Invited Talks

A New Approach to the Analysis of Experimental Atomic Spectra

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Atomic spectroscopy is a vital field providing crucial reference data for applications ranging from astrophysics to fusion research and industrial applications. Despite its importance, the number of groups and people active in the field has been decreasing steadily over the past few decades and it is unlikely that this is going to change any time soon. Although we can, and should, advocate for more funding for atomic spectroscopy, it is incumbent on us to ensure that we are applying our limited resources in the most efficient way possible. One way we can do that is by sharing data and by improving the software tools that we use.

Many of the spectra recorded on our spectrometers can be used for multiple purposes – for example spectra recorded for the analysis of a neutral atom may include many lines of the singly-ionized atom, and can be used to measure wavelengths, oscillator strengths, and hyperfine structure. Reuse of these data has frequently relied on ad-hoc collaborations, but this has proved inefficient when the history of the data processing has been lost or inadequately documented, as is often the case when groups rely on summer students to boost their dwindling resources. Much of the software that is used to analyze atomic spectra is old, having been written in the 1970's and 1980's by titans of the field, who made the most of limited computer resources using computer languages that are rarely taught to students now. Since these codes contain valuable knowledge regarding the analysis of spectra, there is an unwillingness to re-write them, and instead, each researcher writes a custom wrapper to analyze their data, repeating the same basic tasks that have been done before. There is a better way.

We are working on new software and data formats using the Hierarchical Data Format 5 file format (HDF5 [1]). This format is designed for heterogeneous data and facilitates easy sharing, cross-platform support, version control, and the ability to store metadata with the data. We anticipate that this format will enable easier sharing of spectral data and better logging of analysis that has already been performed. Extensive python libraries are available that will enable us to embed previous knowledge in a way that can be understood and extended by future researchers. Our software is initially focusing on the measurement of branching fractions and oscillator strengths using spectra from Fourier transform spectrometers, but we plan to extend its scope to replace many of our current programs for analyzing other atomic data. This will require a more extensive team than the three coauthors of this paper, and thus we are actively seeking collaborators for this project. I shall describe our vision for the structure of the HDF5 files used for our data and the programs that we are developing for their analysis.

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The Imperial College Spectroscopy Group: High Accuracy Atomic Data for Astrophysics

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Modern advancements in telescopes and astronomical spectroscopy have revolutionised our understanding of the universe, providing us with unprecedented high-resolution astronomical spectra across many spectral regions. However, the accurate interpretation of these spectra, collected at great effort and expenditure of resources, crucially depends on the availability of precise laboratory atomic data. The Imperial College (IC) Spectroscopy group has taken up the challenge of meeting this acute need by employing Fourier transform spectroscopy (FTS) to measure atomic spectra of many astrophysically important elements. Our analyses of these laboratory spectra have resulting in significant improvements in the breadth and accuracy of atomic data.

Our work focuses on measuring new atomic data and enhancing the precision of existing data for a wide range of astrophysically important elements, including the iron group elements, which hold special significance due to their high abundances and multitude of electronic transitions, and, more recently, the rare earth elements, which are involved in r-process nucleosynthesis. Through the analysis of high-resolution spectra, we have achieved substantial reductions in uncertainties for transition wavelengths and energy levels, often exceeding an order of magnitude, while transition probabilities can be measured with uncertainties of just a few percent. The high resolution of FTS also enables line broadening effects such as hyperfine and isotope structure, crucial data for accurate stellar abundance measurements, to be determined.

The significance of our work extends beyond the current state of astronomical research. As the field continues to advance, telescopes such as the Extremely Large Telescope and the James Webb Space Telescope will continue to drive the demand for further improvements in atomic data. To ensure that the IC spectroscopy group can continue our work providing the data vital for these instruments, we are expanding our measurement capability into the infrared with the addition of a new high-resolution Fourier transform spectrometer.

In this talk, we present some of the most recent results of our spectroscopic analyses, discuss our future research plans and emphasize the critical role of accurate atomic data in modern astronomical research.

