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Abstracts of Contributed Talks

Electron recombination with H-like highly charged ions

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The line-profile approach (LPA) [1] is applied to evaluation of the electron recombination with highly charged ions within the framework of QED. Both dielectronic recombination and radiative recombination processes are considered. The interelectron interaction is taken into account partly to all orders of the QED perturbation theory. The radiative corrections to the lowest order (electron self-energy and the vacuum polarization) are also included. With this approach the most accurate contemporary results for the electron recombination cross section on the one-electron uranium and gadolinium ions are obtained.

We performed QED calculation of the total cross section of the electronic recombination of H-like ions of uranium [2] and gadolinium. The cross section is presented as a function of the energy of incident electron. Due to the dielectronic recombination process the cross section shows resonances corresponding to the doubly excited $(2s,2s),(2s,2p),(2p,2p)$ two-electron configurations. These resonances are investigated in details. The interelectron interaction for the *ns*, *np*, *nd*-electrons (the principal quantum number $n \leq 3$) is taken in all orders of QED perturbation theory. The interelectron interaction for the other electrons (including the negative part of the Dirac spectrum) is considered in the first order of perturbation theory. The dominant part of the radiative corrections (self-energy and vacuum polarization) is also taken into account; the self-energy vertex corrections which are not resonant are missing.

Results of the present calculation for uranium are compared with previous calculations [3,4]. The interelectron interaction is taken into account in the present work more precisely compared to the previous works. Since the LPA is *ab initio* QED approach, the QED effects are considered systematically. The major discrepancy between the calculations reveals itself in the lineshapes of the resonances.

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Atomic Data for Singly and Doubly Ionized Fe-peak Species

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Several of the most important astronomical topics today that involve UV and optical astronomical spectroscopy require detailed understanding of singly and doubly ionized iron-peak species (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu). Yet, our present knowledge of the atomic physics and spectra is lagging behind the avalanche of high quality spectra arising from these ions.

We are carrying out a systematic study of each of these species aiming to provide complete spectral models containing radiative rates and collision strengths. The present atomic computations employed a combination of state of the art atomic physics methods, e.g. relativistic Hartree-Fock, the Thomas-Fermi-Dirac potential, and Dirac-Fock computation of A-values and R-matrix with intermediate coupling frame transformation and Dirac R-matrix. We study the advantages and shortcomings of each method.

The obtained spectral data is then benchmarked against observed astronomical spectra. It has been found that the Dirac R-matrix collision strengths yield excellent agreement with observations. By contrast, LS-coupling R-matrix results fail to yield accurate effective collision strengths at around 10^4 K, despite using very large configuration expansions, because of the limited treatment of spin-orbit effects in the near threshold resonances of the collision strengths. The present models are in very good agreement with observed emission spectra, in contrast with previous models. The present work demonstrates that accurate atomic data for low ionization iron-peak species is now within reach.

Infrared atomic oscillator strengths for the study of ultracool dwarf stars, brown dwarfs and exoplanets

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The opacity of ultracool dwarf stars, brown dwarfs and exoplanets peaks in the IR and is characterized by molecular bands, with atomic spectral lines observed in the relatively molecular-free windows. These sub-solar objects (SSOs) are of great interest to the study of galactic dynamics (How much mass is stored in faint SSOs?), star formation (Is there a lower mass limit below which no "stars" form?) and exoplanets (What distinguishes an exoplanet from a brown dwarf?). By determining their fundamental properties, such as effective temperature (T_{eff}), metallicity, and surface gravity, the key differentiating parameters of SSOs can be derived, and their position and status within the HR diagram of luminosity vs. temperature determined. However, the opacity of these objects is dominated by molecular spectra, which are exceedingly difficult to model to the accuracy required to determine SSO spectral classification. Instead, one can use atomic transitions observed in the relatively molecular-free windows. These transitions are comparatively unblended and lie at the peak energy distribution of cool SSOs ($T_{eff} < 2000$K). In addition, the IR atomic lines are easier to observe than lines of the same atoms in the visible where cool SSOs have less flux. Furthermore, the possibility of measuring atomic transitions in Jupiter sized exoplanets has recently been demonstrated by the observation of neutral sodium in the transiting 'hot Jupiters' HD 189733b and HD 209458b [1, 2].

