

# LABORATORY ASTROPHYSICS WHITE PAPER

(BASED ON THE 2006 NASA LABORATORY ASTROPHYSICS WORKSHOP  
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## 1. Preface

Laboratory astrophysics and complementary theoretical calculations are the foundations of astronomical and planetary research and will remain so for many generations to come. From the level of scientific conception to that of the scientific return, it is our understanding of the underlying processes that allows us to address fundamental questions regarding the origins and evolution of galaxies, stars, planetary systems, and life in the cosmos. In this regard, laboratory astrophysics is much like detector and instrument development at NASA and NSF; these efforts are necessary for the astronomical research being funded by the agencies.

The NASA Laboratory Astrophysics Workshop met at the University of Nevada, Las Vegas (UNLV) from 14-16 February, 2006 to identify the current laboratory data needed to support existing and future NASA missions and programs in the Astrophysics Division of the Science Mission Directorate (SMD). Here we refer to both laboratory and theoretical work as laboratory astrophysics unless a distinction is necessary. The format for the Workshop involved invited talks by users of laboratory data, shorter contributed talks and poster presentations by both users and providers that highlighted exciting developments in laboratory astrophysics, and breakout sessions where users and providers discussed each others' needs and limitations. We also note that the members of the Scientific Organizing Committee are users as well as providers of laboratory data. As in previous workshops, the focus was on atomic, molecular, and solid state physics.

The NASA Universe Working Group (UWG) within the SMD requested a White Paper be drawn up outlining the conclusions of the Workshop for presentation at the next UWG meeting in April 2006. Specifically, the request included

1. addressing the major science goals as defined in the 2006 NASA Strategic Plan and then providing details on the critical laboratory astrophysics data requirements that will have to be met, if the desired science results are actually to be achieved,
2. reporting of recent significant astronomical results where the input from laboratory astrophysics was of critical importance, and
3. discussing in detail the specific laboratory astrophysics efforts that will need to be undertaken in direct support of missions and programs that are on the near horizon, specifically *Herschel*, *SOFIA*, *JWST*, *Hubble* servicing, and ALMA (the latter of primary concern to NSF).

These points are addressed in the subsequent sections of this requested White Paper, which also contains a set of recommendations drawn from a consensus view of the Workshop participants.

A number of points figured prominently at the UNLV Workshop, points that were raised in the White Paper from the 2002 NASA Ames Laboratory Astrophysics Workshop. These include: “Laboratory facilities are aging and major funding is required to replace them with modern, state-of-the-art equipment” and “The training of new scientists in laboratory astrophysics is crucial for the future of the field, but the low level of funding is making it more difficult to attract students...”

In the last four years the situation has become even more dire. Laboratory astrophysics has reached a point where it is ceasing to be a viable, productive field. This should be of great concern to NASA and NSF. Without laboratory astrophysics, the scientific return from current and future NASA missions and NSF ground-based observations will diminish significantly. Without laboratory astrophysics the future progress of astronomy and astrophysics is imperiled. Recommendations are provided below that address this issue in a time of limited resources, especially funding.

## 2. General Findings

- A study of the importance of laboratory astrophysics for all of astronomy under the auspices of the National Research Council and involving NASA, NSF, DOE, and DoC/NIST is long overdue.
- There is a strong requirement for a rich, vibrant laboratory astrophysics community that can respond on a “rapid” time scale to ongoing observations over a wide range in wavelengths and physical conditions.
- There is an urgent need to maintain the infrastructure, in terms of both personnel and facilities.

- Databases of atomic, molecular, and solid state parameters that are complete (e.g., wavelength lists for all stages of ionization) and critically evaluated are a necessity.
- In a number of areas, theory and experiment are converging so that the astrophysics, which depends on such data, is more secure.
- There is significant overlap between data needed to study phenomena beyond the Solar System and within it.
- As missions probe earlier moments in the history of the Universe, phenomena associated with high energies (short wavelengths) are observed with missions having instrumentation designed for low energies (long wavelengths).
- The data requirements for advances in astrophysics from NASA missions are more often than not the same requirements for DOE-sponsored research on plasmas and NSF-sponsored astronomical research; the need for critical evaluations of available data highlights the close connection to DoC/NIST.

### 3. Recent Successes

Astrophysical discoveries are propelled forward in part by experimental and theoretical advances in atomic, molecular, and solid state physics. Presented below are selected examples of significant astrophysical results that arose from recent laboratory and theoretical efforts on phenomena involving atoms, molecules, and solids. When possible, we also highlight future avenues for the research.

