defining roles to play within astrophysical frontiers. Panel (a) shows the detections of polycyclic aromatic hydrocarbons in the dense cold interstellar medium by McGuire and co-workers (add refs; see also Cernicharo). For decades infrared spectroscopy of astronomical objects detected broad emission features labeled as the unidentified interstellar bands. These were believed to be associated with polycyclic aromatic hydrocarbons (PAHs). However, despite dedicated laboratory/theoretical efforts, there was no assignment to an individual species. Concurrently, Jones (Faraday discussion) highlighted a key problem with grain formation models. Carbonaceous solids, such as PAHs, are believed to form in the envelopes of asymptotic giant branch stars with elevated C/O ratios. However, the destruction processes in the interstellar medium are too efficient - thus requiring another production mechanism. McGuire and co-workers, through a dedicated program that linked Green Bank Telescope (GBT; NSF-funded) observations to laboratory spectroscopy, detected and identified benzontirile and an emerging host of other PAH molecules, forming in the cold dense interstellar medium. This not only provided the first true spectral identification of a PAH but also, potentially, solved a galactic dust conundrum. This work is just beginning to probe the extent of chemical complexity associated with star-forming regions and offers an exciting astrobiological future.

Panel (b) highlights one of the spectroscopic results from the first year of operations of NASA's James Webb Space Telescope (JWST): the detection of the CH_3^+ cation. In the early 1970's and into the 1980's the detection of molecules in the dense interstellar medium created the field of astrochemistry. This progress directly linked astronomy with chemical laboratory efforts in the fields of spectroscopy, gas-phase chemical kinetics, molecular photoprocesses, solid-state physics, and catalytic chemistry. A key facet of today's chemical networks is that the gas phase chemistry is dominated by carbon with the CH_3^+ cation driving the overall chemistry of gaseous organics. For decades astronomers had searched for this molecule to no avail. In 2023 an international team of researchers detected a series of vibration/rotation lines near 7 microns within a young protoplanetary disk embedded within the Orion Nebula (Berne et al. 2023, Nature). Earlier laboratory work (Schlemmer) showed striking correspondence with CH_3^+ which was confirmed via detailed theoretical and (subsequent) laboratory work, leading to the exciting interdisciplinary (astronomy, physics, chemistry) discovery of the molecule that lies at the heart of molecular chemistry associated with star and planetary birth.

Panel (c) shows the tremendous progress made by the Atacama Large Millimeter/submillimeter Array (ALMA) in uncovering the rich inventory of organic molecules present in young star-forming systems (Jorgensen+2016). The identification of dozens of different organics is of great importance to astrobiology, since this chemically complex material could seed new planets with the building blocks for prebiotic chemistry. While it has been known for several decades that organics can form in space, only with the exquisite sensitivity and spatial resolution of ALMA have astronomers been able to provide detailed assessments of what molecules are present, how abundant they are, and where they are located within these solar system progenitors. In tandem with the observations, these advances are possible thanks to spectroscopic databases that rely on both experimental and computational inputs. While much progress has been made in interpreting these spectra, a recent estimate suggests that a staggering 70% of detected lines have not yet been assigned to any molecular carrier (Taquet+2018). Moreover, there is still significant debate about how these organics form, necessitating further experimental and theoretical investigations of gas-phase and solid-state reaction pathways (e.g. Lopez-Sepulcre+2019). Fully interpreting these fantastic data sets from the NSF-funded ALMA facility requires dedicated experimental efforts in spectroscopy, reaction mechanisms, and chemical kinetics.

Panel (d) illustrates another highly consequential early result from JWST: spectra revealing the presence of icy and refractory materials in young proto-solar analogs. Ices represent the main reservoir of volatiles in star- and planet-forming regions, and therefore have broad-ranging importance to interstellar chemistry and the formation of habitable planets. With higher sensitivity and spectral resolution compared to previous IR telescopes, it was anticipated that JWST would provide a more detailed picture of interstellar ices than ever before– and indeed, early results show hints of trace organics that have never been detected in the ice phase (Yang+2023, Rocha+2023). IR absorption spectra are, however, quite difficult to interpret and require comprehensive libraries of spectral templates measured in the laboratory. It is clear from initial attempts to fit the observed spectra that existing laboratory data is insufficient, and additional solid-state spectroscopic measurements are urgently needed. New mechanistic studies of ice-phase reaction pathways will also be required to contextualize how ice-phase organics are formed. Only with supporting laboratory efforts can we fully unpack the rich information encoded in the JWST spectra.

In summary, these four panels illustrate a few exciting frontiers in the study of the interstellar medium and the emergence of habitable planetary systems. The exquisite data sets from recent NSF and NASA-funded facilities simply cannot be explored to their full extent without a dedicated link to interdisciplinary science and laboratory work.

Findings/Comments/Recommendations: ISM Science Frontiers and Data Needs

Finding: Although laboratory astrophysics is essential in maximizing the scientific potential and impact of new astronomical missions and observatories, funding to support these efforts is not a formal part of mission planning. This lack of coordination may limit the impact of next-generation facilities. With a modest investment into laboratory astrophysics, likely at the level of a percent or two relative to the mission cost, this concern can be greatly mitigated. Given that multi-billion-dollar class missions are increasingly routine, this would appear to be a wise investment.

Finding: The needs of the astrophysics community increasingly require the involvement of multiple stakeholders to properly interpret data; these problems are best addressed by the involvement and coordination of multiple subject matter experts. The single PI model is valuable, but a more coordinated effort can help minimize pitfalls and gaps.

Recommendation: NSF and NASA should explore the feasibility of implementing a laboratory astrophysics for mission planning (LAMP) concept to enable the astronomical community to evaluate the science of a proposed mission/facility in the context of its laboratory astrophysics requirements. By integrating such requirements in the planning and maturation of new missions and facilities it should be possible to retire risk and maximize the scientific potential of next-generation facilities.

Recommendation: Laboratory astrophysics needs its own funding line to ensure modest and stable investment to support the needs of the larger astrophysics community; it cannot be an afterthought, Agencies should provide increased funding opportunities for both single PIs programs and larger collaborative teams.

Recommendation: NSF and NASA should explore the possibility of joint or collaborative programs to meet common needs.

Databases

The observing community makes discoveries through the interpretation of astrometric data in reference to verified laboratory measurements. Reference data must be codified into standard formats and provided publicly to all potential observers, ideally within a rigorous review process. Support of databases from laboratory astrophysics programs has been realized through the paradigm to “advance crucial laboratory measurements [DS2020]”. In this paradigm, specific large projects with set requirements enable focused results within the predefined program objectives. These efforts remain “..woefully incomplete, and there is a small number of active laboratories that contribute to them.” [DS2020]

In the present arena of ‘open science’, astrophysicists are poised to gain access to laboratory astrophysical data at all levels of maturity (Table 2, table columns 1-4), except perhaps the most valuable type of data: critically reviewed multi-sourced data compilations (Table 2, column 5). For infrared/vibrational spectra, HITRAN has taken on this role but overlap for ISM is minimal, for rotational spectra, JPL and Cologne have roles typically directly connected to ISM support, for atomic data, NIST maintains a role through DOC (Department of Commerce) that is typically not supported by NSF/NASA astrophysics, for kinetic and photochemical data, some coverage for ISM needs appears in JPL (Earth and Planetary) and Sandia (combustion) efforts. The expansion of HITRAN into planetary/exoplanetary-relevant data has opened the question of why the primary funding is Earth Science based (true also for JPL) and how any comprehensive effort might be sustained in competition within scientific research programs. For laboratory astrophysics, observational programs, such as those associated with the Herschel project, directly funded laboratories to measure, catalog and publish spectra, but this mechanism waned quickly after the mission ended, resulting in a present lack of responsiveness to community efforts and needs. Attempts at NSF/NASA partnership to connect JPL database curation to ALMA needs failed.

