NASA Laboratory Astrophysics Workshop 2006 Introductory Remarks

Hashima Hasan

Astrophysics Division, NASA Headquarters, Washington DC 20546

hhasan@nasa.gov

1. Introduction

NASA Laboratory Astrophysics Workshop 2006, is the fourth in a series of workshops held at four year intervals, to assess the laboratory needs of NASA's astrophysics missions - past, current and future. Investigators who need laboratory data to interpret their observations from space missions, theorists and modelers, experimentalists who produce the data, and scientists who compile databases have an opportunity to exchange ideas and understand each other's needs and limitations. The multi-wavelength character of these workshops allows cross-fertilization of ideas, raises awareness in the scientific community of the rapid advances in other fields, and the challenges it faces in prioritizing its laboratory needs in a tight budget environment.

Currently, we are in the golden age of Space Astronomy, with three of NASA's Great Observatories, Hubble Space Telescope (HST), Chandra X-Ray Observatory (CXO), and Spitzer Space Telescope (SST), in operation and providing astronomers and opportunity to perform synergistic observations. In addition, the Far Ultraviolet Spectroscopic Explorer (FUSE), XMM-Newton, HETE-2, Galaxy Evolution Explorer (GALEX), INTEGRAL and Wilkinson Microwave Anisotropy Probe (WMAP), are operating in an extended phase, while Swift and Suzaku are in their prime phase of operations. The wealth of data from these missions is stretching the Laboratory Astrophysics program to its limits. Missions in the future, which also need such data include the James Webb Space Telescope (JWST), Space Interferometry Mission (SIM), Constellation-X (Con-X), Herschel, and Planck. The interpretation of spectroscopic data from these missions requires knowledge of atomic and molecular parameters such as transition probabilities, f-values, oscillator strengths, excitation cross sections, collision strengths, which have either to be measured in the laboratory by simulating space plasma and interactions therein, or by theoretical calculations and modeling. Once the laboratory data are obtained, a key step to making them available to the observer is the creation and maintenance of critically compiled databases. Other areas of study, that are important for understanding planet formation, and for detection of molecules that are indicators of life, are also supported by the Laboratory Astrophysics program. Some examples are: studies of ices and dust grains in a space environment; nature and evolution of interstellar carbon-rich dust; and polycyclic aromatic hydrocarbons. In addition, the program provides an opportunity for the investigation of novel ideas, such as simulating radiative shock instabilities in plasmas, in order to understand jets observed in space.

A snapshot of the currently funded program, mission needs, and relevance of laboratory data to interpreting observations, will be obtained at this workshop through invited and contributed talks and poster papers. These will form the basis for discussions in splinter groups. The Science Organization Committee will integrate the results of the discussions into a coherent White Paper, which will provide guidance to NASA in structuring the Laboratory Astrophysics program in subsequent years, and also to the scientific community in submitting research proposals to NASA for funding.

2. NASA's Laboratory Astrophysics Landscape

Proposals for the Laboratory Astrophysics Program are solicited through the Science Mission Directorate's omnibus solicitation, Research Opportunities in Earth and Space Science (ROSES). The program element in ROSES that the Laboratory Astrophysics Program is a sub-element of is the Astronomy and Physics Research and Analysis (APRA) Program. The solicitation is open to all investigators and proposals are competitively selected through a peer review process. A typical investigation is funded for three years, so that approximately one third of the program is reviewed every year. Programmatic balance between different Laboratory Astrophysics research areas is achieved by the Selection Official by reviewing all the selectable proposals, investigations in the second and third year of funding, and aligning them with NASA's strategic priorities.

In Fiscal Year (FY) 2006, 33 investigations were funded for a total of ∼\$3.8M. Of these, 4 could be broadly categorized as infrared investigations, 9 as those supporting interstellar medium (ISM) studies, 5 in the area of submillimeter spectroscopy, 8 in the area of UV/Optical atomic processes, 2 in the area of UV/Optical molecular and dust formation processes, and 5 in the support of X-ray missions. Given below are extracts from the abstracts of the proposals submitted by investigators. Full abstracts can be found through links on the NASA web page for research solicitations, the url for which is http://nspires.nasaprs.com/external/

2.1. Infrared Investigations

Peter Bernath (University of Arizona) is analyzing laboratory spectra of astrophysically-relevant molecules using a Fourier transform spectrometer, FTS. Molecules of interest include hot water and transition metal-containing diatomics. The laboratory spectra of water, CaH, MgH, FeH, TiH, VO, CN and C_2 molecules will be analyzed to provide improved spectroscopic parameters and molecular opacities. This work is required in order to calculate the spectral energy distributions of cool stellar and sub-stellar objects. The next generation of NASA missions in the submillimeter, infrared and near infrared regions will provide spectra of exquisite sensitivity but (generally) moderate resolution. Interpretation of these spectra will require simulations based on data supplied by this investigation.

