Workshop on Astrophysical Opacities

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Book of Abstracts

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On the importance of atomic data and opacities in evaluating the effects of atomic diffusion in stars

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Atomic diffusion processes may significantly change the distribution of chemical elements inside the stars. Being slow, these processes gain importance in zones where the mixing processes are very weak or absent, i.e. in the radiative zones. However, the modified abundances in these stable zones may contaminate zones where mixing occurs. In some cases, the internal structure of the star can be affected, mainly through the local opacity changes which depend on the local chemical composition. One of the main ingredients in evaluating diffusion velocities in stars is the radiative acceleration which accounts for the momentum transfer from the photon flux to atoms. Radiative accelerations are closely dependent on atomic properties of each species entering the mixture composing the local plasma, and so, their calculations are closely related to the available atomic data and opacity tables. I will give an overview of the various methods used to compute radiative accelerations and I will show some examples of the crucial roles of large atomic and opacity data banks for their calculations.

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Experimental methods for stellar interior opacity measurements at the Z facility

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Laboratory opacity experiments have been developed at the Sandia Z facility over the last fifteen years. Model predictions for iron opacity are notably different from measurements performed at conditions similar to the boundary between the solar radiation and convection zone [J.E. Bailey et al., Nature 517, 56 (2015)]. In this presentation we describe the experimental methods, some of the tests performed to assess the reliability and accuracy, and possible directions for future research.
++ Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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What helioseismology has taught us about opacities and EOS

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Helioseismology has allowed us to determine the structure and dynamics of the Sun to an unprecedented accuracy and precision. This allows us to test different solar models against the Sun to determine which model is good. By comparing models constructed with different physics, we can determine which physics inputs work better, and thus use the Sun as a laboratory to test the physics of stellar material. In this talk I shall describe what we have learned about stellar opacities and the equation of state using helioseismic data.

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Molecular line lists and absorption cross sections based on laboratory measurements

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Molecular opacities are based on line lists for small molecules and absorption cross sections for larger molecules. In this talk research results from our laboratory will be surveyed on the preparation of line lists for diatomic molecules such as CN, NH, OH, OH^+, C_2, etc. using experimental measurements with a Fourier transform spectrometer for line positions and ab initio dipole moment functions for line intensities. Our measured line lists for high temperatures for small polyatomic molecules such as methane and ammonia will also be presented as well as measurements of infrared absorption cross sections for small hydrocarbons such as ethane and propane.

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An overview of molecular opacities

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The atmospheres of cool astronomical objects are full of molecules. The spectra of cool stars, brown dwarfs, planets and exoplanets are dominated by molecular bands and the classification of these objects depends largely on molecular features. Compared to atoms, molecules have many more lines because of vibrational and rotational degrees of freedom, which lead to complex spectra from the microwave to the ultraviolet. For small molecules opacities are based on line lists, while for large molecules absorption cross sections are needed. This talk will survey the experimental and computational approaches to the preparation of line lists and cross sections, illustrated by applications to selected astrophysical problems.

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Radiative association of $^{36}Ar^+$ and $^{38}Ar^+$ with hydrogen

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In a recent paper [Barlow *et al.*, Science **342,** 1343 (2013)], the ArH^+ ionic system has been detected in the Crab Nebula. We accordingly propose to examine in this work the radiative association of the argon ions $^{36}Ar^+$ and $^{38}Ar^+$ with atomic hydrogen and calculate the related temperature-dependent rate coefficients. To do so, we have to construct the transition dipole moments and the potential-energy curves via which both Ar^+ and H species approach each other. The corresponding data points are borrowed from the most recent and reliable calculations of Stolyarov and Child [PCCP **7,** 2259 (2005)]. Once the curves are constructed, the rate coefficients are computed quantum mechanically and analyzed in the temperature range $1 - 10000$ K.

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Temperature-dependent mobility coefficients of ground and excited N^+ ions moving in cold helium plasma

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The atmospheric chemistry revealed the importance of the ionic nitrogen in the ionosphere. This is why, over the last few decades, the diffusion and mobility phenomena of this ion have been widely investigated experimentally at different temperatures. More recent experiments of ionic open-shell systems, such as C^+ and N^+ ions, evolving in very weakly ionized plasmas have been performed at Tokyo Metropolitan University with flow-drift tubes. In particular, the mobility measurements of ground and metastable-excited nitrogen ions N^+ diffusing in neutral helium could not be explained theoretically at very low temperatures. The present work suggests improving the above calculations by using a more elaborate gas mobility model for solving the Boltzmann equation, namely, the three-temperature theory, in which full quantal momentum-transfer cross sections are introduced. Indeed, employing the two-temperature theory, most of the previous theoretical works determined, with classical transport cross sections, the reduced mobility coefficients K_0 of N^+ ions in terms of the ratio E/N of the electric field strength to He gas number density, although the classical approach should cease to be valid at very low temperatures. To determine the quantum-mechanical cross sections, we first computed with MOLPRO the corresponding NHe^+ interaction potentials that dissociate into the ground $N^+(^3P)$+He and metastable $N^+(^1D)$+He asymptotes. The generated potential-energy curves are smoothly connected to specific long- and short-range forms. Higher multipole expansions may be added as temperature goes to 0. Moreover, the accuracy of the obtained potential curves is verified by looking at their spectroscopic parameters, as the well depths and their minimum positions. Once the NHe^+ potentials are known, they are used to solve the radial wave equation and, thus, obtain the energy-dependent phase shifts. These phases should therefore allow the computation of the individual full quantum-mechanical cross sections effective in diffusion.
The next step is devoted to the mobility calculations with the average transport cross sections among the triplet states for N^+ (^3P) ions and among the singlet states for $N^+(^1D)$ ions, both moving in cooled He. To achieve this purpose, we have utilized the Fortran code GC.F of Viehland based on the Gram-Charlier series. The calculations could yield, in particular, the zero-field reduced transport mobility K_0, which may be considered as a probe for the quality of the NHe^+ internuclear potentials. The present work produced the value 18.2 $cm^2V^{-1}s^{-1}$. This value is comparable to 20.0 ± 1.2 of McFarlan *et al.*, 20.0 of Fhadil *et al.*, 17.1 of Sanderson *et al.*, and 17.3 of Tanuma *et al.* Finally, the computations show the obtained first-set data of the mobility results compare quite well with values from literature.