Table 2: Categories of data and metadata necessary for critical evaluation and compilation of databases. Open science data (left four columns) and expert data compilation (right column). Open science data will become available through the traditional paradigm to "advance crucial laboratory measurements [DS2020]"; no astrophysics specific support exists for expert data compilation.

Raw data	Calibrated Data	Analyzed Data	Published Data	Data Compilation	
Spectra, absorption profiles	Corrected spectra, concentration profiles	Quantum assignments, line-by-line parameters, reaction rates, photochemical rates	Analyzed data + extrapolative predictions with uncertainties	Sum of literature-wide analyzed data and standardized gap filling/extrapolation	Data
Gas/material info, spectral range, pathlength, time ranges	Calibration factors, unit equivalences, identified impurities	Mathematical basis, rate equations, limiting factors, assumptions	Comparisons to literature, peer-reviewed	Subject matter expert commentary, source materials, recalibrations, additional literature comparisons	Meta-data

Findings/Comments/Recommendations: ISM Databases

Finding: Atomic and molecular data are produced regularly, albeit not typically tailored for astrophysical use. Standardization, regularization, and accessibility are paramount. Observing communities utilize databases through tailored algorithmic interfaces.

Finding: Support mechanisms for database construction and curation include research programs and large observing projects.

Finding: Atomic and molecular databases serve multiple communities in an interdisciplinary environment not encapsulated in the otherwise also interdisciplinary field of laboratory astrophysics

Recommendation: Expand support mechanisms to enable long-term database maintenance and curation, providing means to deal with IT evolution, physical server space, and equipment. Share this burden with other disciplines that benefit from the databases.

Finding: Kinetics and photochemistry databases for ISM do not exist at an adequate level. Active efforts to critically evaluate reaction rates exist only for Earth Science purposes.

Financial Support, Workforce Development, and Infrastructure

The ISM consists of a diverse array of extreme, heterogeneous, nonequilibrium environments that differ widely from terrestrial conditions. To measure relevant physical properties under such exotic conditions requires custom instrumentation that often requires years of development and specialized training. For ISM-relevant experimental laboratory astrophysics work, these instruments often consist of vacuum pumps/chambers, cryogenic equipment, molecular beams, lasers, spectrometers, optics, and sensitive electronics. Instruments as a whole consist of many small/mid-scale pieces of equipment (of order $10,000-$500,000). At national laboratories, instruments are developed and maintained through regular institutional equipment budgets. In academic institutions, where most of the student training occurs, equipment primarily comes from start-up funds from Chemistry and Physics departments.

Based on community feedback, academic researchers struggle to acquire funding to maintain existing equipment and to develop new instrumentation. This challenge arises from a confluence of factors. Universities do not typically provide funding for new equipment after the initial startup investment; PIs support their research programs through external grants. While both NSF AAG and NASA APRA in principle allow for equipment purchases, the reality of rising personnel costs and core inflation coupled with the relatively flat award sizes from grant programs leaves little room for equipment. The cost of developing a new instrument is too high to be supported through the astrophysics grant programs, but often too low and too specialized to be supported through other funding mechanisms for major and/or shared instrumentation. A single MRI award has been made for laboratory astrophysics by NSF AST in the past 10 years ($800k, a shared merged-beam endstation to be coupled with synchrotron facilities).

As evidenced by the large fraction of ISM-relevant work being carried out in academic chemistry and physics departments, laboratory astrophysics requires expertise from chemists and physicists. The requisite measurements and calculations are expensive and challenging, but they do not always directly address questions at the forefront of the fields of chemistry or physics as was often the case in prior decades. The limited available funding for laboratory astrophysics necessitates that researchers based in these departments look to other disciplinary funding programs which generally will not support a project whose primary objective is motivated by astronomical needs. Instead, researchers must shift their scientific focus toward other fundamental chemistry and/or physics questions that may be of limited astronomical relevance. These other commitments, coupled with the challenges of developing new capabilities, limits academic efforts to respond to emerging data needs from missions. In the longer term, chemistry and physics departments may not continue to invest startup funding and salary lines in laboratory astrophysics groups if they do not envision sufficient extramural funding to be available in those areas, creating a threat to the US laboratory astrophysics workforce.

Laboratory astrophysics provides an excellent environment for training highly skilled scientists whose contributions to the national scientific workforce extend well beyond space science. Trainees are prepared for a variety of careers that require critical thinking, solving complex problems, analyzing large quantities of data, and developing/maintaining complex technical equipment. They then move on to positions in areas of high national priority, including semiconductors, national defense, artificial intelligence/machine learning, and energy.

It is difficult to estimate the number of research groups actively engaged in ISM-relevant laboratory astrophysics in the US. A review of NSF and NASA funding awards shows that approximately 25 unique PIs have received funding in academic institutions as well as an additional 5-7 PIs at government institutions over a period of 10 years for NSF and 5 years from NASA. Assuming these represent roughly half of the active groups working on ISM laboratory astrophysics, the total number is likely near 50+/-10 groups in universities and 12+/-3 in national laboratories. The funded universities were almost exclusively R1 institutions, and the government labs were located at NASA Goddard, NASA Ames, SETI, and the Harvard-Smithsonian Center for Astrophysics. It is important to note that boundaries among ISM, planetary, and stellar/nuclear research are not always clear, and overlap may exist between groups identified here and those discussed in the other subreports.

A representative (though not necessarily average) ISM research group at a university involves the participation of approximately 3 graduate students, 5 undergraduate students, and 1 postdoctoral scholar over a 5 year period. Given the average duration of appointments, this equates roughly to 2-3 undergraduate students and 3 graduate students at any given time, occasionally joined by a postdoctoral scholar. Government laboratories over a 5 year period involve 2.5 undergraduate students[2], 2 graduate students, 4.5 postdoctoral scholars, and 5 staff scientists. These numbers are based on a community survey that received 21 responses from groups who self-identified as working in the area of ISM research at academic institutions and 14 responses from government laboratories. As above, considerable overlap exists; of these 35 responses, 24 identified at least one of the other two areas in addition to ISM as a significant area of research focus.

Supporting this workforce has become increasingly difficult, as the average award size (150-175k/year) from the research grants programs has remained approximately constant, even as core inflation has increased by 30% over the last 10 years. Barring an increase in award size, PIs will increasingly have to operate with smaller teams and restrict the scope of projects. In addition, the short timeframe (3 years) of a research grant and the low funding rate (<20%) present major challenges in maintaining continuity, which is critical in laboratory experimental efforts.

Fieldwork facilities (e.g. NASA CSBF and AFRC) are subsidized at the top level and proposals using those facilities are prioritized, this is done to maintain capability.

[2] Undergraduate and graduate student involvement in national laboratories takes place primarily in the form of summer internships, as the national laboratories do not grant degrees.

Laboratories are not similarly subsidized/supported at the programmatic level, local institutions are expected to maintain capability. In lieu of institutional support, laboratory PIs allocate fewer resources to personnel development. This results in fewer PhDs per dollar invested.

Findings/Comments/Recommendations: ISM Facilities, Infrastructure, and Workforce Development

Finding: Funding increases for laboratory astrophysics grant programs recommended by the past three decadal surveys have still not materialized for ISM-relevant research. Average award sizes and the number of awards have generally remained flat over the time period reviewed.