- Abundance determinations for old metal-poor halo stars using the *Hubble Space Telescope* and ground-based observations suggest that two different rapid neutron-capture processes may exist for nucleosynthesis beyond the iron peak (Cowan et al. 2005, ApJ, 627, 238). This insight is the result of new laboratory oscillator strengths for high  $Z$  elements (e.g., Ivarsson et al. 2003, A&A, 409, 1141). The new data have also allowed for improvements in radioactive dating using Th/Eu ratios and are yielding reasonable cosmochronometric age estimates for halo stars (Snedden et al. 2003, ApJ, 591, 936).
- X-ray emission from comets is due to charge exchange between solar wind ions and neutrals in cometary comae (e.g., Cravens 2002, Science, 296, 1042; Beiersdorfer et al. 2003, Science, 300, 1558). It is now also predicted that up to half of the diffuse soft X-ray background may not be extra-solar but may actually be due to solar wind charge exchange with geocoronal and interstellar neutrals (Robertson & Cravens 2003, J. Geophys. Res., 108, 8031). These findings suggest that charge exchange involving higher principal quantum numbers and emission at UV/visible wavelengths and involving simple molecules like H<sub>2</sub>O may be important as well (Greenwood et al. 2001, Phys. Rev., A 63, 062707).
- In the well-studied AGN NGC 3783, the warm absorber density and location have been found, respectively, to be smaller and closer to the central black hole than expected (Krongold et al. 2005, ApJ, 622, 842). This discovery is a major success of theoretical atomic physics, which identified the numerous unknown absorption lines in the high

resolution *Chandra* and XMM-*Newton* spectra of warm absorbers. These lines were shown to be inner-shell absorption transitions for the low charge states of Fe and were also used as a powerful new plasma diagnostic (Behar et al. 2001, ApJ, 563, 497).

- Measuring the atmospheric temperature of the extra-solar planets TrES-1 (Charbonneau et al. 2005, ApJ, 626, 523) and HD 209458b (Deming et al. 2005, Nature, 434, 740) with the *Spitzer Space Telescope* is partly a success of stellar atmosphere spectral synthesis and laboratory studies of molecular opacities. Transit searches for extra-solar planets also use synthetic stellar spectra as templates against which to correlate measured radial velocities (Konacki et al. 2003, Nature, 421, 507), a method which is at the core of NASA's future *Kepler Mission*. For these and other cases, the increasing completeness of the calculated line lists and opacities (Bautista 2004, A&A, 420, 763) has been a critical factor.
- Using the *Kuiper Airborne Observatory (KAO)*, important molecules have been detected in the interstellar medium (ISM) whose emission had been inaccessible by ground-based astronomy. Of particular note are  $\text{H}_2\text{D}^+$ , a cornerstone species in the ion-molecule theory of interstellar chemistry, HCl, a fundamental hydride, and  $\text{H}_3\text{O}^+$ , a direct tracer of the water abundance (e.g., Zmuidzinas et al. 1995, ASP Conf. Ser., 73, 555; Timmermann et al. 1996, ApJ, 463, L109), as well as the pure rotational lines of  $\text{NH}_3$ , OH, and CH (e.g., Stacey et al. 1987, ApJ, 313, 859). The *KAO* has also been invaluable in detecting ro-vibrational transitions of heavier species such as  $\text{C}_3$  in molecular clouds (e.g., Giesen et al. 2001, ApJ, 551, L181). Studies of these species have led to breakthroughs in our understanding of the molecular component of the interstellar medium. These discoveries were only made possible by preceding high resolution, laboratory spectroscopy (e.g., Brown et al. 1993, ApJ, 414, L125; Harrison et al. 2006, ApJ, 637, 1143). Such laboratory measurements are needed for the sensitive spectral-line surveys proposed for *Herschel*.
- High rotational lines of CO (up to  $J = 45$ ) have been discovered in the Orion-KL Nebula using the *KAO* and the *Infrared Space Observatory* (Gonzalez-Alfonso et al. 2002, A&A, 386, 1074). These spectral lines gave the first early glimpses of the process of high mass star formation with associated shocks and high velocity outflows (e.g., Hollenbach et al. 1995, ASP Conf. Ser., 73, 243; Ceccarelli et al. 1996, ApJ, 471, 400). These studies would not have been possible without previous high resolution laboratory spectroscopic work; the understanding of the dynamics in this environment rests on past investigations of collisional excitation. This and the preceding example reveal the exciting results anticipated at sub-millimeter wavelengths with *SOFIA* and *Herschel* and from new approaches to molecular synthesis on grains in shock-heated regions (Madzunkov et al. 2006, Phys. Rev., A 73, 020901(R)).
- *FUSE* observed UV absorption of  $\text{H}_2$  and HD in the ISM from a range of excited rotational levels (Snow et al. 2000, ApJ, 538, L65; Ferlet et al. 2000, ApJ, 538, L69), providing new insights into the physics and chemistry of translucent clouds and a tool to evaluate the ISM deuterium abundance. These observations and their interpretations

were made possible by laboratory studies of the electronic transitions and processes relevant to the formation of H<sub>2</sub>.