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The role of opacity in calculating the structure and evolution of protoplanetary disks

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Stars are born surrounded by protoplanetary disks, formed as rotating molecular cloud cores collapse conserving angular momentum. The makeup of these disks is originally similar to the ISM, namely, around 99% gas and 1% solid grains, “dust”. These proportions change with time with most of the gas ending in the stars and planets or being photoevaporated, and solids remaining in rocky planets and smaller bodies or in cores of giant planets. Understanding the details of this evolution is at the forefront of current research. At the same time, the advent of high spatial resolution instruments has provided astonishing images of substructures in protoplanetary disks, giving further clues to disk evolution. A key parameter affecting evolution – determining the development of instabilities, the location of condensation fronts of volatiles and refractory materials, the chemical structure, the drift of material towards the star or leaving the disk –

is the disk temperature. Disks are heated mostly by absorption of radiation fields from the central engine: the photosphere and the X-rays and UV radiation due to magnetic activity on the stellar surface, plus the high-energy fields resulting from the accretion shock formed as the stellar magnetic field brings disk material onto the star. The ability of disk matter to absorb these radiation fields – its opacity – is therefore a crucial factor determining disk structure and evolution. I will review the current understanding of disk opacities and how they are used in disk modeling. These include both gas – molecular and atomic – and dust opacities, from the X-rays to the far-IR. Directly related to this is the equation of state appropriate to disks because the dust and gas phases are linked. For instance, molecular hydrogen, the dominant component of the disk, forms on grain surfaces so formation rates are dependent on grain mass abundance and size distribution. Condensation fronts of different species may induce the formation of pressure traps conducive to planet formation; the location of those fronts depends on the density-temperature structure of disks as well as on the exposure to desorbing radiation fields. I will describe these and other effects, as well as refer to the databases of molecular and dust opacities most frequently adopted in current efforts.

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Measuring iron spectral opacities in solar conditions using a double ablation front scheme*

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It has been known for practically two decades that facilities like OMEGA should be well adapted to study the stellar plasma physics. Experiments on various laser facilities (LULI2000, OMEGA, ORION) and on pulsed-power devices (Z pinches at the Sandia laboratory and Imperial College) have put in evidence the astrophysical problems to solve, the challenges ahead and the different techniques to be developed to produce reliable benchmarks [1,2]. A novel technique for opacity measurements in solar conditions is investigated. It is developed in the context of iron opacity measurements near solar interior temperatures and densities, a problem that has recently highlighted discrepancies between theory and observations [3]. This new scheme takes advantage of the stability of thermodynamic parameters induced by Double Ablation Front structures [4], obtained by the interaction of an intense laser pulse with a medium-Z target.
We propose an experimental design based on the current laser and diagnostics capabilities of the OMEGA laser system in Rochester. Extensive simulations suggest the capability to bring an iron sample to an electronic temperature of 170 eV and electron density of 1.5e23 /cm3 during more than 500 ps. The scheme is specially designed to minimize the longitudinal and lateral density and temperature gradients in the sample down to 5% of the on-axis values, in a plasma volume of 300 microns in diameter. Maintaining homogeneous plasma parameters during such a long timescale compared to typical hydrodynamic times ensures Local Thermal Equilibrium in the sample, allowing for a reliable spectral opacity measurement. We further assess the robustness of the technique with respect to hydrodynamic perturbations (from laser imprint or target surface roughness) and to hot electrons (from the non-linear laser-plasma interaction).
This experimental platform was first checked on OMEGA during a shot-day on October 2016. The target was designed with tracer layers of selenium and aluminum to infer the thermodynamic parameters of the target near the sample of interest. While spectral features of the selenium tracer were identified in the experiment, an unexpectedly large quantity of high-energy X-rays produced by the backlighter source produced significant noise in the spectrometer and prevented any opacity measurements. We present results from a follow-up experiment on OMEGA conducted in July 2017.
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[3] J.E. Bailey et al., Nature 517, 56 (2015)
[4] V. Drean et al., Physics of Plasmas, 17, 122701 (2010)
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Los Alamos opacity data for astrophysical applications

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A new set of Los Alamos OPLIB opacity tables for the elements hydrogen through zinc have recently been released [1] and are available online [2]. Our tables have been computed using the Los Alamos ATOMIC code [3,4], which make use of atomic structure calculations from the Los Alamos suite of atomic physics codes [5] that include fine-structure detail for all the elements considered. The equation-of-state model used in our opacity table calculations, known as ChemEOS [6,7], is based on the minimization of free energy in a chemical picture. Recent publications by us [1,8] have compared our calculations to available experimental opacity data and to other opacity calculations. Our tables have also been used in some recent stellar modeling calculations [9,10]. This poster presentation will give an overview of our opacity calculations and provide some examples of comparisons to other work and of selected stellar modeling applications.
The Los Alamos National Laboratory is operated by Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under Contract No. DE-AC5206NA25396.
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Opacity enhancement due to diffusion-induced element accumulation inside B-type stars

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A number of Main Sequence B-type stars, like ν Eri, κ Cen, a Car, κ Vel, present oscillations which may be accounted for by opacity mechanisms, provided that the stellar opacity be larger than the standard computed one, at least in some specific layers. This has been studied by several authors, who computed "ad hoc" opacity profiles able to reproduce the observations. Here we show that atomic diffusion, which causes the elements to move selectively inside stars under the main effects of gravity and radiative accelerations, may be the reason for these opacities enhancements. The radiative accelerations on specific elements are the result of the photon absorption, which depend on the ionisation stage. For this reason, the elements accumulate in layers close to the region where they are the most important contributors to the global opacity. This increases the opacity at the right place in a natural way. We present preliminary results obtained for a 9.5 $M_{\odot}$ model.

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Hydrodynamical instabilities induced by atomic diffusion in F and A stars

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Atomic diffusion, including the effect of radiative accelerations on individual elements, leads to important variations of the chemical composition inside the stars. The accumulation in specific layers of the elements, which are the main contributors of the local opacity, leads to hydrodynamical instabilities that modify the internal stellar structure and surface abundances. In this talk we show that the modification of the initial chemical composition by atomic diffusion has important effects on the internal stellar mixing and leads to different surface abundances of the elements. This leads locally to an increse of the Rosseland opacity by a factor three in some cases. These processes could no longer be neglected in stellar evolution models as the observations are more and more precise. Especialy with the future space missions as Tess and Plato.

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A quantitative comparison of opacities calculated using the distorted-wave and R-Matrix methods

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The present debate on the reliability of the opacities for astrophysics, ignited initially by the solar convection zone problem, has reached the present climax with the new measurement of the Fe opacities on the Z-machine at the Sandia National Laboratory (Bailey et al. 2015). In order to understand the differences between all the theoretical results, on the one side, and experiments on the other as well as the differences between the different theoretical results, very detailed comparisons are needed. Many ingredients enter the calculation of opacities. Deconstructing

the whole process and comparing the differences at each step should quantify the importance and impact of each of them on the final results. We present here such a comparison using the two main approaches to calculate the initial atomic data (R-matrix vs DW approaches) and quantify the effect on the populations, line broadening and extrapolation for Fe XVII and Ni XIV opacities.