Finding: Even a short-term disruption in funding can have an outsized impact on the viability of laboratory astrophysics efforts since most groups are not well-funded. Funding disruptions lead to a lack of continuity in personnel, limiting knowledge transfer as senior laboratory personnel depart and increasing the risk of equipment failure due to the loss of institutional knowledge.

Recommendation: Agencies should consider NIH MIRA-style awards. A MIRA has a 5-year term with a fixed annual budget (250k or 300k/year), and the goal is to have a high renewal rate. A MIRA serves as a solid reliable base level of funding that also provides flexibility to PIs in allocating resources between personnel, supplies, travel, and equipment as the needs of a project change. However, without an increase in program budgets, implementation of such a system will decrease funding rates to an even more unacceptable level.

Finding: Of the NASA/NSF awards through the APRA and AAG programs, approximately 2/3rds of the awards made to academic institutions went to PIs based in either a Chemistry department or a Physics department that is not joint with astronomy.

Finding: ISM-related laboratory astrophysics research based in chemistry and physics departments plays a major role in workforce development for astrophysics. In addition, the technical training provided by laboratory astrophysics translates well to broader areas of the STEM workforce.

Finding: A significant fraction of laboratory astrophysics is performed by groups who have no formal training in astronomy or astrophysics. The astrophysics community must "pay its own way"; they cannot expect others to produce data that is useful to the field without dedicated and stable investment. This situation will only get more acute in a prolonged and highly constrained budget environment.

Finding: A mismatch exists between the availability of specialized laboratory astrophysics research equipment, which is often most readily available at government research facilities, and student trainees who are based at academic institutions. PIs at academic institutions have limited access to funding mechanisms for developing and upgrading mid-scale equipment, and government laboratories lack access to student trainees because the limiting existing mechanisms for funding student participation through collaborations with academic institutions do not adequately meet the needs of both parties.

Recommendation: Agencies should provide funding opportunities for personnel affiliated with national laboratories working on database development and/or laboratory astrophysics efforts to train undergraduate students through internship programs. Current mechanisms provide funding for students, but not staff time. This investment will benefit the academic sector by equipping incoming graduate students with domain-specific knowledge and experience from the beginning of their careers.

Appendix F

Report from the Planetary and Exoplanetary (PlEx) sub-group

Gerardo Dominguez (California State University, San Marcos), Iouli Gordon (Chair, Center for Astrophysics | Harvard & Smithsonian), Sarah Horst (John Hopkins University), Nikole Lewis (Cornell University), Ella Sciamma-O'Brien (NASA Ames Research Center)

A forefront science theme identified in the ASTRO2020 decadal report was "Worlds and Suns in Context" with a priority area of "Pathways to Habitable Worlds". This science theme focuses on "The quest to understand the interconnected systems of stars and the worlds orbiting them, from the nascent disks of dust and gas from which they form, through the formation and evolution of the vast array of extrasolar planetary systems so wildly different than the one in which Earth resides". The ASTRO2020 panel on Exoplanets, Astrobiology, and the Solar System highlights that the priority area of "Pathways to Habitable Worlds" would benefit significantly from collaboration across disciplinary boundaries (e.g. exoplanets, solar systems, earth science, biology, and chemistry), and ongoing support for enabling observations, theory and laboratory work. Here (see Table 1), we identify and discuss some of the core questions and priority areas identified by the ASTRO2020 decadal that will require laboratory work to address. We note that the topical area of planetary and exoplanetary science in the context of laboratory astrophysics is somewhat complicated by divisional divides at NSF and NASA (e.g. the Astrophysics and Planetary Science Divisions at NASA). Here, we focus on the scope specific to the ASTRO2020 report and the charge of the AAAC Laboratory Astrophysics Taskforce but note that cross-divisional efforts will be crucial to meet the laboratory work needs of planetary and exoplanetary.

Figure 1 shows how the best-case scenario works for identifying molecules in the atmosphere of exoplanets or modeling their photochemistry and climate. The ab initio calculations typically provide completeness of the line lists, including at higher temperatures where experiments and their interpretations are challenging. The experiments, however, provide more accurate parameters, especially for well-isolated lines. Therefore, the best-case scenario is to use ab initio data to assign experiments, and then the latter can be used to refine the ab initio models. In the end, the best line list is obtained through the combination of theoretical and empirical data. The broadening parameters are then typically measured and extrapolated using semi-empirical methods. There are efforts to calculate the broadening parameters with ab initio methods, but at the moment, these calculations are computationally expensive. The resultant line lists are validated and deposited to spectroscopic databases in well-defined format, and parameterizations. The planetary scientists then calculate opacities, which are later fed into the radiative transfer models that are used to interpret spectra from telescopes. Unfortunately, recent exoplanetary observations have shown unidentified features, therefore highlighting that the observation preceded relevant laboratory work.

Table 1: Summary of Science Needs, as stated in ASTRO2020 Decadal and Corresponding Laboratory Experimental Data Needs

2020 Decadal	Science Needs	Laboratory Astrophysics Needs
Exoplanetary Atmospheres Missions/facilities that target exoplanet atmospheres/surfaces: HST, JWST, Ariel, Pandora, US ELTs, NOIRLabs telescopes, HWO	What are exoplanetary atmospheres, clouds, and haze particles (that can settle to the surface) composed of? What are the atmospheric circulation and radiative properties that regulate exoplanetary atmospheres and their climate? Photochemistry in different layers of the atmosphere. Interaction with radiation from the parent star	Chemical Reaction Rates of gases at non-terrestrial conditions Energies, Oscillator Strengths, Collisional parameters for calculating opacities of gases at a variety of thermodynamic conditions (including high temperatures), Collision Induced Absorption (CIA) of temporary collisional pairs Haze and Cloud Formation Surface/Atmosphere Interactions Optical Emission and Scattering

Habitability Missions/facilities that target habitability: JWST, HWO, LUVIOR	How do habitable environments arise and evolve within the context of their planetary systems? How can signs of habitable life be identified and interpreted in the context of their planetary environments? False positives for potential biosignature gases.	Theoretical and Experimental Line lists for biosignature molecules and interfering species at near-terrestrial temperatures Oscillator Strengths Optical Emission and Scattering Haze and Cloud Formation Theoretical calculations of planetary atmosphere chemistry and evolution will be needed to interpret biosignature gases detected in exoplanet spectra
Exoplanet interiors	How do bulk planetary properties and formation and thermal histories affect planetary interior and magnetic fields? How does a planet's interior structure and composition connect to its surface and atmosphere?	Geophysics and Geochemistry Mineral Physics High-pressure experiments

Protoplanetary Disks and **Planet Formation** Missions/facilities that target planet-forming regions: ALMA, JWST, NOIRLabs Telescopes, HWO	What is the composition of protoplanetary disks? How are volatiles distributed during and after planet formation?	Characterization of volatiles and organics: ● Theoretical and Experimental Line lists ● Millimeter wave spectroscopy and Far IR spectroscopy (low T) of gases and dust analogs ● Optical constants of protoplanetary disk dust analogs in the FIR and submm for interpretation of ALMA and future observatory data ● Reaction rates for relevant gases, ices, and solids ● Surface chemistry, grain/ice interactions Fluid dynamics?
Solar System object (for comparative analysis and precursor science)	How do planetary atmospheres evolve? Atmospheric dynamics to understand atmospheric evolution Atmospheric chemistry (Earth, Venus, Titan, Pluto, Jupiter, Saturn, for comparative analysis)	Theoretical calculations General Circulation Models (GCM) to interpret observations of Venus, Mars, Earth, Titan and better model exoplanets Lab experiments (gas phase and solid phase) under “planetary conditions”