We discuss our recent measurements of oscillator strengths in the IR for neutral species [3]. In particular, we show how Mn I transitions can be used to determine SSO properties even when the atomic transitions are blended with molecular features. In addition, we discuss the relevance of atomic data to the study of ultracool dwarf stars, brown dwarfs and hot Jupiters.

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Polarization of the Lyman-α_1 x-ray line emitted by hydrogen-like Ti^{21+}, Ar^{17+} and Fe^{25+} ions excited by electron impact.

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Using the relativistic convergent close-coupling method we have calculated the polarization of the Lyman-α_1 x-ray line emitted by hydrogen-like Ti^{21+}, Ar^{17+} and Fe^{25+} ions excited by electron impact. We find that account of Breit relativistic corrections is important to resolve the discrepancy between experiment and theoretical calculations.

The RCCC method involves solving a set of relativistic partial wave Lippmann-Schwinger equations for the T-matrix

$$T_{fi}^{\Pi J}(k_f\kappa_f, k_i\kappa_i) \;=\; V_{fi}^{\Pi J}(k_f\kappa_f, k_i\kappa_i) + \sum_n \sum_\kappa \int\!\!\!\!\!\!\diagup\!\!\!\!\!\!\int k^2 dk \frac{V_{fn}^{\Pi J}(k_f\kappa_f, k\kappa) T_{ni}^{\Pi J}(k\kappa, k_i\kappa_i)}{E - \epsilon_n^N - \epsilon_{k'} + i0}, \tag{1}$$

with the notation as specified in [1].

Magnetic sublevel excitation cross sections of the $2p_{3/2}$ state from the ground $1s_{1/2}$ state are required to determine the polarization of the $2p_{3/2} \rightarrow 1s_{1/2}$ line. These cross sections are related to the polarization by the following expression

$$P = \frac{3(\sigma_{1/2} - \sigma_{3/2})}{3\sigma_{3/2} + 5\sigma_{1/2}}, \tag{2}$$

where σ_{m_f} is the cross section for excitation to a magnetic sublevel.

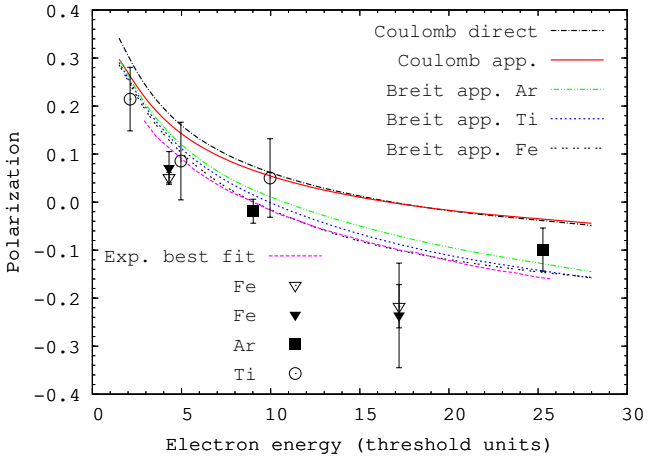

FIG. 1: Polarization of Lyman-α_1 emission line of Ar^{17+},Ti^{21+}, and Fe^{25+}. Present calculations are compared with experimental data of Nakamura et al. [2] and Robbins et al. [3]. Presented Coulomb potential calculations are for Ti^{21+} ion (results for Ar^{17+} and Fe^{25+} ions are practically the same). The two sets of experimental results for Fe^{25+} pertain to the two experiments outlined in Robbins et al. [3].