Bailey, J.E. et al., 2015, Nature 517, 56-59

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Effects of the plasma environment on the atomic structure and K-lines of oxygen ions

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The observed widths and shifts of X-ray emission K-lines from accreting black holes imply that they are formed in a region very close to the compact object [1]. The intensity of these lines can give some insight into the effects of special and general relativity in the emitting region as well as information about some properties of the compact object itself. Magnetohydrodynamics simulations of accreting black holes computed by Schnittman *et al.* [2] reveal that the plasma conditions in such an environment should be characterized by an electronic temperature ranging from 10^5 to 10^7 K and an electronic density ranging from 10^{18} and 10^{21} cm^{-3}. Such physical conditions may affect the atomic structure and processes corresponding to the ionic species present in the plasma.

The main goal of the present work is to estimate the effects of plasma environment on the atomic parameters associated with the K-vacancy states in cosmologically abundant elements as oxygen ions within the astrophysical context of accretion disks around black holes. In this purpose, multiconfiguration Dirac-Fock computations have been carried out for these ions by considering a time averaged Debye-Hückel potential for both the electron-nucleus and electron-electron interactions in order to model the plasma environment, using a combination of the GRASP92 [3] and of the RATIP [4] codes.

A new set of results related to the plasma environment effects on ionization potentials, transition energies and radiative emission rates is reported for all the ionization stages of oxygen, from O I to O VII. The variations due to the plasma environment effects which have been computed for these parameters, relatively to the isolated ion, are in very good agreement with those obtained by another independent computational approach, namely the Breit-Pauli relativistic approximation as implemented in the AUTOSTRUCTURE code [5,6]. Our results predict that the ionization potentials are lowered by several eV and that the transition wavelengths are slightly redshifted, whereas no significant variation have been observed for the radiative rates.

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Rayleigh scattering as an opacity source in stellar atmospheres

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There are many different opacity sources in the stellar atmospheres. Because of limited computational time and memory the less important opacity sources are usually neglected in stellar atmosphere models. Rayleigh scattering is one of such opacities that are frequently neglected in model atmospheres. But this neglect could not be valid for every case. We study influence of the Rayleigh scattering by hydrogen, helium, and selected metals on computed stellar atmospheres of hot stars with solar chemical composition and some types of CP stars

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The problem of the high iron abundance in accretion disks around black holes

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In most accreting black hole systems copious X-rays are emitted from the inner-most regions commonly observed accompanied by a reflection spectrum, which shows signatures of energetic photons being reprocessed by the optical thick material of an accretion disk. Given their abundance and fluorescence yield, K-shell lines from iron are the most prominent in the X-ray reflected spectrum. These line profiles can be grossly broadened and skewed by Doppler effects and gravitational redshift. Consequently, the modeling of the reflection spectrum provides one of the best means to measure the spin of the black hole among other physical quantities. The accuracy of these spin estimates is called into question because fitting the data requires very high iron abundances, typically several times the solar value. Meanwhile, no plausible physical explanation has been proffered for why these black hole systems should be so iron rich. The most likely explanation for the super-solar iron abundances is a deficiency in the models, and the leading candidate cause is that current models are inapplicable at very high densities ($> 10^{18}$ cm^{-3}), due to the lack of atomic data appropriate for this regime. Here we present the current observational evidence for the super-solar abundance of iron in many black hole systems, and show the effects of high density in the state-of-the-art reflection models. We also briefly discuss our current efforts to produce new atomic for high-density plasmas, which are required to improve the present photoionization models.

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Solar opacities, their uncertainties and the standard solar model

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Plasma effects in the extreme properties of the solar interior are a major source of uncertainty in the calculation of solar opacities. With the decade old problem of solar opacity in mind, I use the atomic code STAR to show a recent study of two major plasma effects on the solar profile, namely ionic correlations and line broadening. These effects are untested in the relevant thermodynamic conditions, and use crude approximations whose applicability at this regime is unclear.
The atomic code STAR is used to study the sensitivity of solar opacities to line broadening. Variations in the solar opacity profile, due to an increase of the Stark widths resulting from discrepancies with OP, are compared with the required opacity variations of the present day Sun, as imposed by helioseismic and neutrino observations. The resulting variation profile is much larger than the discrepancy between different atomic codes, agrees qualitatively with the missing opacity profile, recovers about half of the missing opacity nearby the convection boundary, and has a little effect in the internal regions. Since it is hard to estimate quantitatively the uncertainty in the Stark widths, we show that an increase of all line widths by a factor of about ~ 100 recovers quantitatively the missing opacity. These results emphasize the possibility that photoexcitation processes are not modeled properly, and more specifically, highlight the need for a better theoretical characterization of the line-broadening phenomena at stellar interior conditions and of the uncertainty due to the way it is implemented by atomic codes.
In addition, we find that taking into account the ionic structure results in about 10% increase in the Rosseland opacity near the convection zone, which mimics the missing opacity profile required by helioseismology and neutrino observations. Such effects induce about 15% increase in the Rosseland opacity for the iron monochromatic opacity which was recently measured at the Sandia Z facility, where the temperature reached that prevailing in the convection zone while the density is 2.5 times lower.
As a result, we argue that the solar opacity problem is hindered due to the large uncertainties. Thus, we propose a method to measure opacities at solar temperatures and densities that were never reached in the past via laboratory radiation flow experiments, by using plastic foams doped with permilles of dominant photon absorbers in the Sun. The method is an ideal candidate to experimentally study Rosseland opacities of the solar mixture.

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HITRAN and HITEMP databases: the quest for accuracy and completeness of reference molecular spectroscopic data

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The HITRAN database is an international standard for reference molecular spectroscopic data. It is widely used in many fields of engineering and science including astrophysics. In this talk the new edition (HITRAN2016) will be introduced. It features almost 50 molecules in the line-by-line section of the database, over 300 molecules in the cross-sectional part, as well as aerosol and collision-induced absorption sections. The amount of lines, spectral parameters and their accuracy have increased substantially. In addition new tools including the online interface www.hitran.org and HITRAN Application Programming Interface (HAPI) were introduced. The upcoming new edition of the HITEMP database which is a sister to HITRAN database but suitable for much higher temperatures will also be discussed.