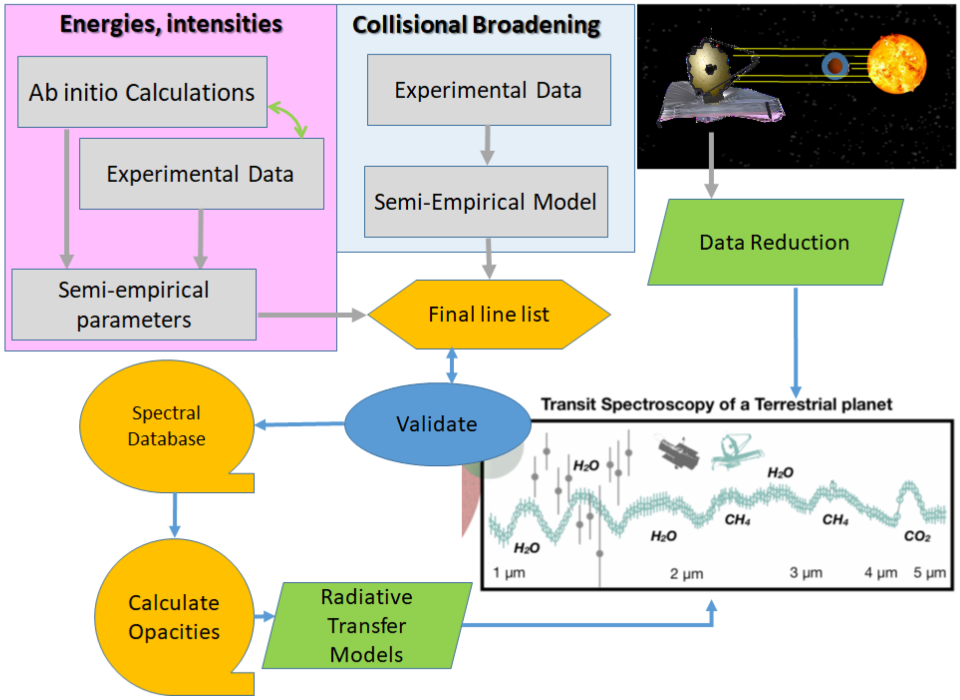

Figure 1. *The pathway from calculations and laboratory spectra to identifying molecular features in the spectra of exoplanets.*

With these identified laboratory astrophysics needs (many of which are reflected in the Fortney et al. [1] white paper) in mind, in the following sections, we assess the current status of relevant laboratory/database efforts, the current and future needs in planetary and exoplanetary laboratory astrophysics, national resources that could be leveraged to meet those needs, and new approaches to consider to support planetary and exoplanetary laboratory work better.

1. (Exo)planetary-Relevant Experimental, Theoretical, and Database Resources

1.1. Experimental facilities

Various experimental setups have been developed in the last 4 decades to simulate the chemistry in (exo)planetary atmospheres using different energy sources (plasma, UV irradiation, proton irradiation…), different temperatures (from 100 K to 1500 K), and different gas mixtures to simulate different environments.

For gas phase characterization, the main diagnostic is high-resolution spectroscopy in the UV-IR to characterize the spectral signatures of molecules in different thermodynamic (P, T) conditions for direct comparison to observations or to use in models. Fourier transform spectrometers and different laser techniques are the most common tools. The majority of existing laboratories can obtain spectra only at room temperature. Obtaining spectroscopy at other conditions, particularly at very low to very high pressures and temperatures, requires specialized instrumentation and facilities that are not readily available in most labs, although notable exceptions exist. Some specialized labs may have such capabilities that theorists and/or experimentalists may not be aware of. These experiments allow for building semi-empirical line lists suitable for interpretation and modeling spectra of exoplanets. Some experimental setups also use mass spectrometry diagnostics to investigate chemical pathways in exoplanet-relevant gas mixtures.

In the solid phase, haze/cloud particle analogs produced in the laboratory can be characterized with many different techniques: mass spectrometry, UV-FIR spectroscopy, scanning electron microscopy, x-ray photoelectron spectroscopy, x-ray absorption near-edge structure spectroscopy, atomic force microscopy, surface energy measurements, as well as vapor pressure measurements of various relevant ices and solids. Producing and characterizing solids require specialized experimental facilities that are not traditionally found in astronomy departments (but may be found in atmospheric chemistry laboratories).
The solid phase measurements needed to support astronomical observations include:
- Optical constants of atmospheric ice, aerosol, and surface analogs from 5K-300K
- Laboratory simulations of planetary surface chemistry (ice, grains)
- Laboratory degradation studies of biotic biomarkers and abiotic organic compounds

1.2. Theory/Models

Theoretical simulations of (exo)planetary atmospheres (gas and haze/cloud particles) include:

- Quantum chemical calculations of rovibrational line lists for characterizing exoplanet atmospheres and spectroscopic constants for molecular species
- Calculating atomic and molecular opacities for exoplanet atmospheres using line lists for various compositions
- Quantum chemical calculations of IR spectral properties of aerosol and cloud particle analogs
- Advanced theoretical simulation of the scattering and absorption properties of porous, heterogeneous aggregates

- Modeling exoplanet atmospheres: A thorough summary of 50 modeling codes has been carried out [2]. Most commonly-used US-developed codes include PandExo (community tool for transiting exoplanet science with the JWST & HST), PICASO (Planetary Intensity Code for Atmospheric Scattering Observations), Virga (cloud model for exoplanets and brown dwarfs), Planetary Spectrum Generator (PSG, radiative transfer and observational simulator).
- Global Circulation Models (Exoplanet, Mars, Venus, Giant planets, etc.),

Theoretical simulations of (exo)planetary surface (composition and processing) and interior include:

- Quantum chemistry calculations (rate constants, branching ratios, etc) and molecular dynamics simulations to explore formation and destruction pathways of complex organic molecules and ices.
- Theoretical calculations to simulate magma-atmosphere interfaces and interiors in exoplanets

1.3. Databases

A comprehensive list of the Databases relevant to exoplanetary research is provided in Appendix D. While there are many databases that exist, they face the following issues:

- Users of databases benefit from well-developed formats and formalisms of the databases. Curation of the data takes a burden away from users to navigate diverse information They also appreciate user support from the database providers on how to obtain and use the data. It is important to enable user interaction with the database provider to identify and address data and software needs. For instance, managers of the HITRAN database get about three questions per day (there are over 30,000 users).
- Once a database exists, it needs continuing support for maintenance and further development of database content, accompanying software tools, user support, and documentation. Curation of the databases is also very important, and the survey of users has clearly indicated this. One aspect of curation encompasses checks that the data are in consistent units, formats, and formalisms. Some of the other validation efforts include checking if the parameters are within their physical boundaries and if all the selection rules are satisfied. Databases ensure the legacy value of Laboratory Astrophysics data and, therefore, require long-

term support. At the moment, none of the databases outside of national labs have guaranteed support. With that, databases require dedicated infrastructure and expertise in the underlying science, including quantum mechanics but also servers, data science practices, website development, etc.

- A need for a publicly accessible “Database of Databases” and “Database of Facilities” has been identified in the surveys.