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Analysis of Nickel and Low–Z Impurity EUV and SXR Radiation from NSTX and Comparison with Laser Plasma Spectra*

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Spectroscopic emission measurements of medium- and low-Z impurity ions, which are always present in MCF plasmas produced by tokamaks, help to survey, understand and minimize the effect of impurities on plasma performance. Recent improvement of the EUV diagnostics on NSTX has provided new higher resolution spectra from the L-shell emission of nickel, iron, copper, and argon [1]. Such spectra, rich in both medium Z and low-Z impurity lines, require a detailed modeling of various elements.

This work mainly focuses on studying Ni EUV spectra. An element of astrophysical significance, nickel is also one of the important plasma impurities. Here we analyze the nickel EUV spectra recorded at the NSTX tokamak (typically Ni X-XIII) and the compact laser plasma facility ”Sparky” at UNR using a non-LTE Ni model, newly updated with more ion configurations to better identify the EUV spectral lines and estimate plasma parameters. The model is based on FAC atomic data which were compared with HULLAC data. Iron emission lines (Fe VIII-X) in the spectra have been also considered.

Additionally, a collection of low-Z EUV spectra from recent experiments at NSTX and compact laser plasma facility “Sparky” at UNR were modeled, compared and analyzed. This work utilized new non-LTE kinetic models of Li, Be, and B, as well as C and O models which have been updated with more high-Rydberg states. These spectra help benchmark spectroscopic models and better identify impurity spectra and plasma conditions.

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The derivation of kinetic equations for anisotropic plasmas from the impact approximation

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Historically, the theoretical foundation for modeling anisotropic plasmas proceeded along two different lines. On the one hand, Fujimoto and coworkers [1] considered cylindrically symmetric plasmas and developed the population-alignment radiative-collisional (PARC) model. The PARC model was derived using semi-classical collision physics within the framework of the impact approximation. This model is based on the theory of multipole relaxation kinetics in gases where heavy-particle collisions played the most important role. On the other hand, Dubau, Inal and coworkers [2, 3] introduced on intuitive grounds the magnetic sublevel to magnetic sublevel rate equation scheme. The formal structures of the two schemes were related to each other by Dubau [2]. The purpose of the present work is to derive both theories on a fully quantum mechanical basis from the wide-frequency-range, impact approximation as formulated by Ben-Reuven [4], which is based on the general binary collision theory for the relaxation matrix by Fano [5]. This derivation opens the opportunity to improve the above schemes by the incorporation of memory-effects, finite density effects, and coherency effects.

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Spectral analysis of polarized light from the motional Stark effect in a high-temperature plasma*

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A diagnostic based on the motional Stark effect (MSE) provides internal magnetic field measurements in magnetically-confined plasmas. A high-energy beam of neutral hydrogen atoms is injected into the plasma, with a component of the atom velocity perpendicular to the magnetic field. The atoms experience a Lorentz electric field and emit Stark-split line spectra that are recorded and analyzed. Magnetic fields in the Madison Symmetric Torus (MST) reversed-field pinch plasma are small relative to other fusion research devices, so the components of the Stark spectrum are not widely separated. Thus the conventional MSE diagnostic technique that relies on photoelectric modulator polarimetry to infer the direction of the polarization of the Stark components is not feasible on MST. Instead, the entire Stark spectrum is recorded and analyzed using a newly refined atomic emission model. A new analysis scheme has been developed to infer both the polarization direction and the magnitude of Stark splitting, from which both the direction and magnitude of the local magnetic field can be derived. Improved modeling of the relative magnitudes and positions of the Stark multiplets is underway using the Atomic Data and Analysis Structure (ADAS). This improvement is expected to reduce the systematic uncertainty of the measured magnetic field.