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Balancing completeness and accuracy in opacity calculations

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Opacity calculations of multi-electron ions in hot, dense plasmas, such as iron in the solar photosphere, require a complete accounting of myriad radiative transitions. One strategy for developing generally reliable and computationally tractable opacity models is to simplify some portion of these transitions while preserving a high level of fidelity in others. This approach ensures both completeness, which is a fundamental requirement of opacity models reliable enough to use in astrophysical applications [1], and spectroscopic accuracy, which is important for comparisons with high-resolution benchmark experiments such as those from Sandia's Z facility [2,3].

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X-ray absorption by interstellar atomic gases near the K-edges of C, O, Ne, Mg, and Si, and the L-edge of Fe

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As a part of an ongoing theoretical atomic physics and laboratory astrophysics research program at WMU, we have calculated highly accurate atomic photoabsorption cross sections using the most robust theoretical methods available. These include the widely used Belfast R-matrix, C. F. Fischer's MCHF, and Strathclyde AUTOSTRUCTURE computer program packages, and are further optimized to treat all additional relevant inner-edge atomic effects (e.g., Auger and radiative damping, orbital relaxation effects, pseudorbitals, etc.) To date, atomic C, O, Ne, and Mg, in neutral and ionized forms, have been studied in great detail, combining R-matrix and MCHF analyses with experimental measurements and X-ray observations. These final calibrated atomic data provide reliable absorption models for interpreting interstellar X-ray absorption spectra, as will be discussed.
Present X-ray absorption studies of interest are now focused on the heavier, more complicated third-row atomic systems. These include the Si K-edge region (≈1.85 keV), where the theoretical atomic photoabsorption cross section is needed for a better understanding of the observed near-threshold Chandra spectrum (Corrales, et al. 2016). Another important third-row system is atomic Fe, with L-edge photoabsorption peaking near the fine-structure-split $3p^{-1}(^2P_{3/2})$ and $3p^{-1}(^2P_{1/2})$ thresholds at ≈ 710 and 720 eV. Therefore, computing reliable R-matrix data for this region requires a relativistic treatment beyond our previous s-vacancy calculations.

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Prediction accuracy, consistency, and limitation of IR computations based on ab-initio theory and high-resolution experimental data

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The fast-growing infrared databases are still not complete or accurate enough to subtract the IR contributions of simple astrophysical molecules so that scientists may identify more "hidden flowers", or to carry out accurate IR simulations at very high temperature. Reasons include, but not limited to, the spectrum complexity, experimental difficulty, and the lack of robust theoretical models. In last 10 years, we have extended the "**Best Theory + High-resolution Experimental Data**" strategy from water to NH_3, CO_2, and SO_2. It allows us to combine the accuracy of experimental line positions with the consistency of high quality *ab-initio* theory. In this way, we have been able to make IR predictions with accuracy similar to what we have for the reproduction of existing data, i.e. $0.01-0.02$ cm^{-1}, for line positions and less than 10% for line intensity deviation. This means the generated IR lists may become reliable alternatives for missing IR bands or minor isotopologues. Recent experiments have verified the accuracy and consistency of our IR predictions. In this talk we will introduce the procedure of this strategy, present examples of verified IR data, and discuss both the advantages and current limitations of our approach. The computed IR data was also used to identify the defects and unreliable extrapolations of existing H_eff models, so it can help improve the opacity databases.

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The role of opacities in stellar pulsation

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We review the role of opacities in classical stellar pulsation - specifically in Cepheids and RR Lyres: two groups of pulsating variable stars that have crucial roles in the age and distance scale. We review the success of a previous revision of astrophysical opacities in ameliorating the Cepheid bump mass discrepancy and assess the possible impact of a further increase in Rosseland mean opacities of about 15% in stellar evolutionary and pulsation models in the context of the large quantities of accurate variable star light curves that are now available. This new data will permit much more rigorous assessment of the impact of new opacities. We close with a brief discussion of opacities in B star pulsation.

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Dielectronic recombination calculations for silicon-like ions and the S^{2+} Orion Nebula abundance conundrum

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To model the spectral features observed with astronomical observatories, an accurate and complete description of relevant atomic processes occurring in stellar environments is required. Among these are the important dielectronic recombination (DR) and radiative recombination (RR) processes, which we have investigated for the entire silicon-like isoelectronic sequence. We report reliable DR and RR rate coefficients that are used in spectral modeling codes to determine chemical abundances of elements in photoionized and collisionally ionized plasmas. These theoretical

investigations also serve as a benchmark for measurements being carried out at national and international accelerator laboratories.
In our study, a perturbative, multi-configurational Breit-Pauli (MCBP) method, implemented within an atomic structure and collision code, AUTOSTRUCTURE, is used to compute the DR and RR rate coefficients for the ground and metastable initial levels of silicon-like ions that are relevant to astrophysical and magnetic fusion plasmas. The final DR results are also compared with available experimental results and are found to be in overall good agreement. A further investigation used the multi-configurational Hartree-Fock (MCHF) method to determine the low-lying resonance positions of S^{+}. These play an important role in the low-temperature DR of S^{2+} in the Orion Nebula where the rate coefficient is sensitive to the theoretically predicted resonance energy values. This work is part of an assembly of a DR database required in the modeling of dynamic-finite density plasmas.

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Equations of state for opacity calculations

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Radiative opacities are important quantities that contribute to the prediction of radiation transport in astrophysical objects. To calculate these opacities requires a knowledge of all electron energy level populations that can contribute significantly to photoabsorption and photon scattering in the mostly plasma environments of these objects. This can be a daunting task. Unlike a conventional equation of state that relates thermodynamic variables to uniquely describe the macroscopic state of an equilibrium solid, liquid, or gas, an "opacity equation of state" requires all the statistical thermodynamic details that are the ultimate basis of that conventional equation of state. The range of temperatures (T) and densities (ρ) required for these opacity calculations can also be extraordinarily large. Therefore it is often necessary to combine results that work well for more limited $\rho - T$ domains to produce equation of state quantities that cover a very large range of $\rho - T$ space.
We will give an overview of some of the more common equations of state that are currently used to produce opacities for astrophysical applications, and will go into some detail on the particular approach used for the recently updated Los Alamos National Laboratory opacity tables that cover the elements hydrogen through zinc. Our method uses a chemical picture with occupation probabilities that depend on the plasma environment to construct a free-energy function that we then minimize to obtain the equilibrium populations of energy levels and ionic species. This method guarantees thermodynamic consistency.