2. Summary of Findings and Recommendations

2.1. Existing resources

Finding #1: *A number of experimental facilities conducting exoplanet-relevant research exist throughout the National Laboratories, NASA centers, and, to a lesser extent, Universities. Few theoretical groups carry out calculations for exoplanet research. With that, even for studies of the Solar System planets, there is still a lack of laboratory data, while the incredible chemical and thermodynamic diversity of the exoplanetary atmospheres calls for substantially more data. As an example, in the search for life, including that in anoxic atmospheres, over 15 thousand molecules have been identified as potential biomarkers [3], but only about 50 of them have reliable line lists, and low-resolution cross-sections exist only for about 500 molecules.*

Finding #2: *Standardized and curated databases play a crucial role in planetary and exoplanetary research. There is a need to salvage existing databases, expand their scope, and ensure their accessibility.*

Recommendation #1: The creation of a “Database of Databases” and a “Database of Facilities” would bring awareness to what is available and enable collaborations.

2.2. (Exo)planetary Laboratory Workforce and Funding Opportunities

There is a lack of demographic data indicating how the laboratory astrophysics workforce has evolved over the years, however, surveys and panel discussions indicate a sense within the community that the workforce is aging and that current PIs and university departments do not have the resources required to prevent the workforce from dwindling further by training and retaining the next generation. A substantial fraction of laboratory astrophysics funding and research are present at NASA centers, and that is a common destination for a larger fraction of mid-career researchers remaining in the field. However, these laboratories do not have easy access to training opportunities for undergraduate and graduate students.

Finding #3: *There is a need for funding mechanisms for*

1) attracting and supporting the training of the new generation for laboratory astrophysics study (support lab exchange, dedicated PhD and postdoc opportunities), and

2) retaining the workforce by creating long-term job opportunities (hiring in lab astro at universities, national labs, and NASA centers)

Finding #4: *Although there is a clear need for laboratory data to support the exoplanet research and there is a very substantial public interest, the available funding avenues are very limited. Traditional NASA programs that support Laboratory Astrophysics, including Astrophysics Research and Analysis (APRA) and Astrophysics Data Analysis Program (ADAP), do not accept proposals aiming to support exoplanetary research. The only program that accepts such proposals is the Exoplanetary Research Program (XRP), which is very broad in its scope, and funds only 1-2 proposals a year to support relevant laboratory studies. The situation at NSF is even more dire, and only a handful of proposals were funded in the last decade. Planetary-relevant studies (with the potential to leverage exoplanets) can be funded through other very competitive NASA programs that support research of the Solar System planets, including Planetary Data Archiving and Restoration Tools (PDART) and Solar System Works (SSW). These programs, however, also provide only limited support for laboratory research needed by exoplanetary science.*

Finding #5: *Laboratories engaged in laboratory astrophysics research are often housed in departments (e.g., astronomy departments) that have smaller start-ups and laboratory funding mechanisms than other university departments where laboratories are housed (e.g., chemistry). Additionally, once start-up is spent, it is challenging for PIs to purchase new equipment except through extremely competitive federal funding programs (e.g., NSF MRI).*

Recommendation #2: In order to increase coordination, it may be helpful if NASA and NSF adopted funding models that support the acquisition and staffing of instrumentation that serves the needs or gaps that are common to both planetary and exoplanetary communities and that simultaneously provides opportunities for the broader community to acquire data at these facilities. NSF's National Facilities and NASA's Planetary Science Enabling Facilities (PSEF) have mechanisms for offering PI-run instrumentation to the broader community and may serve as a model or catalyst to encourage additional leveraging of expensive laboratory instrumentation to serve both the planetary and exoplanetary communities while reducing redundancy. A benefit of shared facilities is that they can provide training opportunities for graduate students, postdoctoral scholars, and (perhaps) even more experienced researchers looking to learn a new analytical skill or method. The NSF-UCLA Secondary Ion Mass Spectrometry (SIMS) (https://uclasims.epss.ucla.edu/) facility is an efficient and inclusive model that can be adapted. The facility has traditionally offered summer workshops that train graduate students and postdocs the opportunity to learn how to run the main instrument as well as how to process the raw data acquired from this instrument.

Recommendation #3 A NASA call for proposals should be offered to specifically support laboratory research for exoplanetary science. This could be offered on a biannual rather than annual basis. Nevertheless, this is essential to enable further progress in this field.

Recommendation #4 Funding should be allocated to the standardized databases to ensure their longevity and curation. This could be done on a quadrennial renewal basis. In particular, these funds should be used on trained personnel who will be able to maintain, update, and curate the data as well as provide software support for the databases.

2.3. Interdisciplinary efforts and fostering collaborations

Finding #6: *A general lack of communication has been identified between observational astrophysicists, laboratory astrophysicists, and physical chemists who produce relevant data but do not have channels of communication. This communication gap becomes evident when crucial reference data, such as spectroscopic data, is lacking, especially during ongoing missions like the James Webb Space Telescope (JWST). A concrete example of this data deficit is the recent discovery of unidentified features in the JWST spectra of various exoplanets, comets, and protoplanetary disks. One of the reasons behind this challenge is the scarcity of interdisciplinary proposals, primarily because there are no clear channels for collaboration. Additionally, there is often a lack of awareness about the potential contributions that scientists from different disciplines can offer to advance research objectives. The problem is certainly recognized among astronomers. The chart below shows the response to the corresponding section of the questionnaire.*

Recommendation #5 This issue can be addressed by facilitating better communication and collaboration among astrophysicists and physical chemists, particularly in the context of space missions, to ensure that critical data gaps are filled and research goals are met more effectively. The previous items could be addressed at joint meetings, but there are far too few in particular at the planetary/exoplanetary community. No workshops exist where scientists from different disciplines can interact and learn from each other. Organizing such meetings or special sessions at bigger conferences should alleviate some of the communication issues.

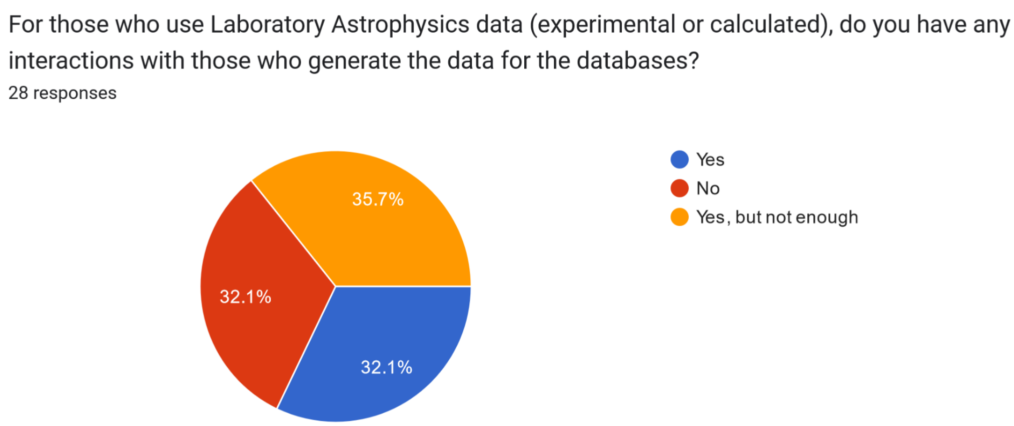

***Figure 2**. Response to the laboratory astrophysics User survey, evaluating the degree of interactions with producers of laboratory astrophysics data, including experiment and theory. A total of 31 responses were received.*

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Appendix G
Report from the Stellar, Nuclear, and Plasma Astrophysics (SNP) sub-group

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Background

Stellar, Nuclear, and Plasma astrophysics (SNP) forms a vital part of astrophysical research. The SNP research area addresses a wide range of important astrophysical questions, including determining the origin and evolution of elements in the Universe, stellar structure and evolution, stellar activity, stellar explosions, stellar populations, nucleosynthesis, cosmic chemical evolution from the first generation of stars to the present, plasma environments from low-density nebulae through to stellar interiors, the nature of dense matter probed by neutron stars, and the complex environments of colliding neutron stars. These areas are often interdisciplinary collaborations, with observers and modelers requiring accurate atomic, molecular, and nuclear data upon which their interpretation of astrophysical plasma environments is based.