- Aromatic infrared bands (AIBs), commonly dubbed “PAH bands”, are now routinely observed with the *Spitzer Space Telescope* and used to probe dust in extragalactic environments (Hogg et al. 2005, ApJ, 624, 162; Wu et al. 2006, ApJ, 639, 157) and to measure redshift (Yan et al. 2005, ApJ, 628, 604; Weedman et al. 2006, ApJ, 638, 613). Such emission measured in a recent *Spitzer* survey of elliptical galaxies indicates that the carriers, attributed to polycyclic aromatic hydrocarbons (PAHs) and their derivatives, are a probe of recent merger activity in these galaxies (Kaneda et al. 2005, ApJ, 632, L83). It certainly looks like the AIB emission is correlated with star formation (Lutz et al. 2005, ApJ, 625, L83; Wu et al. 2005, ApJ, 632, L79). This progress has only been possible thanks to laboratory emission and absorption spectra of PAH-type species, including ions. Furthermore, the signature of individual PAH-like molecules can now be sought in astronomical spectra at UV and visible wavelengths, making it possible, for the first time, to detect specific aromatic compounds in space.
- The analysis of the first cometary and interstellar sample return from the Stardust mission will provide key information on grain formation and processing in space. Observations with *ISO* and *Spitzer* have revealed the presence of specific minerals (e.g., crystalline silicates) in a variety of Galactic environments, including outflows from evolved stars and protoplanetary disks (Waelkens et al. 1996, A&A, 315, L245; Waters et al. 1996, A&A, 315, L361). This work is critical to understanding dust processing during its lifetime, and is only possible thanks to laboratory measurements of the infrared spectra for candidate grain materials (Begemann et al. 1994, ApJ, 423, L71; Jäger et al. 2003, J. Quant. Spectr. Rad. Transf., 79-80, 765).
- Studies of dust and ice provide a clear connection between astronomy within and beyond the solar system (Strazzulla et al. 2005, Icarus 174, 31). Planetary surface temperatures are derived from ice measurements in the NIR (Grundy et al. 2002, Icarus, 155, 486), while planetary atmospheres (Europa, Ganymede,...) are explained by laboratory studies of ices (Hansen et al. 2005, Icarus, 176, 305).

While examples listed above demonstrate the rich astrophysics enabled by laboratory astrophysics, they are by no means the only notable advances. We are limited here only by the constraints of space.

#### 4. Current and Future Needs

We now turn our attention to the needs to reach the next level of understanding of the Universe, near and far. The discussion is guided by the 2006 NASA Strategic Plan. Of most relevance to laboratory astrophysics are items in Strategic Goal 3, sub-goals 3B, 3C, and 3D. Particular areas of research include (1) the origin, structure, evolution, and destiny of the Universe, (2) the potential for life elsewhere, and (3) the nature of solar activity and its effect on the solar system.

## 4.1 Atoms and Ions in Astrophysics

Astrophysics needs vast quantities of atomic data. Data are needed for all the cosmically abundant elements as well as for the rarer elements in order to tease out the chemical evolution of the Universe. We discuss in general the atomic data needs of the astrophysics community and give some specific, but not exclusive, examples.

Analyzing and modeling cosmic spectra begin with identifying the observed lines which may be seen in emission or absorption. This requires **accurate and complete wavelengths across the electromagnetic spectrum** for spectral line identification, wind velocity determinations, and investigating variations in the fine structure constant over the age of the Universe. The need includes bandpasses that are commonly considered the realm of ground-based observations. For example, the *James Webb Space Telescope* will observe many objects whose ultraviolet and visible lines have been redshifted into the IR.