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STAR - a new STA code for the calculation of solar opacities

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We present a novel implementation of the STA model, called STAR (STA-Revised), which was written from scratch. The model is based on the theory of Bar-Shalom and Oreg [1] with various improvements. A comparison with other atomic codes was performed and a good agreement was reached. The model is used to calculate and analyze solar opacities. We also implemented a model for the solution of the HNC equations for the calculation of ion-correlation functions for mixtures. We present first calculations of ion-correlation functions for the solar mixture in the solar center and near the convection zone base. These calculations will be used in the future to estimate the effect of the ionic structure of the plasma, on the calculation of solar opacities.

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METUJE global hot star wind models

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We describe our own global (unified) hydrodynamical models of expanding atmospheres of hot stars. The models solve hydrodynamic, kinetic equilibrium (also known as NLTE), and comoving-frame (CMF) radiative transfer equations consistently from the (nearly) hydrostatic photosphere to the supersonic wind. The model input parameters are the stellar effective temperature, radius, mass, and metalicity. For these stellar parameters, our code predicts the photosphere and wind structure and in particular the wind mass-loss rate and terminal velocity. The photospheric emergent flux and thermal structure nicely agree with the TLUSTY model atmospheres.

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Testing the opacities using the SED variability of chemically peculiar stars

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Opacity variation across the stellar surface is the key aspect of the spectral energy distribution (SED) variability in chemically peculiar stars. The opacity variations are caused by the presence of surface spots with enhanced (or depleted) abundance of individual elements. Simulations of the SED variability of chemically peculiar stars with abundances derived from Doppler mapping provide a detailed test of the continuum (bound-free) and line opacities in the model atmospheres. The effect of opacities on the SED is most pronounced in the ultraviolet region. We simulate the ultraviolet and visual SED variability of selected chemically peculiar stars using model atmospheres calculated for actual surface abundances and compare the predicted SED with observational results. We show that the simulations can reliably predict the observed SED and its variability provided that complete bound-free and bound-bound opacities are used. Therefore, the variability of chemically peculiar stars may serve as a test of opacities included in model atmospheres.

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Including all the lines: data releases for spectra and opacities

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I present a progress report on including all the lines in the line lists, including all the lines in the opacities, and including all the lines in the model atmosphere and spectrum synthesis calculations. The increased opacity will improve stellar atmosphere, pulsation, asteroseismology, nova, supernova, and other radiation-hydrodynamics calculations. I also report on using stellar atlases to verify the line data and spectrum calculations, and as tools for extending laboratory spectrum analyses to higher energy levels. All the data are available on my website kurucz.harvard.edu.
In updating previous calculations I generally compute three times as many levels, including all the most recent laboratory data, and produce ten times as many lines. With the addition of heavier elements that were not previously computed I expect to have more than one billion atomic lines. I already have production programs that can tabulate opacity spectra and opacity distribution functions (ODFs), and a model atmosphere program ATLAS9 that uses ODFs for opacity, and ATLAS12 that uses opacity sampling for any number of atomic and molecular lines.
I have redone my calculations from the 1980s for elements up through zinc to produce about 544 million lines as of October 2016. Of these more than 2.11 million lines are between known energy levels so have good wavelengths for computing spectra. The completed ions are listed in /atoms/completed. I am now working on the heavier elements and will have many more lines by the time of the workshop. New line lists for predicted lines, gfpred*, and for lines with good wavelengths, gfall*, are in the directory /linelists/gfnew. The gfall* lists include data from the literature when they are available. My old molecular line lists have been supplemented or replaced with new line data that many authors have generously placed on the web.

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The Belgian Repository of fundamental Atomic data and Stellar Spectra

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Accurate atomic data is a vital component of almost every branch of astrophysics. All models and descriptions of stellar evolution, atmospheres, formation and internal structures are governed by the fundamental atomic data available to the astrophysical community. As such, errors and uncertainties in adopted atomic data can systematically propagate throughout the entire field of astrophysics.
The Belgian Repository of fundamental Atomic data and Stellar Spectra, BRASS, aims to take the first, crucial steps towards removing systematic errors in atomic input data required for quantitative stellar spectroscopy. We will thoroughly assess the quality of fundamental atomic data available in the largest repositories, such as wavelengths and oscillator strengths, by comparing very high-quality observed stellar spectra, taken using the Mercator-HERMES and ESO-VLT-UVES spectrographs, with state-of-the-art theoretical spectra. BRASS will offer both critically-evaluated atomic transition data and high-quality stellar spectra, spanning the entire visible wavelength range for BAFGK spectral types, via an online public interactive interface under development.
To date we have compiled atomic line transition data, for ions of up to 5+ and in the visible wavelength range, from major online repositories including NIST, VALD, and multiple data providers currently in the VAMDC portal. We have cross-matched multiple literature occurrences of atomic transitions for over 75,000 individual lines in preparation for our systematic quality assessment and revealed a significant scatter in literature log(gf) values of up to 2 dex. Almost 2000 unique atomic lines, spanning the BAFGK spectral types in the visible wavelength range of 4200-6800 Angstroms, have been selected for quality assessment work currently underway.

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The Belgian Repository of fundamental Atomic Data and Stellar Spectra: a status update of BRASS

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BRASS is an international networking project of the Federal Government of Belgium for the development of a new public database providing accurate fundamental atomic data of vital importance for stellar spectroscopic research. We present an update of its mid-term development status. The BRASS database will offer atomic line data we thoroughly test by comparing theoretical and observed stellar spectra. We are in the course of performing extensive quality assessments of selected atomic input data using advanced radiative transfer spectrum synthesis calculations which we compare in detail to high-resolution Mercator-HERMES and ESO-VLT-UVES spectra of very high signal-to-noise ratios of hot and cool stars (BAFGK-types). We have retrieved about half a million atomic lines required for the detailed spectrum synthesis calculations from the literature and in online databases such as VAMDC, NIST, VALD, CHIANTI, TIP/TOPBASE, SpectroWeb. The atomic datasets have been cross-matched based on line electronic configuration information and organized in a new online repository that will become publicly available at brass.sdf.org. The validated atomic data, combined with the observed and theoretical spectra will also be interactively offered in BRASS. The combination of these datasets is a novel approach for its development, which will provide a universal reference for advanced stellar spectroscopic research. We present an overview of the BRASS Data Interface developments allowing online user interaction for the combined spectrum and atomic data display, line identification, and line equivalent width measurements.