Figure 1. Two James Webb Telescope images of the Ring nebula. Left is the Near-Infrared Camera (NIRCam), right is the Mid-Infrared Instrument (MIRI), showing the wealth of information from different wavelength bands.

“Laboratory Astrophysics” consists of laboratory experiments and theoretical calculations dedicated to the understanding of our universe, providing atomic, molecular and nuclear data, and benchmarking models, thus complementing astronomical observations and astrophysical/astrochemical modeling. As such, Laboratory Astrophysics forms an important foundation for SNP research, with a wide range of data required. This in turn is built upon the laboratory astrophysics infrastructure of experimental facilities and theoretical groups. The ASTRO decadal reports of 2010 and 2020 both indicated the critical importance of Laboratory Astrophysics. As stated in the 2020 decadal report:

“Laboratory astrophysics is a critical but often hidden and underappreciated cornerstone of the enabling research foundation. It has been chronically underfunded; concerns were raised in both the 2000 and 2010 decadal surveys, but the problem persists. Research in this area needs to be regarded as a high priority, and the existing approaches are not sufficiently advancing the field. A multi-step recommendation in this area urges the agencies to identify the need for supporting laboratory data to interpret the results of new astronomical observatories, identify resources, and consider new approaches or programs for building the requisite databases. The recommendation also points out the need to include not only experts in laboratory astrophysics but also users of the data to identify the highest priority applications.“

It is clear from section 4.5.5 of the Astro2020 Decadal survey, the 2018 NASA LAW report, and the 2023 white paper on nuclear structure, reactions, and astrophysics, that support and development of Laboratory Astrophysics is critical for a wide range of stellar, nuclear, and plasma astrophysics. We do not repeat here the long list of individual scientific questions that require laboratory astrophysics data; however, we list some illustrative examples in the table below. In the remainder of this report, we present recommendations based upon an overview of these well-documented needs. We direct the reader to these reports for a detailed list of scientific questions, missions, wavelength ranges, and their connection to laboratory astrophysics needs.

Themes and Associated Telescopes/Missions	*Science Questions*	*Application to Laboratory Astrophysics*
Multi-messenger astronomy (JWST, HST, LIGO, VIRGO, FERMI, SWIFT, BlackGEM, DECam, GOTO, the Vera C. Rubin Observatory's LSST, ULTRASAT, VISTA, and WINTER)	Determining the origin and evolution of heavy elements in the Universe. What are the dynamics of Neutron star mergers?	For heavy elements: - Lab measurements of nuclear reaction rates - Atomic opacity calculations and oscillator strengths - Electron-impact collision calculations and measurements for excitation, ionization, and recombination
Sources of X-rays and UV emission (XRISM, CHANDRA, XMM-NEWTON, ATHENA)	What is the source of high energy radiation in accreting black holes? What are the conditions and dynamics in supernova explosions?	Inner-shell photo- and electron-impact ionization of K- and L-shell electrons. High-accuracy atomic structure measurements and calculations for satellite lines in atomic systems.
Photoionized plasmas (JWST, HST, ground-based optical spectroscopy)	What is the mechanism for the abundance discrepancy factors in planetary nebulae and H II regions? What are the abundances of complex atoms in photoionized plasmas?	Photo-absorption data for gas-phase molecules containing O and Fe. Improvements in the accuracy of low-temperature dielectronic recombination rate coefficients.

		Improved electron-impact data for Fe-peak elements.
Stellar interiors **(TESS, GONG network)**	What is the nature of stellar structure, stellar evolution, and stellar populations?	Nuclear reaction rate coefficients and opacities for astrophysically abundant elements.
Accreting neutron stars (XRISM, XMM-Newton, Chandra, ATHENA)	What is the compactness of neutron stars?	Nuclear reaction rates on unstable neutron deficient isotopes.
Stellar explosions including Novae and Supernovae (COSI, INTEGRAL, NuSTAR, Kepler, XRISM, CHANDRA, XMM-NEWTON, ATHENA)	What is the contribution of explosive nucleosynthesis to the origin of the elements? How do supernovae explode?	Nuclear reaction rates on stable and unstable nuclei, including weak interaction rates. Improved Fe-peak element electron-impact data for non-equilibrium ionization balance conditions.
The solar wind interaction with atmospheres of comets and planets **(JWST, XRISM, SWIFT, XMM-NEWTON, CHANDRA, IRTF, SOAR, Keck)**	What is the role of the interaction of the solar wind with atmospheres?	Charge-exchange data for the range of solar wind velocities of H and He on the atoms and molecules present in cometary and planetary atmospheres. High-resolution measurements of molecular spectra for species in cometary and planetary atmospheres.

Table 1: A sample of scientific areas and missions within SNP that have unresolved science questions and laboratory astrophysics data needs.

The science goals for current and future ground-based observatories (e.g., ALMA, ELTs), as well as space science missions (e.g., JWST, NGRST, HWO), can only be realized if the fundamental physics needed for interpretation of the astrophysical data obtained with these facilities are determined robustly. For example, data obtained with JWST need more molecular data for IR spectroscopy. Data obtained with the ELTS, as well as UV, X-ray, and gamma-ray missions need atomic and nuclear data. Some of these data are completely missing, while for others they are not accurate enough compared to the observational accuracies (to be) achieved by the facilities.

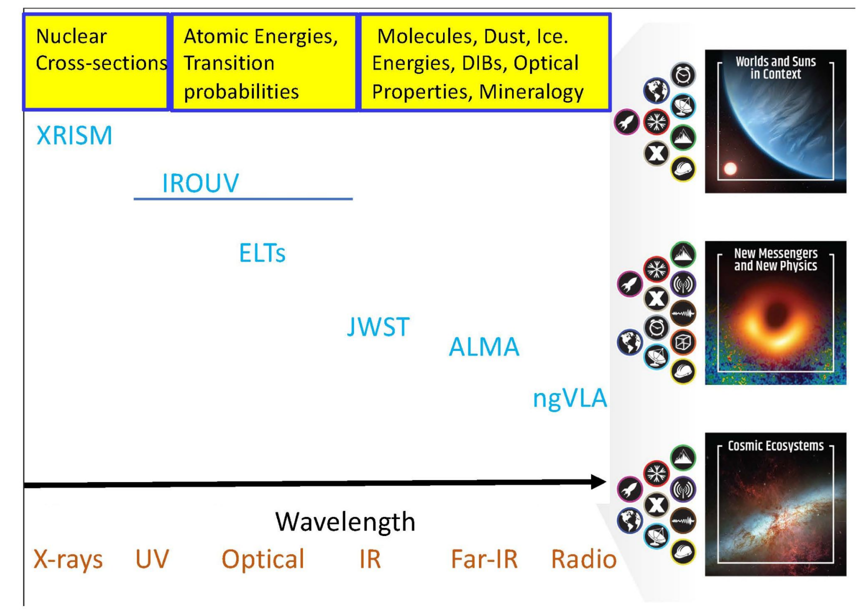

Figure 2. Progress in different areas of laboratory astrophysics is essential for the interpretation of data obtained from key current/future missions pertaining to the important themes recommended by the Astro-2020 Decadal Survey (adapted in part from a figure from the Astro-2020 Decadal Survey).