The next step toward understanding the properties of an observed cosmic source depends on accurate knowledge of the underlying atomic processes producing the observed lines. **Oscillator strengths and transition probabilities** are critical to a wide variety of temperature and abundance studies from infrared to X-ray wavelengths. Many existing data for the heavier elements are still notoriously unreliable. These current limitations on the atomic data available for mid-Z elements make it difficult to determine the nature of the r-process. For example, non-LTE spectral analysis of the prototypical super-soft source Cal 83 provides stellar parameters indicating a massive hot white dwarf. This is of great interest as such sources are the likely progenitors of Type Ia supernovae. But a detailed chemical analysis of Cal 83 is not possible with currently available data in the soft X-ray domain. **Inner shell photoabsorption and fluorescence yields** are needed for studies of X-ray photoionized plasmas such as AGN and X-ray binary winds, and for finding the hot interstellar and intergalactic gas. *Chandra* searches for the “missing baryons” in the warm hot intergalactic medium (WHIM) have been enabled by new laboratory studies of inner-shell transitions; however, many line identification issues remain. Rate coefficients for **electron impact excitation** approaching 10% accuracy are necessary for the most important line ratio diagnostics yielding temperature, optical depth, density, and abundance. Recent theoretical and laboratory studies of the important ion Fe XVII suggest for the first time that this is possible, confirming the quantitative analysis of resonance scattering in the elliptical galaxy NGC 4636 and suggesting that conventional chemical-enrichment models for ellipticals are not correct. **Proton impact excitation** is important because ions in hot post-shock material decouple from radiatively cooling electrons and may remain hot enough to produce line emission through collisional impact, as seen in SN 1006. Atomic data for these processes also appear to be important for our understanding of colliding winds in hot star binaries. There is a crucial need for **state specific cross sections for dielectronic and radiative recombination and for charge exchange**. Complete spectral models require accurate predictions for the line emission from all recombination processes. Temperature and abundance determinations in a wide range of cosmic sources make use of this line emission. Observations of the WHIM are contaminated by X-ray emission from the

heliosphere, requiring accurate data for X-ray line emission due to charge exchange. These data will be needed to analyze X-ray emission from stellar winds within astrospheres, which if detected would provide a diagnostic of the stellar wind composition.

Turning the observed line strengths into elemental abundances requires accurate ionization balance calculations. Cosmic plasmas can be divided into two broad classes: photoionized and electron-ionized. Photoionized gas is formed in objects such as AGNs, X-ray binaries, planetary nebulae (PNe), H II regions, the intergalactic medium, Wolf-Rayet nebulae, and luminous blue variable nebulae. Electron ionized gas is formed in objects such as stellar coronae, supernova remnants, the interstellar medium, and gas in galaxies or in clusters of galaxies.

Modeling the ionization structure of each class of plasma requires accurate data on many processes. Photoionized gas requires reliable low temperature **dielectronic recombination** (DR) and electron ionized gas high temperature DR. Calculating reliable low temperature DR is theoretically challenging and for some systems laboratory measurements are the only way to produce reliable data. For high temperature DR, few benchmark measurements exist for L-shell and M-shell ions. Density dependent DR rate coefficients are needed for dense plasmas but are sorely lacking. For decades astrophysicists have had to rely on theoretical **photoionization** calculations of varying degrees of sophistication. The development of third generation synchrotron light sources has opened up the possibility of measuring photoionization cross sections for many astrophysically important ions. High energy electrons or photons can lead to the production of an inner shell hole which then decays via the sequential emission of single or multiple electrons (most often) and/or photons (less often); past data sets have used inaccurate approximations for the **Auger yield**. Some modern theoretical work has been carried out for K-shell vacancies, but more work remains, especially for L-shell vacancies. **Charge exchange (CX) recombination** with H and He and **CX ionization** with  $H^+$  and  $He^+$  have been shown to be important for many systems, but few modern calculations or laboratory measurements exist at the relevant temperatures. Data are also needed for low charge states of elements such as Se and Kr in order to study nucleosynthesis in PN progenitor stars. The recommended **electron impact ionization** (EII) data are highly suspect. Recommended data derived from the same scant set of measurements and calculations can differ by factors of 2 to 3. Much of the published experimental data include contributions from an unknown metastable fraction in the ion beams used. The recommended EII data have not undergone any significant revision or laboratory benchmarking since around 1990. Little data also exist for **three-body recombination**, the time reverse of EII, which is important in high density plasmas.

Implicitly included in all the above data needs is the potential for developing new plasma diagnostics. One particularly exciting possibility is that of an X-ray line diagnostic for magnetic field strength. It may also be possible to measure the equation of state of neutron stars using a simultaneous measurement of the gravitational redshift and pressure broadening of atomic absorption lines. This will require accurate Stark profile data for highly charged heavy ions in very dense plasma ( $10^{19}$  to  $10^{23}$   $\text{cm}^{-3}$ ). Experimental and theoretical work

such as this offers the potential to open up new areas of astrophysical research.