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Aerosol optical properties in exoplanet and brown dwarf atmospheres

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The formation of clouds and hazes in exoplanet and brown dwarf atmospheres shapes their observed spectra. The species that condense readily in these atmospheres range from the common, like water and ammonia ices, to the more obscure, like sodium sulfide and potassium chloride. One of the most important dust species is silicate, including enstatite and forsterite. Optical properties for these species are required in order to model their effect on the emergent spectra of these objects. Some of these optical properties are well-constrained, but others are less well measured and are currently included in models using interpolation to fill in gaps in wavelength coverage. As the JWST era approaches, we will probe infrared wavelengths with interesting spectral features, including silicates at ˜10 microns as well as various oxide and sulfide species. Accurately determined optical properties will aid in the interpretation of long-wavelength spectra of these objects; it is possible that spectra from JWST will allow us to directly measure the compositions of some of these exoplanet and brown dwarf clouds using their vibrational features. The photochemical hazes that may form in warm exoplanet atmospheres have particularly poor constraints on their optical properties. While proxies for Titan's hazes have been created and

studied in the lab, the hazes that form in exoplanets will naturally look quite different, as they are species that condense at much hotter temperatures than Titan's haze. Since many planets large and small appear to have hazy atmospheres, this is an area that requires much more study. Lab experiments are needed to determine first what the composition of these hazes is likely to be, and then determine their indices of refraction across a broad wavelength range.

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Systematic measurements of opacity dependence on temperature, density, and atomic number at stellar interior conditions

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Model predictions for iron opacity are notably different from measurements performed at matter conditions similar to the boundary between the solar radiation and convection zones [1]. The calculated iron opacities have narrower spectral lines, weaker quasi-continuum at short wavelength, and deeper opacity windows than the measurements. If correct, these measurements help resolve a decade old problem in solar physics. A key question is therefore: What is responsible for the model-data discrepancy? The answer is complex because the experiments are challenging and opacity theories depend on multiple entangled physical processes such as the influence of completeness and accuracy of atomic states, line broadening, and contributions from myriad transitions from excited states. To help determine the cause of this discrepancy, a systematic study of opacity variation with temperature, density, and atomic number is underway. Measurements of chromium, iron, and nickel opacities have been performed at two different temperatures and densities. The collection of measured opacities provides constraints on hypotheses to explain the discrepancy. We will discuss implications of measured opacities, experimental errors, and possible opacity model refinements.
R. More is retired from the National Institute for Fusion Science, Toki, Gifu, Japan.
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Reconstruction of light-curve anomalies of radio pulsars

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The wave propagation [1] theory based on Kravtsov & Orlov approach outlined the general aspects of the theory of radio light curve and polarization formation for radio pulsars. It allowed us to describe general properties of mean profiles such as the position angle of the linear polarization *p.a.* and the circular polarization for the realistic structure of the magnetic field in the pulsar magnetosphere. However, some radio pulsars indicate clear deviation from that correlation. In this work we apply the theory of the radio wave propagation in the pulsar magnetosphere for the analysis of anomalous light curves and polarization profiles. We show that within our theory the circular polarization of a given mode can switch its sign, without the need to introduce a new radiation mode or other effects.

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Radiative-opacity calculations for stellar astrophysics

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The opacities computed by different codes for astrophysical applications may show significant differences. In this work, we discuss some important issues, such as the number of configurations, levels and lines included in the calculations, the accounting for configuration interaction or the breakdown of statistical methods. The essential role of laboratory experiments to check the quality of the computed data is underlined. We review some X-ray and XUV laser and Z-pinch photo-absorption measurements as well as X-ray emission spectroscopy experiments involving hot dense plasmas produced by ultra-high-intensity laser irradiation. The measured spectra are compared with results of the fine-structure atomic code SCO-RCG [1] and with MCDF (Multi-Configuration Dirac-Fock) calculations. A particular attention is paid to iron, which plays a crucial role in the understanding of astero-seismic observations of Beta-Cephei- and SPB- (Slowly Pulsating B) type stars, as well as in the Sun [2]. For instance, in Beta-Cephei type stars, the opacity peak of the iron group, at a temperature of about 200,000 K, excites acoustic modes by the "kappa mechanism". An analysis of the recent and unexplained iron opacity measurements performed on the Z machine of Sandia National Laboratory [3] in conditions close to the ones of the tachocline (boundary between the convective and radiative zones of the Sun) is presented. We comment on several theoretical aspects related to that experiment concerning the roles of collisional excitation and auto-ionization, the modeling of Stark broadening [4], the accounting for Rydberg states or the calculation of photo-ionization [5].

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5

Plasma effects on the atomic structure and X-ray K-lines of astrophysical interest

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X-ray emission lines from accreting black holes, most notably K-lines, have observed widths and shifts which imply an origin very close to the compact object [1]. The intensity of these lines can provide insight into the effects of special and general relativity in the emitting region as well as insight into some properties of the compact object itself. Magnetohydrodynamics simulations of accreting black holes computed by Schnittman et al. [2] seem to reveal that the plasma conditions in such an environment should be characterized by an electronic temperature ranging from 10^5 to 10^7 K and an electronic density ranging from 10^{18} and 10^{21} cm^{-3}. This may affect the atomic structure and processes corresponding to the ionic species present in the plasma.
The main goal of the present work is thus to estimate the effects of plasma environment on the atomic parameters associated with the K-vacancy states in cosmically abundant ions within the astrophysical context of accretion disks around black holes. In order to do this, relativistic atomic structure calculations have been carried out by using the multiconfiguration Dirac-Fock (MCDF) method, in which a time averaged Debye-Hückel potential have been considered for both the electron-nucleus and electron-electron interactions for modeling the plasma environment. Those computations have been performed by using a combination of the GRASP92 code [3] for obtaining the wavefunctions and the RATIP code [4] for computing the atomic parameters, taking into account the plasma environment.
A new set of results related to the plasma environment effects on ionization potentials, transition energies and radiative emission rates is reported for some iron and oxygen ions. A comparison between the atomic parameters obtained by using the MCDF method and another independent computational approach, namely the Breit-Pauli relativistic approximation as implemented in the AUTOSTRUCTURE code [5,6], will also be discussed in detail.

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4

Lifetime measurements using two-step laser excitation for high lying even-parity levels and improved theoretical oscillator strengths in Y II

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Accurate oscillator strengths for electric dipole transitions in singly ionized yttrium (Y II) are needed for the determination of the yttrium abundance in stellar atmospheres. A recent example is the determination of the abundance ratio [Y/Mg] in solar twins that provides a sensitive chronometer for Galactic evolution [1,2]. Moreover, high excitation lines have additional diagnostic value because they can probe both non local thermodynamical equilibrium (NLTE) and 3D effects in stellar atmospheres [3].
We report here new time-resolved laser-induced fluorescence lifetime measurements for 22 highly excited even-parity levels in Y II. To populate these levels belonging to the configurations 4d6s, 5s6s, 4d5d, $5p^2$, 4d7s and 4d6d, a two-step laser excitation technique was used. Our previous pseudo-relativistic Hartree-Fock model [4] was improved by extending the configuration interaction up to $n = 10$ to reproduce the new experimental lifetimes. A set of oscillator strengths extended to transitions depopulating these 22 even-parity levels in Y II is presented and compared to the values found in the Kurucz's database [5].