Benjamin McCall (University of Illinois at Urbana-Champaign) proposes to obtain laboratory spectra of buckminsterfullerene, C_{60}, and its positive ion C_{60}^+ in the gas phase, using continuous-wave cavity ringdown spectroscopy with infrared lasers. The laboratory spectroscopy of C_{60} will directly enable a sensitive search for interstellar and circumstellar C_{60} using TEXES at NASA's IRTF and eventually using EXES on the Stratospheric Observatory for Infrared Astronomy (SOFIA). The laboratory spectroscopy of C_{60}^+ will enable us to test the controversial hypothesis that C_{60}^+ is the carrier of two of the enigmatic Diffuse Interstellar Bands (DIBs) in the near-infrared. Together, this work will enable the first census of the fraction of cosmic carbon that is tied up in the form of fullerenes. Mc Call will also develop an ultrasensitive new technique (SCRIBES: Sensitive, Cooled, Resolved Ion BEam Spectroscopy) that will allow us to record the spectra of molecular ions with a sensitivity approaching the limit of single molecule absorption spectroscopy.

Anne Hofmeister's (Washington University) work is focused on distinguishing grain-size and temperature effects on the infrared fingerprints of astrominerals. Characterizing dust properties will further our understanding of many aspects of astrophysics, since it is an essential part of star formation processes; is key to understanding mass loss from aging stars; and contributes to interstellar processes such as gas heating and the formation of molecules. Improved laboratory data will be obtained, and an analysis performed of available astronomical databases using the new information. The results will be applied against available ISO data and up-coming Spitzer data. One goal is to identify Al_2O_3, which is known to exist in pre-solar grains in meteorites, but the astronomical evidence is equivocal and interpretations are controversial. As the data are published, the information would be disseminated though websites maintained by the participating universities.

Perry Gerakines (University of Alabama at Birmingham) is producing a database of laboratory infrared spectra of ice mixtures containing carbon dioxide. Mixtures representative of solid CO_2 in interstellar icy grain mantles in a wide variety of environments will be studied. These spectra will be used primarily in the analyses of IR data obtained with the Spitzer Space Telescope We will draw upon existing knowledge of interstellar solid CO_2 as obtained in the analyses of data from the Infrared Space Observatory, with which we have extensive experience. Existing databases will be refined to include a more systematic study of ice compositions and effects of ice thermal history. Optical constants, of wide use to the general astronomical community, will be calculated from the IR transmission spectra for use in scattering calculations. Data will be distributed via the Internet to the general community.

2.2. Interstellar Medium Processes

Theodore Snow (University of Colorado) is continuing his program to measure chemical reaction rates involving large molecular ions with astrophysically common reactants. The motivation for this work is two pronged - the identification of diffuse interstellar bands, and the study of reactions that may be relevant to dense interstellar clouds, such as: reactions with anions of polycyclic aromatic hydrocarbons (PAHs), which may be chemically and energetically important in dense clouds. In a parallel collaborative effort chemical models relevant to the reactions and products measured in the laboratory, will be developed. The research will have impact on the interpretation of data from Spitzer, SOFIA, JWST, Herschel and the HST instrument, Cosmic Origins Spectrograph (COS).

Vidali Gianfranco (Syracuse University) plans to investigate the formation of molecular hydrogen in different simulated astrophysical environments. Knowledge of surface science techniques will be applied to obtain information on the mechanisms and efficiency of formation of H_2 in different conditions of composition and morphology of grains. Measurements done in the past will be extended to amorphous silicates of various composition (from Fe- to Mg-rich) and to carbonaceous materials obtained using various methods. The new information obtained will be used in models of H_2 formation in various ISM environments. An understanding of H_2 formation routes and degree of internal excitation following its formation on grains is needed for the analysis of data of H_2 transitions obtained in space-based observations using, for example, ISO, HST, and FUSE. It also impacts analyses of observations of molecules in dense clouds using infrared space observatories (ISO, Spitzer, SOFIA, Herschel).