The work of Laboratory astrophysics is often at the fundamental level of determining atomic, molecular, and nuclear cross-sections. These data are then processed into the form used in modeling and diagnostics codes, such as rate coefficients, opacities, or generalized coefficients. It is important to note that much of this fundamental work can lead to scientific breakthroughs, such as the discovery of a new molecule in space. In addition, the laboratory astrophysics work is archived in databases for use by the community. The work of curating, vetting, maintaining, and updating these databases is significant, requiring expert knowledge. The laboratory astrophysics data needed by the community covers many disciplines. For example, the interpretation of the spectra from neutron star mergers requires accurate atomic opacity and collision data, and nuclear data, all of which are integrated into models that include both plasma physics and general relativity. These data are urgently needed to help understand the origin of the heavy elements in the Universe, especially given the ongoing and expected future advances in multi-messenger astronomy related to kilonovae. These include advances in kilonova localization from ground-based wide-field instruments such as BlackGEM, DECam, GOTO, the Vera C. Rubin Observatory's LSST, ULTRASAT, VISTA, and WINTER; in concert with advances in LIGO/VIRGO sensitivity and improvements of the localization capabilities of the world-wide network of gravitational wave detectors; ongoing gamma-ray burst monitoring; as well as the extended capabilities of detailed followup spectroscopy for well-localized events, for example with JWST.

In the rest of this document, we summarize the current status and needs of the laboratory astrophysics community, to allow support of critical observational astrophysics, along with recommendations. The topics are divided into workforce development, databases, and facilities and infrastructure.

Findings and Recommendations

1. Workforce Development

The information used for the workforce development was gathered from NSF-AAG and NASA laboratory astrophysics funding awards, NSF-Physics and DOE Office of Science funding for nuclear physics, two community surveys (one to the laboratory astrophysics community and one to the data users), as well as discussions and presentations from the LATF meetings.

Laboratory astrophysics trains a workforce with multiple skills. On the experimental side, laboratory astrophysics researchers are experts in many areas (such as optics and electronics); on the theory side they have code development and testing, and on the observational side, they have expertise in using optics, coding, statistics, and synthesizing knowledge in multiple areas to bear upon the ultimate laboratory– the entire Universe. In all areas (experimental, theoretical, observational), laboratory astrophysics researchers have skills in processing and analyzing large datasets. All of this takes many years of training, and it is important to have a pathway from undergraduate research to graduate positions, to post-doctoral researchers, to permanent positions at national labs and Universities.

In addition, to maintain the US's competitiveness at the international level in the STEM fields, it is essential to train the workforce with critical-thinking skills, deep scientific understanding, and experience in hands-on laboratory skills and data science. Such expertise can easily be transferred to industrial settings, strengthening the country in cutting-edge areas of national need such as energy research and national security. Laboratory astrophysics is an excellent resource for this area of workforce preparation.

a. Atomic and Molecular Workforce Development

Considering the funding data, the picture shows a mixture of positive and negative aspects. The PIs are mostly mid-career and senior researchers, with some early career faculty, and a mixture of proposals from National Labs and Universities. In general, there is reasonable support for undergraduate and graduate students. Only a small number of laboratory astrophysics grants request postdoctoral researchers, possibly due to an effort by the PIs to keep their grant proposals close to the average funding levels per grant. There have only been a small number of early career awards, and many laboratory astrophysics permanent positions are researchers who have to split their time between laboratory astrophysics and funding sources from other disciplines.

There is funding for both atomic and molecular projects, and for both experiment and theory, with more funding being allocated to molecular projects and for experiments. Only a small fraction (~5%) of projects bring together observations with theory/experiment, with the other projects archiving data that can be used by the community to analyze observations. Thus, there is a need for more multi-institute projects that involve observations, and for projects that include both theory and experiment. This reflects a need for more communication between the theoretical/experimental communities and the observational community and the limitations of what can currently be supported by the average laboratory astrophysics grant.

A major problem in hiring faculty in experimental laboratory astrophysics at universities is the lack of adequate startup funds. Setting up and maintenance of equipment in a new lab by an early-career faculty member needs substantial investment, which Physics or Chemistry departments at many universities (both R1 and R2) are not able to provide. In addition, many national lab facilities have world-class equipment but need early career staff to continue and maintain their research programs.

In summary, the level of funding support decreases as the career path of students progresses from undergraduate to graduate to postdoctoral to permanent positions. The workforce is currently below the critical mass required to maintain expertise in many of the specializations within Lab Astro.

b. Nuclear Workforce Development

A significant number of graduate students are attracted to laboratory nuclear astrophysics. Though data are uncertain, we estimate per year about 80-90 graduate students are being supported, the majority (~60) by NSF with the largest groups at Michigan State University, The University of Notre Dame, and Florida State University. This reflects the important role that laboratory nuclear astrophysics plays in attracting students into low-energy nuclear physics and thus in developing the Nation's nuclear workforce. It also shows the important workforce development role of university laboratories, both large national user facilities such as FRIB but especially also the smaller university-based accelerator laboratories that contribute a large fraction. In addition, about 25 postdocs are supported, roughly equally divided between NSF, DOE nuclear physics awards, and DOE national laboratories. There is a need for stronger support of the low-energy nuclear and nuclear astrophysics research workforce given the new opportunities from accelerator facility investments and increased needs in astronomy. Similarly to the Atomic and Molecular workforce, there is a need for strengthening connections to the astrophysical and observational community, along with opportunities across funding agencies and disciplines.

Recommendation 1.1: A focus on workforce development, to address the loss of critical mass in the workforce. Of particular need is early career support via post-doctoral fellowships, early career awards, and support for start-up funds at universities.

Recommendation 1.2: Support for more connections between the observational community and the laboratory astrophysics experiment and theory communities, including more interagency collaboration. This could include more support for

laboratory astrophysics REU and graduate fellowships that involve observational aspects, as well as more grants that involve observational collaborations.

2. Databases

There are many atomic, molecular, and nuclear databases (~72) available for Laboratory Astrophysics – see Appendix D and the figure below. The data represents a huge amount of effort on careful measurements and calculations. This includes structure, transition rates, and collision data. The databases are much more than a simple archiving of tables of numbers, but represent specialized knowledge in the evaluation, vetting, and curation of the data, as well as modeling and visualization tools.

The large number of available databases does not imply completeness of available data. While much progress has been made in the processes and atomic, molecular, and nuclear systems included in these databases, it is also true that these recommended data can have limited coverage. This has necessitated the creation of many specialized databases targeting various limited wavelength regions, plasma conditions, and data formats. Many databases are compendiums of un-evaluated data lacking internal and inter-database consistency. There is a need both for the generation of data missing from databases – particularly on the molecular side – and improvements and evaluation of existing data. For example, there is a significant backlog of evaluating nuclear data for astrophysics, converting them into data usable for astrophysical applications, and incorporating them into databases. This work requires high expertise in both experimental and theoretical physics and elaborate methodology, but often lacks the necessary workforce.