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Relativistic distorted-wave and Dirac *R*-matrix calculations of the x-ray line polarization of the 3*C* and 3*D* lines in Fe XVII

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Access to accurately calculated polarization data is crucial in the interpretation and analysis of certain electron-beam ion trap (EBIT) experiments. We have recently performed a detailed study of the magnetic sublevel, electron-impact excitation cross sections (or collision strengths) and resulting line polarizations of the $3C$ and $3D$ transitions in Fe XVII. These lines are of particular interest in providing x-ray diagnostics for a variety of astrophysical plasmas [1]. This study employed both the relativistic distorted wave (RDW) [2] and Dirac R-matrix (DARC) [3, 4] methods, which were used to calculate magnetic sublevel collision data and polarizations for an assortment of atomic models of varying complexity. Our comparisons display very good agreement between the RDW and background DARC results for both the collision strengths and polarizations. Furthermore, the background contribution of the polarization is found to be relatively insensitive to the details of the atomic models that were investigated.

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Polarization properties of the Ly-alpha line from sulphur and nickel plasmas driven by high-intensity, ultrashort-duration laser pulses

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We report on an experimental and theoretical investigation of the polarization properties of the Ly-alpha line in sulphur and nickel. In separate experiments, the Vulcan petawatt laser of the Rutherford Appleton Laboratory was used to irradiate S and Ni targets. The intensity on target for both the Ni and the S shots was 5×10^{20} W/cm^2 assuming that the laser beam contains approximately 30 % of the energy in the FWHM. The resulting Ly-alpha line emission was processed by two HOPG crystals and two image plates, set to simultaneously record the two orthogonal states of linear polarization of the Ly-alpha spectral lines. The lower-energy (J=1/2) component was used as an unpolarized reference check on the calibration of the two instruments. The higher-energy component (J=3/2) was observed to be partially polarized, which is a signature of an anisotropic electron distribution. We interpret the experimental data with the help of a magnetic-sublevel population atomic kinetics model that allows us to connect the observed polarization properties of the Ly-alpha with the characteristics of the electron distribution consisting of a beam of energetic electrons and a colder return current.

Configuration Interaction in Statistically Complete Hybrid-Structure Atomic Models

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Spectroscopic accuracy and statistical completeness are equally important elements of the collisional-radiative atomic models widely used for astrophysical applications and laboratory plasma diagnostics. However, it is difficult to include both elements in models of complex, multi-electron ions: while spectroscopic accuracy requires fine structure calculations that can access configuration interaction and metastable-level effects, statistically complete models at that level of detail are computationally intractable. Hybrid-structure atomic models [1] in which configuration interaction effects are extended from a subset of fine structure states to configurations and superconfigurations [2] offer one way to simultaneously meet the demands of model accuracy and completeness. Details of extending configuration interaction effects in this way will be presented along with sample calculations of emission spectra from M-shell tungsten and L-shell iron.

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Oscillator strength measurements of atomic absorption lines from stellar spectra

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We develop a new method to determine oscillator strength values of atomic absorption lines with state-of-the-art detailed spectral synthesis calculations of the optical spectrum of the Sun and of standard spectral reference stars. We update the log(gf)-values of 1014 neutral lines observed in the disk-integrated KPNO-FTS spectrum of the Sun and high-resolution echelle spectra (R=80,000) of Procyon (F5 IV-V) and Eps Eri (K2 V) observed with large S/N ratios of ∼1,500 using the new Mercator-HERMES spectrograph at La Palma Observatory, Spain.

We find for 531 Fe I lines and 65 Si I lines in the sample a systematic over-estimation of the literature log(gf)-values with central line depths below 15 %. We employ a curve-of-growth analysis technique to test the accuracy of the new oscillator strength values and compare calculated equivalent line widths to the Moore, Minnaert, & Houtgast atlas of the Sun.

The online SpectroWeb database displays the observed and synthetic spectra interactively and provides the new log(gf)-values together with important atomic line data. The graphical database is under development for stellar spectra of all spectral subtypes observed with large dispersion and S/N ratios.