Gary Ferland (University of Kentucky) is computing rovibrational excitation and dissociation cross sections and rate coefficients for collisions of H, H_2 and He with H_2 and HD for all transitions between all bound rovibrational levels of the target molecules. The results of this proposal will then enable models, such as the very widely used and tested computer code CLOUDY, to reliably simulate astrophysical environments, leading to deeper examination and understanding of their physical properties, such as cooling processes, molecular emission, and nonequilibrium effects in molecular gaseous nebulae and other molecular environments. Thus, it will be possible to extract the maximum scientific return from the significantly improved observations of such environments from NASA's Spitzer Infrared Telescope Facility, and other upcoming infrared astrophysics missions such as SOFIA, the James Webb Space Telescope, Herschel, and Astro-F.

Phillip Stancil (University of Georgia) is performing theoretical investigations of atomic and molecular processes for applications to M, magnetic white, and cool white dwarfs are proposed. In addition, collision processes relevant to the ejecta of Type II supernovae will be computed. The data will be provided to stellar and nebula modelers for testing of the resulting calculations, as existing experimental or theoretical data are lacking in most cases, and for predicting of spectra for comparison to observations. All data will also be made available on the WWW. The results from this work are critical to development of advanced non-thermal and non-chemical equilibrium models which will aid in the analysis of observations from the current and next generations of space- and ground-based telescopes enhancing the scientific return from NASA astrophysics missions.

Swaraj Tayal (Clark Atlanta University) aims to provide accurate extensive radiative and collisional atomic data for astrophysically important ions for analysis and interpretation of spectroscopic observations from the International Ultraviolet Explorer (IUE), HST, Astro-1,2, Extreme Ultraviolet Explorer (EUVE), and FUSE. The UV and visible lines provide powerful diagnostic tools to advance the understanding of the physical and chemical conditions of a variety of astrophysical environments such as atmospheres of stars.

Thomas Gorczyca (Western Michigan University) is focusing his efforts towards obtaining improved simulations of astrophysical plasmas through the computation of new atomic data. Calculations of dielectronic recombination (DR) and fluorescence and Auger yields due to a 1s vacancy, needed for modeling shocked gas in supernova remnants and X-ray photoionized plasmas are being performed. The new atomic data will be disseminated to the astrophysics community via the web page http://homepages.wmich.edu/∼gorczyca/atomicdata and will be used by the authors in the non-equilibrium plasma simulation code CLOUDY to enable more accurate interpretations of ionized emission/absorption line gas. This work will be relevant to the interpretation of spectroscopic data from a range of past, present, and future satellite observatories including IUE, HST, EUVE, ISO, HUT, ORFEUS, Einstein, EXOSAT, ROSAT, ASCA, FUSE, GALEX, Chandra, XMM, JWST, Spitzer, Suzaku, and Constellation-X.

Hantao Ji (Princeton Plasma Physics Laboratory) is performing a laboratory study of Magnetorotational Instability (MRI) in a Gallium disk. The goal is to demonstrate MRI, study its properties, and compare experiments with numerical and analytical modeling. The astrophysical importance of MRI is that it is now believed that it drives accretion in disks ranging from quasars and X-ray binaries to cataclysmic variables and perhaps even protoplanetary disks.

John Laming (Naval Research Laboratory) is studying instabilities of radiative shocks. Shocks will be launched by high power laser irradiation of a target either in a shock tube to study ID instabilities or in a gas cell to study multi D instabilities of blast waves. The results are expected to be of importance to astrophysical fields ranging from stellar wind and interstellar medium shocks, to those occurring in accreting objects such as T Tauri stars, white dwarfs and other compact accretors, as well as core-collapse supernovae.

Mark Bannister (Oak Ridge National Laboratory) is performing a series of laboratory measurements and theoretical calculations of electron-impact ionization (EII) in support of a wide range of past, present, and future NASA flight missions. EII is the dominant ionization mechanism in supernova remnants, galaxies, clusters of galaxies, and stellar atmospheres. These measurements will provide new EII rate coefficients with uncertainties of less than

15%. The new atomic data will be used to benchmark state-of-the-art EII calculations using time-dependent close-coupling, R-matrix with pseudostates, and distorted-wave techniques. Once the theoretical and experimental results converge, calculations will be made for the needed EII rate coefficients for the remaining unmeasured ions in the relevant isoelectronic sequences. These data will be fit with the standard fitting formulae used by the astrophysics community for ionization balance calculation. Results will be widely disseminated.