To conclude, the above discussion brings to the fore two important issues. First, interpreting astrophysical spectra from neutral to highly charged ions generally requires large modeling codes (e.g., radiative transfer codes, photoionization codes, collisional ionization codes). Many of these are publicly available. These codes incorporate vast amounts of theoretical atomic data, which themselves often come from large atomic codes, as well as data derived from laboratory measurements. A collaboration among astrophysicists (observers, theorists, and modelers) and atomic physicists (theorists, and experimentalists) has proven highly successful not just in the examples highlighted here but for many other cases. Such collaborations are vital for maximizing the scientific output of past, present, and future NASA spectroscopic missions. Second, the need for closer coordination with other agencies and departments is clearly evident. A significant body of atomic research has been funded by NSF and DOE in the past, but the scope and accuracy required for today's research in astrophysics and fusion physics demands a renewed effort. Many studies on stellar abundances and atmospheres are conducted at ground-based observatories. With respect to ground-based observations, NSF is the most appropriate source for funding work on the necessary laboratory data for wavelengths, oscillator strengths, and collision cross sections. Moreover, reliable results require critically evaluated compilations, which have been accomplished with great success in the past by DoC/NIST and DOE laboratories, especially Oak Ridge National Laboratory. This must continue with NASA and NSF support.

## 4.2 Molecular Astrophysics

Over the past 30 years, space-based and ground-based astronomy have shown that the Universe is highly molecular in nature. In fact, half of the mass in the inner 10 kpc of our Galaxy is thought to be composed of molecular material. The discovery of over 130 different chemical compounds in interstellar gas, with the vast majority organic molecules, reveals the complexity of interstellar chemistry. Protogalaxies and the first stars are predicted to have formed from primordial clouds where  $\text{H}_2$  and HD controlled the cooling and collapse of these clouds. Subsequent stars and planetary systems are known to form out of the most complex molecular environments; therefore, it is inevitable that interstellar chemistry is intimately connected to the origins of life.

An understanding of the molecular component of the Universe requires a two-fold approach. First, the chemical compounds, their abundances, and how they are distributed in astronomical sources need to be determined. Second, molecular formation mechanisms including reaction pathways and dynamics need to be understood. Attaining these goals is crucial in guiding future missions designed to observe molecules and to interpret results from past and current missions. We now discuss the needs for laboratory data.

**High resolution laboratory spectroscopy** is absolutely essential in establishing the identity and abundances of molecules observed in astronomical data. It is extremely important for laboratory measurements to have a resolving power higher than the astronomical



instruments at sub-millimeter and terahertz wavelengths, namely, 1 part in  $10^7$  to  $10^8$ . Given the advancements in detector technologies, astronomical spectra obtained in this frequency region will be extremely complex. Such will be the case for spectra obtained toward star-forming regions with *Herschel*. Furthermore, all the main functional groups known to organic chemists have now been observed in interstellar molecules, suggesting that interstellar chemistry contains the organic complexity seen on Earth. This result indicates that the origin of life may have begun in the gas phase chemistry of interstellar clouds. Laboratory spectroscopy is crucial in making the link between interstellar molecules and simple biological compounds that could seed life. It is also crucial in making the link between interstellar molecules (gas phase) and dust (solid phase) that is discussed in the following section.

For molecular data obtained from NASA missions to be of practical use, **accurate assignments of observed spectral features** are essential. The problem here is two-fold. First, the transitions of known molecules need to be assigned in these spectra, including higher energy levels and new isotopic species. Second, the spectra of undiscovered species that promise to serve as important new probes of astronomical sources need to be identified, such as the following. **Hydrides**, including metal hydrides and their ion counterparts, have transitions unique to the sub-mm/IR, and hence are excellent targets for space astronomy. **Organic ions and radicals**, including large aromatic species, serve as molecular probes and key intermediaries in chemical reactions that lead to more complex molecules. The simplest, and most fundamental, of these molecules also have important transitions in the sub-mm/IR. **Biogenic compounds**, including possible radical intermediates, directly tie into questions of the origin of life.

The spectroscopic study of such molecules, many of which cannot be produced in large abundance in the laboratory, **requires the development and application of state-of-the-art ultra-sensitive spectroscopic instruments** (e.g., velocity modulation, cw and pulsed cavity ringdown, time-of-flight mass spectrometers). Construction and implementation of these instruments is costly and time-consuming, and data production from these devices cannot be turned on and off at will. Efficient utilization requires continued support.

Detecting the possible presence of a species, however, is not sufficient since it must be reconciled with other physical properties of the medium. Even the steps leading to formation of simple species, such as  $\text{CH}^+$  and  $\text{H}_3^+$ , have not been fully resolved. To understand the chemical composition of these environments and to direct future molecular searches in the framework of future NASA missions, it is important to **untangle the detailed chemical reactions and processes** leading to the formation of new molecules in extraterrestrial environments. The data necessary to understand ion-molecule and neutral-neutral reactions leading to carbon-bearing and hence biologically relevant molecules in the interstellar medium and in planetary and cool stellar atmospheres involve the use of ion storage rings, flowing afterglow and selected ion flow tubes, crossed beams machines, and setups establishing low temperature kinetics. Data are urgently needed for (1) **products** of bimolecular reactions, (2) **intermediates of these reactions** that can be stabilized by three-body reactions in denser media such as cometary, planetary, and stellar atmospheres and gravitationally-

collapsing gas of protostellar objects, and (3) reactive/inelastic **rate coefficients, with pressure and temperature dependent branching ratios**. These data will establish credible chemical models of interstellar, planetary, and stellar environments. The chemical models in turn are imperative to predict the existence of distinct molecules in extraterrestrial environments, thus guiding future astronomical searches of hitherto unobserved molecular species. Even for the simplest of molecules,  $H_2$ , many uncertainties remain in its formation and destruction mechanisms, from primordial to solar-metallicity gas. The former may limit our ability to understand protogalaxy and structure formation at high redshift, a major scientific goal of *JWST*.