3D model atmospheres and needs for accurate atomic data

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The determination of chemical abundances in stars hinges on the availability of accurate atomic data, as well as an accurate description of their atmospheric structure. 3D hydrodynamical model atmospheres are developing into a standard tool in astrophysics for deriving high-fidelity chemical abundances in cool stars where gas-dynamical effects influence the thermal and kinematic properties of the atmospheres. We discuss our experiences when working on abundance analyses of the Sun and metal-poor stars, and identify cases where the achievable accuracy is limited by the quality of the available atomic data. Our wish-list for improved data spans the range of rather basic information - namely whether particular spectral lines are present in a wavelength range - to accurate wavelengths, oscillator strengths, and collisional cross-sections.

Kinetics of parabolic states of hydrogen beam in fusion plasmas

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We present simulation results for populations of the excited states of hydrogen beam in fusion plasmas [1]. The calculations were performed with the collisional-radiative model NOMAD [2] extended to include the parabolic Stark *nkm* states up to n=10 where n is the principal quantum number. The goal of this work is a self-consistent description of the motional Stark effect, beam–emission spectroscopy, relative populations of magnetic sublevels and beam-attenuation processes.

Calculation of the cross sections between the *nkm* states is based on (i) atomic-orbit-close-coupling method (AOCC) in the parabolic basis for excitations from the hydrogen ground state to the first excited states ($n\leq3$) and (ii) unrestricted Glauber approximation for the collisions involving all other transitions. For the first time the ionization from the m-resolved excited states induced by electric field was included in simulations.

The simulation results are compared with the experimental data from JET [3, 4]. A good agreement is found for the ratio of intensities of Balmer-α components. Our results demonstrate strong deviations from statistical population distributions in the whole range of operation of present fusion devices, including ITER plasmas. This also results in the reduction of total beam emission at intermediate densities. Finally, it is shown that the ionization by electric field reduces the H_α emission for the heating beam for ITER at the level of about 30%.

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SPECTROSCOPIC ANALYSIS OF M-SHELL TUNGSTEN BENCHMARKED WITH LLNL EBIT DATA AND COMPARED WITH Z-PINCH PLASMA EXPERIMENTS*

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Two different sets of experiments featuring tungsten x-ray spectral data are presented and analyzed. The first of these data sets was taken on an electron beam ion trap (EBIT) at Lawrence Livermore National Laboratories (LLNL) at varying electron beam energies between 2.5 and 3.9 keV. Emphasis is given to understanding the change of ionization balance between experiments with different electron beam energies and its usefulness in identifying spectral features. Non-LTE kinetic modeling with HULLAC atomic data was used in the analysis. In particular, 3-4 and 3-5 transitions in Ni-, Zn-, Cu-, Ga-, and Ge-like W ions were modeled independently and then the ionization balance was derived.

In addition, tungsten x-ray spectra were also studied in high-energy-density plasma conditions on Zebra, the 1.6 MA pulse power generator at the University of Nevada, Reno. The above-mentioned LLNL EBIT data and modeling was employed to identify various tungsten spectral features and to estimate ionization balance, with particular focus on planar tungsten arrays.

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Dielectronic recombination and satellite line spectra of highly-charged tungsten ions