2.3. Submillimeter/THz Studies

In anticipation of the launch of SOFIA and Herschel, several investigators are producing laboratory data in the submillimeter and THz regime. Eric Herbst's (Ohio State University investigations are aimed at enriching the database of laboratory submillimeter-wave spectra so that assignment and analysis of astronomical spectra in this wavelength region can become more routine. The submillimeter-wave spectra of a wide variety of molecules will be measured and analyzed. Geoffrey Blake (California Institute of Technology) is continuing his laboratory studies to characterize the rotational spectra of key hydrides (especially water, ammonia, and their isotopologues) and the rotation-torsion interactions in complex species known to exist in star-forming cores. Lucy Ziurys (University of Arizona) is assembling a complete database of highly accurate rotational rest frequencies for metal hydride molecules of astrophysical interest. John Pearson (Jet Propulsion Laboratory) is obtaining precise laboratory data on the rotation spectrum of CH^+ and its $^{13}CH^+$ and CD^+ isotopomers. His group will also improve the accuracy of the known transitions of ^{13}CH and CD from approximately 10MHz to 100kHz. Brian Drouin (Jet Propulsion Laboratory) is measuring the state-to-state collision rates and pressure broadening of water with dihydrogen as a function of temperature for the lowest ortho and para rotational transitions of water. This data is central to interpretation of SWAS and Herschel water spectra.

2.4. UV/Optical Atomic Studies

James Lawler (University of Wisconsin, Madison) is developing a Spatial Heterodyne Spectrometer (SHS) in the vacuum ultraviolet (VUV) and using it in the 300 nm to 100 nm wavelength range for the measurement of basic atomic data including atomic transition probabilities, hyperfine structure constants, and isotope shifts of lines from singly and multiply ionized iron group ions. This laboratory project supports VUV astronomy with Hubble Space Telescope and other missions at low red shift, and supports future research with the James Webb Space Telescope at high red shift.

James Babb (Harvard-Smithsonian Center for Astrophysics) is studying the pressure-broadening of alkali atom resonance lines for modeling atmospheres of extrasolar giant planets and white dwarfs.

Steven Federman (University of Toledo) is determining oscillator strengths of ultraviolet atomic and molecular transitions. Laboratory data on lifetimes, branching fractions, and oscillator strengths will be acquired through beam-foil techniques and absorption studies with synchrotron light source; these data will be interpreted using appropriate theoretical tools. Relevant to analysis of data from HST, FUSE, SOFIA, Spitzer, Herschel.

Steven Manson (Georgia State University) is calculating photoabsorption and recombination rates for astrophysically important species over a broad range of wavelengths from the UV/Visible to the X-ray using a variety of state-of-the-art methodologies to augment the existing atomic database in this area. This work will support HST, FUSE, Chandra, XMM, CHIPS and future space missions.

Sultana Nahar (Ohio State University) is computing large-scale radiative data mainly for Fe ions using the state-of-the-art relativistic R-matrix method. The calculations will constitute a multi-wavelength database useful across a wide spectral range and will be made available electronically to the astrophysical community for analysis of observations from a number of space missions ranging from far-infrared to X-ray.

Ara Chutjian (Jet Propulsion Laboratory) is using the JPL Highly Charged Ion Facility to measure absolute electron-impact cross sections (collision strengths) in those highly charged ions that are detected in stars, quasars, planetary nebulae, and the shock-heated ISM. Emphasis includes ions emitting in the EUV through X-ray regions to accommodate the enormous data returns from HST, FUSE, and EUVE; and from the high-resolution X-ray spectrometers aboard Chandra and XMM-Newton. There is a concomitant need for laboratory measurements and benchmarking of the various theoretical calculations in distorted-wave, multistate R-matrix, Breit-Pauli, etc. approximations. The JPL measurements will include ions/charge/states/transitions that are numerators or denominators in electron temperature and density diagnostics of the emitting plasma. Work will continue on excitation cross-sections for the He-like C V, N VI, and O VII X-ray triplets. First measurements anywhere were published by JPL on absolute excitation cross sections for the Fe X coronal red line. Work will continue on absolute measurements on Fe XII - Fe XVI, including the coronal green line in Fe XIV. All measurements are compared to the latest theoretical results in distorted-wave or R-matrix calculations. This work supports the many spacecraft data streams described above, as well as new missions such as Suzaku and Constellation X.