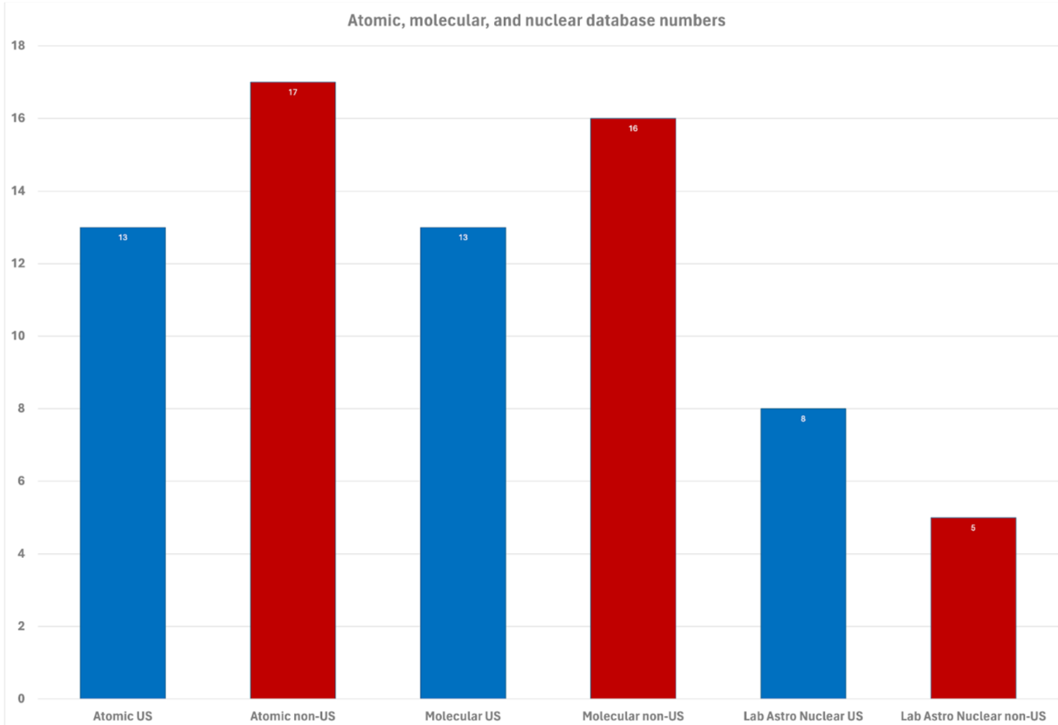

Figure 3: The number of existing databases per laboratory astrophysics subject are at US (in red) and non-US institutions (in blue).

Much of the data in the databases was generated from work in the core disciplines (e.g., AMO, chemistry, nuclear physics, and condensed matter). As the community survey indicated, there is a need to better connect the data users to these communities. There is an associated need to better connect the projects supported by funding in these core disciplines to those supported by funding in astronomy and astrophysics. Laboratory astrophysics is a natural vehicle to bridge this gap, because laboratory astrophysics researchers are connected to the work in these core disciplines, and to the work done by astrophysical observers and modelers. This synergy should be leveraged and enhanced by identifying existing common resources, as well as more cross-disciplinary and interagency funding opportunities. Workshops that bring together astronomers with researchers who generate data and curate databases critical for astronomy could be ideal venues to foster such collaboration and coordination.

There are a number of databases that gather data from a wide range of sources (e.g., HITRAN and VAMDC), a useful resource for the community. Comparing data from multiple sources, many with different data formats, is a formidable task. Such work should be encouraged and supported. It is also important that such databases ensure that it is easy for the information for crediting the original source to be provided to the data user for use in references in any publications.

There is a need for uncertainties on the archived data, a task that would require a huge amount of work. Among the listed atomic databases, only one (the NIST ASD) contains critically quantified uncertainties on the evaluated and recommended data. Similarly, only one nuclear astrophysics database (STARLIB) includes uncertainties. Efforts are underway for the development of methods to assign uncertainties to theory data in atomic, molecular, and nuclear physics. It should become the normal practice that uncertainties are provided with any experimental or theory data archived in the databases, however this requires significant increases in effort and support. The community surveys reflected a strong need by the astrophysics community for the databases, as well as a need for more communication between the user communities and those generating the data.

It should also be noted that while significant portions of the databases are from data that was calculated or measured as part of non-astrophysics funding (e.g., DOE-FES, Chemistry programs), this situation is becoming rare. As a result, it is becoming more important that astrophysical funding be made available to support the laboratory astrophysics data needed for current and future missions. More inter-agency supported work that connects the astrophysical data needs with the fundamental programs would also help with this situation.

Recommendation 2.1: Approaches for long-term support for the curation and development of the existing databases with emphasis on critical data evaluation and uncertainty quantification should be pursued. This includes supporting the specialized database workforce as well resources to connect and search the databases.

Recommendation 2.2: Facilitated workshops bringing together researchers who rely on laboratory astrophysics data with those generating and curating the data should be held to help identify the most pressing needs and priorities for current and future astronomical missions. Given that laboratory astrophysics is uniquely positioned to bridge the gap between astronomy and core disciplines such as chemistry, AMO, nuclear physics, and condensed matter physics, the workshops should also highlight interdisciplinary efforts, synergies, as well as cross-disciplinary and interagency funding opportunities that could help address the

critical data needs and enable astronomical discoveries.

3. Facilities and Infrastructure

In this document we define “infrastructure” as the set of institutions and funding mechanisms that enable laboratory astrophysics activities, and “facilities” as the experimental and computational resources that are needed to carry out laboratory astrophysics investigations.

The infrastructure consists of a network of national labs (e.g., GSFC, JPL, NIST, LLNL, LANL, SNL), DOE OS-supported national user facilities (for nuclear astrophysics, e.g. FRIB and ATLAS), and Universities that contribute to laboratory astrophysics research. The University infrastructure includes groups usually within astronomy, physics and astronomy, physics, or chemistry departments. It is often the case that the resources at these facilities were built up from funding that includes some outside of Lab Astro, such as direct funding for chemistry or for nuclear programs. This network, along with the federal support of the national labs, national user facilities, and the federal grant programs mentioned in section 1, represent a history of infrastructure development that has led to the experienced researchers, equipment, and theoretical/computational tools that currently exist.

There are many facilities used for Laboratory Astrophysics. They can also be split into Federal and University facilities, following the infrastructure that supports them. While there exists much specialized equipment, there is a need for Universities to be able to upgrade and improve existing equipment. Often the measurement of a new molecule, or new process requires a change in the equipment.

The agency support includes NSF, NASA, and DOE, with more details being given in section 1. There is an increasing need, due to the interdisciplinary needs of future missions, of inter-agency collaboration on laboratory astrophysics projects. There is also a need for coordination of access by NASA and NSF funded projects to leverage resources from DOE facilities (e.g., EBIT plasma experiments, synchrotron light sources). In plasma and atomic physics, these multi-billion-dollar investments are increasingly geared toward doing specialized research, with both institutional and facility barriers to accommodate laboratory astrophysics users. Devotion of a small fraction of available user time, plus modest resources to ensure access to lab floor space would enable efficient leveraging of these state-of-the-art facilities for laboratory astrophysics measurements.

Recommendation 3.1: Support for experimental facilities in critical areas for current and future missions, as mentioned in the decadal survey and associated white papers. Facilitated workshops would also be useful in identifying specific needs.

Recommendation 3.2: Small levels of funding and lab-time to enable experimental facilities for atomic, molecular, and plasma physics outside of NSF and NASA to make important laboratory astrophysics contributions.

Conclusions

In conclusion, there exists a set of well-motivated and experienced researchers who have the specialized skills to use the infrastructure of existing equipment and theoretical tools to perform high-quality laboratory astrophysics research for stellar, nuclear, and plasma astrophysics. However, the workforce has fallen below the critical mass required to maintain the expertise needed for current and future missions. As a result, the US is in danger of losing competitiveness in this area and the return on investment of future missions will be hampered by a lack of Laboratory Astrophysics data. At the same time, there is a strong desire from the users of the data to connect with those generating the data, and much exciting research and discoveries to be made. The recommendations in this report are focused on the development of the workforce at the critical early career stage and maximizing the use of specialized resources and databases.

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