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Revised and Extended Analysis of Argon V – VII

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This project revisits the spectral analysis of argon's fourth to sixth ionization stages (Ar V-VII). We revised the experimental data's wavelengths, uncertainties, and intensity using the techniques for intensity and wavelength correction of the observed lines proposed by Alexander Kramida [1,2]. These techniques are used on data from a single set of experiments performed at the Centro de Investigaciones Opticas, La Plata, designed to cover the region from the vacuum ultraviolet to visible. We looked for all previously known lines in our reference spectrograms, which produced a table with wavelengths analyzed as a single set. This analysis also includes lines classified for the first time in this work.

Another work front is on atomic structure calculations. The increased computing power of the past decades offers possibilities that were not available when much of the original analysis work was done. More configurations have been used to elaborate isoelectronic sequences to compare experimental and theoretical values and to model least-squares fits with much more configurations. Other methodological additions include atomic core polarization effects in calculating energy and transition rates, statistical comparisons between observed line intensities, and transition rates corrected to take the population of the higher levels into account.

In this presentation, we will summarize the results obtained, including some new data on Ar VII and additions we made in our previous study of Ar V-VI [3,4].

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IT 4

New Astrophysical Opacities from The Opacity Project

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A detailed comparison of the results between two methods used to calculate opacities has been assessed[1]. As well as trying to understand the underlying differences between the measured Fe opacities at the Sandia National Laboratory [2] and prior theoretical calculations, a new set of monochromatic opacities for key Fe ion stages have been calculated. These ion stages are important contributors to the Rosseland opacities for the physical conditions characterizing the base of the Solar convection zone, and have been calculated in the framework of the Opacity Project approach. These new data sets are being tested on solar models. These new results pave the way in defining the best way for future calculations to be integrated into the Opacity Project for a new updated release of monochromatic, Rosseland and Planck mean opacities as well as radiative accelerations.

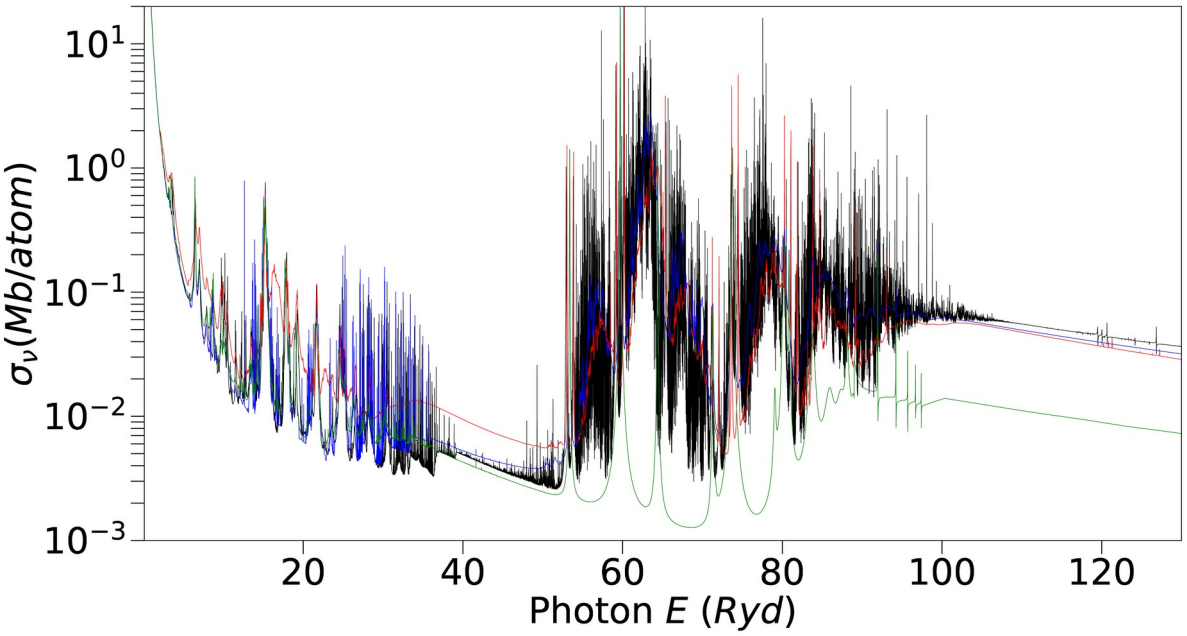

Figure 1: Fe XVII monochromatic opacity cross sections. R-Matrix n=6 (black), AutoStructure with autoionizing states (red), The Opacity Project 1st release 1996 (green),The Opacity Project 2nd release 2005 (blue).