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Update on the iron opacity experiments on the NIF

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Recent iron opacity experiments on the Sandia National Laboratories Z machine have shown up to factors of two discrepancies between theory and experiment. Much effort has been put into looking at the experiment and the opacity theories but a resolution of the discrepancies has not been forthcoming. It is emphasized that the discrepancies present a fundamental theoretical challenge. To help resolve this question an experimental platform for doing opacity experiments is being developed on the National Ignition Facility (NIF). This platform will be able to replicate the experimental conditions of the Z experiments and also extend the measurements to other temperatures and densities. Experiments to date have demonstrated the capability to produce a satisfactory X-ray backlighting source and the ability to achieve the appropriate plasma conditions in the opacity sample. Some initial iron data has been taken but there are still problems with backgrounds and with the spectrometer used to make the measurements. The path forward for reducing the backgrounds and improving the spectrometer will be presented. It is expected that data for comparing with the Z experiments will be available within a year.

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Recalculation of astrophysical opacities: overview, methodology and atomic calculations

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The Opacity Project was launched in 1983 with the goal of calculating astrophysical opacities using state-of-the-art atomic physics based on the coupled channel (CC) approximation employing the powerful R-Matrix (RM) method [1]. Over the next decade, a suite of extended RM codes were developed to compute large-scale bound-bound transition strengths and bound-free photoionization cross sections with unprecedented accuracy. One of the primary features of OP was the precise delineation of *intrinsic* autoionizing resonance profiles whose shapes, extent and magnitudes are determined by myriad channel couplings in the (electron+ion) system. However, CC-RM calculations are of immense complexity and require substantial computational effort and resources. For the often dominant inner-shell transitions they could not be completed owing to computational constraints on the then available high-performance supercomputing platforms. Simpler approximations akin to distorted-wave (DW) type methods used in other opacity models, that neglect channel couplings, were therefore employed to compute most of the OP data.

In recent years a renewed effort has been under way as originally envisaged using the CC-RM methodology [2], stimulated by two independent developments. The first was a 3D Non-LTE analysis of solar elemental abundances that were up to 50% lower for common volatile elements such as C, N , O and Ne [3]. It was suggested that an enhancement in opacities could resolve the discrepancy, particularly in helioseismological models. The second was an experimental measurement of iron opacity at the Sandia Z-pinch device, under stellar interior conditions prevalent at the base of the solar convection zone, that were 30-400% higher in monochromatic opacity compared to OP [4]. The Z results also found nearly half the enhancement in mean opacity needed to resolve the solar abundances problem.

The pilot CC-RM calculations [2] for an important iron ion Fe XVII resulted in 35% enhancement relative to the OP Rosseland mean opacity at the Z conditions. While the enhancement is consistent with subsequently reported results from other opacity models [5,6], there are also important differences in (i) atomic physics, (ii) equation-of-state, and (iii) plasma broadening of autoionizing resonances. The calculations are of immense complexity and require substantial computational effort and resources. The Fe XVII calculations were carried through to convergence by including n = 3 and n = 4 levels of the target ion Fe XVIII. They showed large enhancements in photoionization cross sections, as successive thresholds are included, due to coupled resonance structures and the background. The extensive role of photoionization-of-core (PEC) or Seaton resonances associated with strong dipole transitions in the core ion Fe XVIII is especially prominent. Several sets of the pilot calculations have been carried out: relativistic Breit-Pauli R-Matrix (BPRM) calculations including 60 fine structure levels up to the n = 3 thresholds, non-relativistic calculations including 99 LS terms up to the n = 4 threshold, as well as BPRM calculations with 218 fine structure levels (in progress). One of the aims is to benchmark existing DW cross sections and monochromatic opacities in the non-resonant background and the high energy region above all coupled excitation thresholds.

In addition to the converged CC-RM atomic calculations, we are also investigating occupation probabilities from the Mihalas-Hummer-Dappen equation-of-state employed in the OP work which are orders of magnitude lower for excited levels than other models. A new theoretical method and computational algorithm for electron impact broadening of autoionizing resonances in plasmas, as function of temperature and density, is described. Finally, issues related to completeness and accuracy would be addressed, particularly "top-up" background opacity contributions to the CC-RM opacities from high-n configurations [5-7].

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Monte Carlo simulations of biophysical factors for viability of life in exoplanetary atmospheres

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We propose to adapt the Monte Carlo package GEANT4, developed by CERN, to simulate the effects of radiation fields of stars on exoplanet atmospheres and explore the possibility of DNA-based lifeforms. Stellar spectral profiles from cool dwarfs will be subject to quasi-monochromatic intensity modulations by chemical constituents of exoplanetary atmospheres, represented as phantoms using Earth-like compositions, as well as those that have been observed and theorized on exoplanets. We will enable radiation penetration into the atmosphere using available molecular opacities of prime atmospheric constituents such as H_2O, CO_2, etc. and study biophysical effects on DNA survival and strand breaking at varying elevations.

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The Bedisk and Beray circumstellar disk codes

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I will describe the operation and atomic data requirements of the Bedisk and Beray codes which can be used to compute synthetic spectra and images for a star surrounded by a circumstellar disk. The Bedisk code computes the thermal structure of the disk based on the central star's photoionizing radiation field by enforcing radiative equilibrium in a gas of a user-specified chemical composition. The code has a large atomic data requirement, including transition probabilities, photoionization cross sections, and effective collision strengths for all atoms and ions included. Detailed line spectra, spectral energy distributions, and synthetic images are computed by the Beray code for comparison to observations. I will also discuss several applications of these codes, including to the classical Be stars, to the pre-main sequence Herbig Be stars, and to the post-main sequence sgB[e] stars.

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ATMOS: Resolving ambiguities in the spectroscopic detection of life

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The search for biosignatures requires a sophisticated understanding of exoplanet atmospheres and the molecules within them. Current atmospheric models consider only a few dominant molecules, all of which can lead to false positives in the remote detection of life.