**Quantum mechanical calculations** are an integral tool in laboratory astrophysical studies. There are many examples where calculations aided in the **interpretation of high-resolution spectra**, provided key **collisional excitation cross sections and the most accurate thermo-chemical data**, and delineated **important reaction pathways**. Input from quantum chemical/molecular physics studies are vital, particularly for extra-solar planets, cool stars, star forming regions, and primordial chemistry. As spectral observations of these sources continue to become available, at ever increasing resolutions, models will be necessary to interpret the spectra for information such as temperature, atmospheric composition, etc.

Critical needs in this area include **line lists, excitation rates, and mechanisms for forming and destroying molecules**. Ro-vibrational and/or electronic line lists for CrH, FeH,  $H_2O$ ,  $CH_4$ , and  $NH_3$  and accompanying molecular structure data are woefully incomplete.  $NH_3$  and methanol, which are widely observed in various astronomical environments, are of particular interest since these molecules possess large amplitude motions and their spectra are highly sensitive to their physical environment. Collisional excitation rates of CO,  $H_2O$ , TiO, and hydrides are required to obtain abundance data from line intensities. Alkali broadening profiles due to collisions by  $H_2$  are needed to deduce gravity and effective temperatures in brown dwarfs. Electronic and vibrational spectra of large polyatomic molecular structures (PAHs, other aromatic carbon compounds, carbon chains,...) and oscillator strengths are required to interpret ubiquitous interstellar spectral features such as the IR emission bands (AIBs) and diffuse interstellar bands (DIBs). Molecular formation/destruction mechanisms, such as UV and X-ray photodissociation of molecules, are essential ingredients for the development of non-chemical equilibrium models.

### 4.3 Dust and Ices in Astrophysics

The formation of stars and planetary systems takes place deep inside cold gas and dust clouds, often obscured by hundreds of visual magnitudes of extinction. At high redshifts, the assembly of galaxies through the merging of smaller units is accompanied by large amounts of obscuring dust. In order to properly decipher the mechanisms that occur in these environments, laboratory studies of silicate and carbonaceous dust precursor molecules (in the gas phase) and grains (solid phase) are required as are studies of the interaction between dust

and its environment (including radiation and gas). These interactions play critical roles in the gas physics and dust processing. Astronomical observations and supporting laboratory experiments over a wavelength region that extends from the X-ray domain to the ultraviolet, infrared, and sub-millimeter regions are of paramount importance for studies of the molecular and dusty universe. It is here where stars and planets form and where most of the chemistry of the Universe occurs. Observations at infrared and sub-millimeter wavelengths penetrate the dusty regions and probe the processes occurring deep within them. Moreover, these wavelengths provide detailed profiles of molecular transitions associated with dust. Because of its importance, NASA has launched or will launch and participate in a number of missions centered on this wavelength region (*Spitzer*, *SOFIA*, *Herschel*, and *JWST*), which will chart the star formation history of the Universe, star and planet formation in the Milky Way, the galactic life cycle of the elements, and the molecular and dusty universe. Together these span most of the key questions in modern astronomy.

The ensemble of current (*Spitzer*) and planned (*SOFIA*, *Herschel*, *JWST*) IR/sub-mm missions will bring in enormous quantities of data in spectral regions where little is known. Laboratory studies are essential in order to support the analyses of these data. Understanding the interaction of cosmic dust with its environment requires the laboratory study of the formation and destruction mechanisms of interstellar grains from their molecular precursors. **Determination of the physical properties of grains** is also critical. These include the nature of atomic and molecular binding sites on the surface, the photoelectric yield, probabilities that incident particles (including electrons and ions) stick to the grain, and ionization potentials.

Mid-IR spectra of individual objects such as H II regions, reflection nebulae, and planetary nebulae as well as the general interstellar medium of galaxies as a whole are dominated by a set of **emission features due to large aromatic molecules**. Studies of the IR characteristics of such molecules and their dependence on molecular structure and charge state are of key importance for our understanding of this ubiquitous molecular component of the ISM.