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Kilonova and Neutron Star Merger Plasma

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Neutron star mergers produce not only strong gravitational wave signals but also a substantial amount of neutron rich ejecta. The expanding neutron rich ejecta has been considered as a natural astrophysical environment of rapid neutron capture process (r-process) nucleosynthesis. Radioactive decay of freshly synthesized r-process nuclei continuously heats the ejecta and powers an optical-infrared transient, a so-called kilonova. A kilonova was detected after the first neutron star merger event, GW170817. To model the kilonova emission, we need to compute radiation transfer of the expanding ejecta composed of heavy elements and plasma condition of the ejecta. Here, we review the current status of the kilonova modeling and possible elemental identification in the spectra of the kilonova in GW170817. We also discuss the progress in the plasma modeling of kilonova nebulae [1,2].

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Lanthanide and Actinide Opacity Computations for Kilonova Modeling

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The production of elements heavier than iron in the Universe still remains an unsolved mystery. About half of them are thought to be notably produced by the astrophysical r-process (rapid neutron-capture process) [1], for which one of the most promising production sites are neutron star mergers (NSMs), known as kilonova [2]. In August 2017, gravitational waves generated by a NSM event were detected by the LIGO detectors (event GW170817) [3], and the observation of its electromagnetic counterpart, the kilonova AT2017gfo, suggested the presence of heavy elements in the ejecta [4]. The luminosity and spectra of such kilonova emission depend significantly on the ejecta opacity, which is dominated by millions of lines from f-shell elements produced by the r-process, *i.e.* lanthanides and actinides [5]. Atomic data and opacities for these elements are thus sorely needed to model and interpret kilonova light curves and spectra.

In this context, the present work focusses on atomic data and opacity computations for lanthanides and actinides, for typical ejecta conditions expected one day post-merger, which correspond to the presence of the element first ionization stages only (neutral to trebly-ionized elements). We intend to discuss our new computations of atomic data and expansion opacities for weakly-charged lanthanides and actinides and compare them with previously reported studies (*e.g.*, [6-10]). In order to do so, we used the pseudo-relativistic Hartree-Fock (HFR) method as implemented in Cowan's codes [11], in which the choice of the interaction configuration model is of crucial importance [12]. In particular, we will also discuss the opacity sensitivity to several effects as the core polarization [13] as well as to a calibration procedure in which configuration average energies are adjusted to match data in the literature.

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4f Photoabsorption in Pt II to Pt V

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Platinum is of significant astrophysical interest as it is one of the most abundant elements in the rapid process (r-process) nucleosynthesis peak around mass number A = 195 [1,2]. Its detection in metal-poor stars provides evidence that r-process nucleosynthesis took place at some time in the environment of the star or the location of its formation. There is also interest in isotopic population anomalies [3] where heavier isotopes are seen to dominate the spectrum. The pattern of isotopic composition varies from the widely assumed fractionation formalism, and lighter isotopes are deficient compared to the prediction of a single-parameter fractionation model. While EUV stellar spectroscopy may not be able to unequivocally identify a given ion stage or excitation state of platinum, EUV studies will help laboratory astrophysicists to map laser produced plasma spectra of lowly-ionised platinum in the visible and near infra-red regions of the spectrum which are more accessible to high-resolution, ground and space-based, stellar spectroscopy. EUV photoabsorption of 6th row species is also of interest due to potential applications exploiting their photochemistry.