Peter Beiersdorfer (Lawrence Livermore National Laboratory) , in response to observations of stellar coronae by Chandra and XMM in the extreme ultraviolet region, which have found numerous emission lines that are absent from the spectral models, is performing systematic laboratory measurements of the L-shell line emission spectra of the intermediate ionization stages of magnesium (Mg III - Mg X), aluminum (Al IV - Al XI), calcium (Ca XI - Ca XVIII), and nickel (Ni IX - Ni XXVI). These measurements will establish a complete emission line catalogue of these ions in the 25 to 200 Å region under well controlled laboratory conditions and densities comparable to coronal plasmas ($< 10^{12}$ cm^{-3}), providing line identification, wavelengths, and relative line intensities for specific electron temperatures, adding to the catalogue of silicon, sulfur, argon, and iron lines established earlier. The possibility of using specific Mg III, Si V, S VII, Ar IX, and Ca XI lines as diagnostics of the magnetic field strength in the range of about 0.5 to 10 kG, i.e., in a range comparable to that of classical T Tauri stars, will also be addressed in the measurements. The intensity of the relevant spectral lines for a range of magnetic field strengths will be studied in order to firmly establish the diagnostic utility of these spectra for such novel measurements.

Joseph Reader (National Institute of Standards and Technology) will expand and refine the NIST database on atomic transition probabilities, wavelengths, and energy levels, responding to current and anticipated needs of space astronomy. Results of the critical compilations will be made available through the online NIST Atomic Spectra Database and in hardcopy publications.

2.5. UV/Optical Molecular and Dust Studies

Martin Head-Gordon (University of California Berkeley) is developing a theoretical model of the electronic spectroscopy of PAHs that can play an important role in complementing, focusing and guiding laboratory PAH research in two directions. First, this modeling can help to identify general classes of PAH molecules that have particularly distinctive spectral signatures, that can cause them to be particularly promising as carriers of the DIBs. Second, theoretical modeling will help to enable specific identification of molecules that are believed to be isolated in laboratory spectroscopy experiments.

Farid Salama (NASA Ames Research Center) will provide laboratory data that will permit the analysis of astronomical data for the presence of specific complex organic molecules through their unique electronic spectrum in the ultraviolet, visible and NIR range. He will measure the absorption spectra of selected PAH and fullerene ions for the first time in the gas phase thus allowing a conclusive test for the presence of specific species in the interstellar medium. He will also measure in the laboratory the changes induced in samples exposed to space environment on board the international space station to provide a fundamental diagnostic on the evolution of organic matter. The ultimate goal is to conclusively determine whether or not these large carbon-containing molecules and ions contribute to the interstellar extinction curve, including the DIBs see in absorption.

2.6. High Energy Studies

Steven Kahn (Stanford University) is continuing his program of X-ray spectroscopic laboratory astrophysics measurements using the electron beam ion trap (EBIT) facility at the Lawrence Livermore National Laboratory and the X-ray microcalorimeter detector developed at the Goddard Space Flight Center. Scott Porter (GSFC) is using the EBIT/microcalorimeter to measure absolute cross sections for both direct electron impact excitation and dielectronic recombination, identify spectral signatures of plasmas which are not in ionization equilibrium, measure the composite X-ray emission from plasmas at a specified Maxwellian temperature, and measure X-ray emission from low energy charge exchange collisions. The results will be used to both verify and complement atomic data used in spectral modeling packages that are heavily used in the astrophysics community

Bradford Wargelin (Smithsonian Astrophysical Observatory) is using an EBIT to continue his study of X-ray emission from charge exchange (CX) of highly-charged ions with neutral hydrogen and helium. The primary results of the research will be high-resolution emission spectra and state-specific relative cross sections as a function of ion energy and temperature.

Timothy Kallman (Goddard Space Flight Center) aims to calculate the yet unknown atomic quantities needed for modeling and interpreting data for an important class of cosmic X-ray sources: those in which photoionization dominates the ionization and heating of gas. These include inner shell photoionization cross-sections and line parameters, recombination cascade rates and branching ratios, and data for the element, Ni.

Daniel Savin (Columbia University) is continuing his program to measure low temperature dielectric recombination rate coefficients for photoionized cosmic plasmas such as are formed in active galactic nuclei, X-ray binaries, the intergalactic medium, planetary nebulae, and HII regions.

I would like to acknowledge Doug Hudgins' analysis of NASA's Laboratory Astrophysics Program, which I have used in preparing the last section of this paper.