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We present our recent progress on theoretical studies that involve autoionizing states of tungsten ions. Such autoionizing states have two channels for decay that leads to a necessity of calculation of both radiative and autoionization atomic data and the detailed study of the dielectronic recombination (DR) process, which is an important atomic process in laboratory and astrophysical plasma. The inclusion of such a process in spectroscopic magnetic fusion plasma diagnostics is very essential for correct identification of the lines in impurity spectra and for understanding the main contributors to the total radiation losses. In particular, tungsten will become near Ne-like in the core of the plasma produced by ITER, which allows the use of L-shell tungsten spectra as a core diagnostic. Na-like dielectronic satellites of Ne-like tungsten will thus likely play an important role in the L-shell x-ray diagnostic of future magnetic fusion plasmas. Three atomic codes are used to produce relativistic atomic data (energy levels, radiative transition probabilities, and autoionization rates). These are the relativistic many-body perturbation theory (RMBPT) code, the Multiconfiguration relativistic Hebrew University Lawrence Atomic Code (HULLAC), and the Hartree-Fock-Relativistic (Cowan) code. Branching ratios relative to the first threshold and intensity factors are calculated for satellite lines, and dielectronic recombination (DR) rate coefficients are determined for the excited states. The total DR rate coefficient is derived as a function of electron temperature, and it is shown that the contribution of the highly-excited states is very important for the calculation of the total DR rates. Synthetic dielectronic satellite spectra are constructed, and the atomic properties specific to the relevant tungsten ions are highlighted.

In particular, first we will consider the results for Na-like tungsten (W^{63+}) and Mg-like tungsten (W^{62+}) using all three codes. Then, we move to even higher ionization states and present the results for lithiumlike ions with nuclear charges ranging from Z = 6 to 100, with emphasize on Li-like W (W^{71+}). These calculations were performed using RMBPT and trends of relative intensity factors as functions of nuclear charge Z will be shown graphically and discussed.

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Polarization and Anisotropic Emission of K-shell Radiation from Heavy Few Electron Ions

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Polarization of atomic radiation is indicative of a preferred direction in the radiation production process. This can occur in active galactic nuclei, high temperature plasmas or in accelerator based atomic physics experiments such as electron beam ion traps and heavy ion storage rings. Of fundamental interest is the polarization from K-shell transitions of one and two electron systems due to the simplicity of their theoretical treatment. Recent developments in both experiment and theory have confirmed the need to include relativistic and quantum electrodynamical effects into the excitation/de-excitation process that creates polarized emission of hydrogenlike transitions for low-Z elements such as argon and iron [1], [2], as well as interference effects between the E1 and M2 de-excitation channels in high-Z ions [3]. By extending the measurements to higher-Z where relativity and QED produce comparatively larger effects will allow for more precise measurements of their effects to be performed.

Here we will present and review a variety of polarization and angular emission pattern measurements performed in the experimental storage ring facility at GSI-Darmstadt. These measurements have investigated both the polarization and angular distribution of emitted radiation from the radiative electron capture process and of Coulombic excitation in hydrogenlike and heliumlike heavy ions, utilizing a novel Si(Li) polarimeter, and multiple single crystal germanium detectors arraigned at various angles. Measurements of the degree of linear polarization as well as the alignment (or the degree of non-statistical population of the magnetic sublevels) of the excited states are compared with theory.

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The Universal Atomic Database

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There are a growing number of databases for atomic physics data which tend to fall into two categories: those developed by data producers and those by modelers who use the data. In the former case, the databases are limited to housing just the data produced by the group and in the format that the group prefers. In the latter case, the amount of atomic data is often extensize, but the data is prone to reformatting or other modifications to suit the modeler's needs. Also, the quality of the data included is dependent on the knowledge and time available to the modeler. In both categories, only a single set of data exists for any process, so there is no easy way of listing competing data sets in one place. A new database for atomic processes, the Universal Atomic Database (uaDB), has been developed to remedy these faults and is housed at NASA's HEASARC web page. First and foremost, data inserted into the database is not modified in any way from the source publication. This requires the database to be able to support the same type of data in multiple formats and units. Furthermore, the data and its authors are directly connected in the database, in fact you can click a link taking you to the NASA ADS page of the source reference. This also allows competing data sets to be stored and compared. While the data currently in the uaDB is primary used for astrophysical purposes, no data will be excluded a priori. In my talk, I will give more details about the capability of the database and give a demonstration on how data is searched for and retrieved.