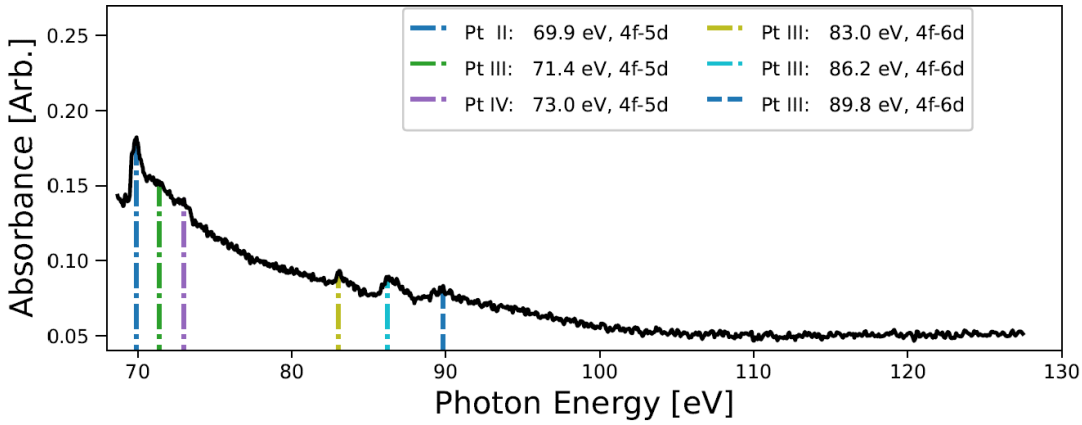

Figure 1: Experimental absorption spectra of laser produced plasmas of platinum, recorded at a delay of 300 ns, showing 4f-nd photoabsorption in Pt^{+}, Pt^{2+} and Pt^{3+}.

In this work we present an investigation into the photoabsorption of platinum laser produced plasmas in the 69 - 128 eV region using the dual laser plasma (DLP) method. In this region 4f → 5d, 4f → 6d and 4f → 7d transitions, broadened by autoionisation, are found in ions Pt^{+}, $Pt2^{+}$, $Pt3^{+}$, and $Pt4^{+}$. Analysis of the spectra was supported by atomic structure calculations using the Cowan suite of codes [4], by relativistic time-dependent local-density approximation (RTDLDA) calculations [5].

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Present Status of the Investigation on the Spectra of Moderately Charged Thulium Ions

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The present contribution reports recent progress on the analyses of vacuum ultraviolet spectra of several thulium ions. The analyses are based on high resolution spectra emitted by a vacuum spark source recorded in the wavelength range of 350-2960Å on the 10m vacuum ultraviolet spectrograph of the Meudon Observatory. On these spectrograms, lines from the three neighbouring ionisation stages, Tm^{2+} (Tm III), Tm^{3+}(Tm IV) and Tm^{4+} (TmV), are present allowing parallel analyses to be carried on. All spectral analyses are supported by parametric calculations using the package of Cowan's codes [1] and provide level compositions, and consequently, transition probabilities and Landé factors.

For the Tm^{4+} ion (TmV), more than 300 lines have been identified for the first time as transitions involving 14 levels of the $4f^{11}$ ground configuration, 37 levels of $4f^{10}5d$, 9 levels of $4f^{10}6p$ and 2 levels of $4f^{10}6s$, all previously unknown. The results confirm the very preliminary report [2] on a few levels of this ion.

The first analysis of Tm^{3+} (Tm IV) was achieved in 2007 [3]. It resulted in the determination of 176 energy levels belonging to the $4f^{12}$, $4f^{11}5d$, $4f^{11}6s$ and $4f^{11}6p$ configurations. However, levels of small J values were missing due to weak intensities of the corresponding transitions. In the present work, we extended the analysis and determined additional levels for these configurations and moreover, new levels belonging to the $4f^{11}6d$ configuration.

The spectrum of Tm^{2+} (Tm III) analyzed by Sugar [4] has been reinvestigated through his unpublished line list ($\lambda > 2000$Å), supplemented by the new experimental data in shorter wavelength region.

For the Tm II spectrum that lies in longer wavelength region, a parametric interpretation of the available experimental levels [5, 6] has been carried out. Calculated Landé g-factors values are compared with experimental values when available.

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Atomic-Structure Calculations for Ultracold Gases of Lanthanides

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Lanthanide elements are widely used as trivalent cations in many modern technological applications. Moreover, some neutral lanthanides, like erbium or dysprosium, have been cooled down to the nanokelvin regime by lasers since about 15 years. Indeed, their magnetic moments make them suitable candidates for *e.g.* quantum simulation of solid-state physics [1,2]. Laser-cooling and trapping require that the atoms are submitted to several electromagnetic fields, and so the detailed knowledge of the atomic spectroscopy – excited energy levels and transition probabilities.