At long wavelengths, the continuum dust opacity is uncertain by an order of magnitude. IR spectral features of interstellar dust grains are used to determine their specific mineral composition, hence their opacities, which determine inferred grain temperatures and the masses of dusty objects, including the interstellar medium of entire galaxies. Emission bands from warm astronomical environments such as circumstellar regions, planetary nebulae, and star-forming clouds lead to the determination of the composition and physical conditions in regions where stars and planets form. The laboratory data essential for investigations of dust include measurements of the **optical properties of candidate grain materials** (including carbonaceous and silicate materials, as well as metallic carbides, sulfides, and oxides) as a function of temperature. For abundant materials (e.g., forms of carbon such as PAHs), the **measurements should range from gas-phase molecules to nanoparticles to bulk materials**. The IR spectral region is critical for the identification of grain composition, but results are also required for shorter wavelengths (i.e., UV), which heat the grains. Previous

studies in the UV have focused on the only identified spectral feature (at 2200 Å), but all materials should show UV spectral signatures. This need will become all the more important with the return of data from COS/*HST*. COS will be searching for the spectral signatures of specific individual aromatics, which provide a link between simpler gas phase species and solids, in the UV and near UV (NUV).

The UV spectral region contains features of important large interstellar molecules, such as organic species that carry the IR emission bands (AIBs) and diffuse interstellar bands (DIBs) and that may be related to the origin of life. Studies of the UV characteristics of such molecules and their dependence on molecular structure and charge state are of key importance for our understanding of this molecular component of the ISM. Identification of UV spectra of large aromatics is especially important to address these issues and represents one of the key science goals of *HST* (COS) and *FUSE*. We draw attention to the far-UV spectral region where *FUSE* operates. Here special coatings and detectors are needed, with the result that laboratory data are lagging far behind the astronomical data. The lack of experimental data in this spectral region has hampered progress in theoretical studies as well as the interpretation of astronomical data. **UV spectra are uniquely capable of identifying specific molecules**, in contrast with the less specific transitions observed in the IR. Laboratory studies provide spectroscopy of large organic molecules (such as PAHs) and their ions in the solid and in the gas phases. This work must be **complemented by quantum theory calculations** so that the laboratory data are properly interpreted.

The UV wavelength region, often used in conjunction with other wavelengths, provides an understanding of the fundamental processes (and especially the energy balance) associated with emissions from planetary atmospheres and magnetospheres, including planetary aurora and dayglow emissions (relevant for all planets and satellites with atmospheres and magnetospheres), as well as comets. Laboratory data on polyatomic molecules and dust grains are needed for modeling planetary atmospheres (a typical recent example is the Cassini-Huygens mission with the return of in-situ measurements from the hazy atmosphere of Titan). Lack of reflectance spectra (UV-visible-NIR) of low temperature frosts/volatile ices has inhibited interpretation of the Galileo data. Unless something is done in the near future, the situation will be similar for Saturn Cassini data. Water is reasonably well studied, and the mid- and far-IR has been done for astrophysical ices, although not at the 50 to 150 K temperatures relevant for solar system objects. **Optical constants/properties** of organic solids (important for most “red” solid bodies in the outer solar system) and of solid sulfur are needed.

New results from *Chandra* and *XMM-Newton* suggest additional areas in need of laboratory astrophysics. Recent astrophysical observations have tentatively identified X-ray absorption by molecules and solids, a new area for laboratory measurements of photoabsorption physics that can lead to differentiation between gas and dust in diffuse media. Detailed examination of **X-ray absorption edges** can, in fact, reveal which specific minerals are present in the ISM.

X-rays detected in the laboratory from olivine and augite surfaces bombarded by highly charged ions (HCIs) indicate that one should be able to detect mineral components when

HCI's collide with a comet or planetary surface (from, for example, the solar wind) and provide wavelengths at which X-ray observations should be made. Such work opens up the possibility of doing “**mineral prospecting**” by **X-ray spectroscopy** using remote spectrometers.

## 5. Recommendations

**Recommendation 1: Conduct a study of the importance and need of laboratory astrophysics for all of astronomy under the auspices of the National Research Council and involving the principal funding sources for astronomical research, NASA and NSF, as well as DOE and DoC/NIST, whose activities encompass similar areas of study.** This is an exciting time for astrophysics, but further progress requires improved atomic, molecular, and solid state data. Laboratory astrophysics, including the related theoretical effort, has reached a point where the field is becoming extinct; the impact on current and future missions will undoubtedly be catastrophic. The report from the NRC should include how the agencies and departments can best work together to maintain this important national resource. Specific items to address include:

1. how to support the development and maintenance of laboratories and their unique instrumentation for ground-breaking research;
2. how to encourage and retain faculty in this area, in terms of ensuring the future supply of laboratory astrophysicists and in maintaining/revitalizing infrastructure in the field;
3. how to foster graduate student participation and PhD theses in these areas, in order to revitalize an aging discipline;
4. how to coordinate the activities of the agencies and departments that benefit from a robust effort in laboratory astrophysics; and
5. how to combine interdisciplinary teams and/or centers, such as present in NASA's Astrobiology Institute, focused on solving specific complex problems and generating comprehensive data to address mission related needs, while continuing a fully funded Astronomy and Physics Research and Analysis (APRA) program to support ground-breaking ideas of individual researchers that could potentially revolutionize aspects of astrophysics and increase the scientific return from expensive NASA missions.