The rich tapestry of life makes use of thousands of molecular species that could contribute towards a biosphere and its associated atmospheric spectrum. A comprehensive analysis of such an atmosphere requires spectral information for each of its molecular components. However, knowledge of molecular spectra currently only exists for a few hundred molecules and, other than a handful of exceptions (e.g. water, CO), most spectra are incomplete. Measuring these molecules experimentally leads to accurate but limited spectra, and it can be difficult, perilous, and sometimes altogether impossible. Theoretical calculations have become a valuable tool in obtaining molecular spectra but, for the majority of molecules, this process remains computationally prohibitive.
Given the relatively low level of accuracy that astronomical observations require, there is value in creating approximate models for the spectra of molecules, particularly for those about which we know very little or nothing at all. ATMOS (Approximate Theoretical MOlecular Spectra) aims to do just that, using a combination of experimental measurements, organic chemistry, and quantum mechanics. ATMOS 1.0, presented here, can identify potential biosignatures with significant spectral features in any given wavelength window.

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The ExoMol project: molecular line lists for the opacity of exoplanets and other hot atmospheres

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The ExoMol project provides comprehensive line lists with the aim of providing data for all molecules likely to be observable in exoplanet atmospheres in the foreseeable future [1]. This is a huge undertaking which involves providing in excess of a hundred of billion spectral lines for a large variety of molecular species [2]. The physics of molecular absorptions is complex and varies between different classes of absorbers, which are therefore divided into following topics (a) diatomic, (b) triatomics, (c) tetratomics, (d) methane and (e) larger molecules. Special techniques are being developed to treat each case. The line lists for a number of key atmospheric species currently available from ExoMol (www.exomol.com) including H_2O, NH_3, CaH, MgH, BeH, SiO, HCN/HNC, KCl, NaCl, CH_4, PN, PH_3, H_2CO, AlO, NaH, ScH, HNO_3, SO_2, SO_3, H_2S and NO. I will present examples of molecular spectra computed using the ExoMol line lists and discuss prospects for future studies.
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The dark side of the Sun

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Is the Sun likely to have a more opaque interior than previously thought? The solar oxygen- (or abundance-) problem can be solved with higher interior opacities, reconciling abundance analysis based on 3D convective atmospheres, with the helioseismic structure of the solar interior. This has been known for more than a decade. But last year we learned that the absorption by just iron, contributes 7% more to the solar opacity at the bottom of its convection zone, than predicted by any opacity calculation so far, and by OP‘05 in particular.
I show, that artificial changes to the absorption (calibrated against the iron experiment) by other elements in a solar mixture OP‘05 opacity, gives the shape and magnitude of change that can restore agreement between modern abundance analysis and helioseismology.
This suggests that improved opacity calculations will solve the solar oxygen problem.‘

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Stellar opacities

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Stellar opacities are fundamental ingredients of stellar evolution. They contribute to the age of stars and determine the transfer of energy in stellar interiors for a great variety of stars. This transfer of energy results from complex and difficult atomic calculations that must be performed for a large number of species and for specific mixtures through a large range of temperature and density.
These ingredients for astrophysics have been known only theoretically for several decades, and the calculations have been developed by a small amount of groups mainly located in the United States even through international teams.
Nevertheless, different approaches (OPAL and OP) have been considered a long time with well-known differences. Such effort has been stimulated by the development of more and more precise measurements of the stellar interiors and the desire to validate the hypotheses contained in stellar evolution codes.
Solar neutrinos and helioseismology have constrained in the nineties new insights, and first experimental opacity measurements have been performed to validate the existing or new calculations. More recently the development of asteroseismology and the dedicated spatial probes (SoHO, COROT, KEPLER...) have encouraged new comparisons between theoretical teams in different countries (mainly USA and France). In parallel the realization of measurements on Z pinch in Sandia and promising ones on high-energy laser facilities (OMEGA, NIF, LMJ) represent new opportunities to progress on accurate opacities for stellar evolution.
This introduction will rapidly describes the history of the last 3 decades, the present situation and the perspectives in this field.

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Single photon double ionization of atomic oxygen

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Double photoionization calculations are performed for atomic oxygen which leaves a residual ion core with a complicated electron structure. An R-matrix with pseudostates (RMPS) method (P. G. Burke, R-matrix Theory of Atomic Collisions, Springer, 2011) is successfully applied to compute the double photoionization cross sections that are in overall agreement with recent experimental results at the Advanced Light Source in Berkeley. In addition to the smooth and linear behavior of these cross sections, strong resonance features are observed similar to double photoionization of atomic helium (Gorczyca et al., JPB, 46, 195201, 2013). In the future, we will expand these RMPS calculations to analyze the inner-shell double ionization of atomic oxygen, which is highly important in astrophysical processes in interstellar medium (Gorczyca et al., APJ, 779, 78, 2013).

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Molecular data for molecular hydrogen plasmas

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Studies of molecular plasmas both in local thermodynamic equilibrium (LTE) and non-LTE require state-resolved (electronic, vibrational and rotationally resolved) transition cross sections or rate coefficients to calculate populations (for non-LTE plasmas), opacities and emissivities. For both electron- and photon-molecule data there is a lack of comprehensive state-resolved data available, particularly for transitions that involve electronically excited states.
Here we present state-resolved results of photodissociation and radiative association of H_2^+ and its isotopologues (D_2^+, T_2^+, HD^+, HT^+, and DT^+). We note that going beyond the commonly utilized "two-level" approximation of H_2^+ could be important in astrophysical models when dealing with radiation temperatures that can access photon wavelengths around 100 nm. For example at these wavelengths, at a material temperature of 8400K, the photodissociation cross section via the (second electronically excited) $2p\pi_u$ state is over three times larger than the photodissociation cross section via the (first electronically excited) $2p\sigma_u$ state.
We will also present the first convergent close-coupling calculations of electron scattering from the hydrogen molecule H_2 [1,2]. These calculations are generally in good agreement with experiment for all major scattering cross sections but differ with commonly "accepted" results by approximately 20% for excitation to the Lyman-Werner levels.
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Converged close-coupling R-Matrix calculations for photoionization of iron ions in astrophysical plasmas

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We have carried out converged close coupling R-Matrix (CCC-RM) calculations for photoionization of Ne-like Fe XVII and demonstrated orders-of-magnitude enhancements in cross section due to successive core excitations. Convergence criteria are: (i) inclusion of sufficient number of residual ion Fe XVIII core states, (ii) high-resolution of myriad autoionizing resonances, and (iii) high-energy cross sections. Distorted wave (DW) calculation has been done for configurations not included in CCC-RM but in OP and OPAL to top up the background opacity, and its contribution will be reported. We will discuss verification of the conventional oscillator strength sum-rule in limited energy regions for bound-free plasma opacity. We will also report preliminary results from R-matrix calculation of photoionization cross section of other L shell iron ions.