**Recommendation 2: Ongoing missions (e.g., *Chandra*, *HST*, and *Spitzer*) and missions that will be initiated in the near future (e.g., *SOFIA*, *Herschel*, *JWST*, and *Beyond Einstein*) suggest a natural ranking for the observational bandpasses of 1) far infrared/sub-millimeter, 2) X-ray and infrared, and 3) UV/visible.** This suggests a similar ranking for laboratory and theoretical efforts over the next few years. However, it is important to keep in mind that there is not always a 1-to-1 correspondence between these observational bandpasses and the needed laboratory astrophysics data. For example, standard UV/visible diagnostics for probing astrophysical environments are redshifted to longer wavelengths in high  $z$  objects. Also, models of chemical

processes involving photons at one wavelength are used to understand environments observed at other wavelengths. Funding should be based on projects considered the most meritorious by peers, as has been done in the past. The highest priority should be given to research most strongly coupled to the needs of NASA missions. Representative examples of laboratory needs coming from the Workshop include the following:

1. far infrared/sub-millimeter spectroscopy of simple hydrides and larger organic molecules; collision cross sections; chemical reaction rates; photoabsorption cross sections; optical constants of solids
2. X-ray and infrared dielectronic recombination, charge exchange, and electron impact ionization data; photoionization cross sections; spectroscopy of solids and ices; surface reactions; particle and radiative bombardment of solids and ices; optical constants of solids
3. UV/visible atomic and molecular spectroscopy, including DIB candidates; oscillator strengths; photoabsorption cross sections; chemical reaction rates; collision cross sections; optical constants of solids

It is important to note that many of the needs cross wavelengths and disciplines: laboratory work on  $N_2$  and hydrocarbons, for example, has proven relevant to the ISM, the atmospheres of Titan and Triton, and the atmosphere of Earth.

**Recommendation 3: Provide higher visibility within astronomical community.** This can be accomplished through the establishment of a Working Group on Laboratory Astrophysics in the AAS. Its Bylaws should include close interaction with IAU Commission 14 on Atomic and Molecular Data. The Working Group can organize sessions at AAS meetings that build upon the success of the recent Topical Session during the Minneapolis Meeting.

**Recommendation 4: Increase support for the NASA Astronomy and Physics Research and Analysis (APRA) program.** The health and vitality of the laboratory astrophysics community depends on continued APRA support. It is important to maintain the core competency of the community and ensure the development of future generations of laboratory astrophysicists. If the current program is cut any further, significant research capabilities will be lost and NASA may not be able to get optimum scientific return from its future, very expensive missions. A viable level of support should be restored for this program.

**Recommendation 5: Mission support of laboratory astrophysics.** Current APRA funding is insufficient to produce all the data needed to ensure successful scientific return from NASA missions. Mission support of laboratory astrophysics through competitively run three year grants would make a significant positive impact on the production of the needed data. Support arising from 1-year grants from observing cycles (e.g., *Chandra* and *Spitzer*) does not address the long-term nature of laboratory work.

**Recommendation 6: Provide adequate funding for databases.** Critically evaluated data are needed by those analyzing astronomical measurements and modeling the

associated environments. True understanding is only possible when collections of the highest quality data on atoms, molecules, and solids are utilized. Here, too, the relevant agencies and departments need to coordinate their efforts. Database compilation and the associated, vital critical compilation, is a skill that is developed over decades in many cases. Long term commitment of funds is essential. In the past, funding of databases and their development was provided as part of the Applied Information System Research Program (AISRP); NASA should consider reestablishing AISRP support for databases. Such a distinction would reduce the conflict reviewers for the ARPA program have in choosing between newly acquired data and compilations of existing data.

**Recommendation 7: Another laboratory astrophysics workshop should take place in 4 years.** Given the fundamental importance of laboratory astrophysics, it is important to monitor the health of the field and to ensure that the laboratory astrophysics community is adequately supporting NASA's space missions. While NASA should continue to be the lead agency, the other agencies and departments (NSF, DOE, DoC/NIST) should be active partners in this workshop.