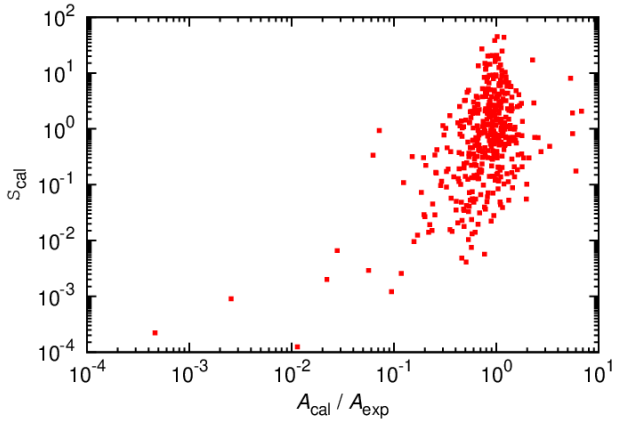

Figure 1: Calculated line strengths $\mathcal{S}_{cal}$ of Er^+ as functions of the ratios between our calculated Einstein coefficients and the experimental ones of Ref. [3].

In this presentation, I will describe the work in which I was involved over the last years, regarding the calculations of atomic properties of interest for laser-cooling experiments, like energies, Landé g-factors, transition probabilities or dynamic dipole polarizabilities. In particular, I will present the *FitAik* program [4], that I have written to calculate A_{ik} Einstein coefficients, using least-square fitting with experimental values. I will focus on the example of Er^+ (Er II), see Figure 1, relevant for experiments with ultracold Rydberg Er atoms [5].

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An Overview of Recent R-Matrix Developments with a Focus on Heavy Neutron-Star Merger and Magnetically-Confined Fusion Elements

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Both magnetically-confined fusion and astrophysical neutron-star merger plasmas require detailed atomic structure and subsequent collisional calculations (electron-impact excitation/ionization) for heavy atomic elements of the periodic table.

For electron-impact excitation we employ the parallel DARC version of the R-matrix codes (see R-matrix review book of P. G. Burke [1]) and this provides sufficiently accurate electron-impact rates to identify lines for near-neutral tungsten targets [2,3]. However, for electron-impact ionization major revision of the codes has been required to address groundstate and metastable ionization of open-shell heavy systems, such as tungsten. This directly impacts one particular fusion application, as by putting higher accuracy constraints known effective ionization will allow us to determine the impurity influx from tokamak plasma facing components.

From an astrophysical perspective, kilonova observations[4] have identified lines of gold and platinum for which parallel DARC codes are ideally suited to explore the LTE/NLTE assumptions of most previous modelling. I shall report upon this within the talk.

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A FAC POTENTIAL FOR AUTOSTRUCTURE

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General atomic structure and collision codes fall into two broad categories: those which describe multi-channel coupled equations which result from the application of a variational principle (Hartree-Fock, Dirac-Fock, and their extension to the continuum, e.g. R-matrix[1]) and those which use a single channel uncoupled equation (generically labelled distorted-wave) where the choice of distorting potential(s) is essentially a free parameter. Examples of the former include Grant and co-workers' GRASP[2], Froese-Fischer's MCHF[3] and Cowan's HFR[4]. Examples of the latter are AUTOSTRUCTURE (AS)[5], FAC[6], HULLAC[7] and the LANL suite[8]. We focus on the latter group. The FAC, HULLAC and LANL codes are very similar being fully-relativistic and utilize a factorization approach[7] for scattering. To a first approximation they only differ in their choice of a unique distorted-wave potential which leads to a set of orthogonal orbitals. Even here, the Dirac-Fock-Slater potential used by FAC and LANL differ only in their detail. AS is fundamentally different in its formulation of the structure problem. It can use multiple distorted-wave potentials which leads to non-orthogonal orbitals which are treated in the same fashion as Cowan's HFR approach for bound orbitals and include the resulting exchange overlaps for the continuum. (The scattering problem is factored using *jK*-coupling.) AS also solves an uncoupled kappa-averaged Dirac equation akin to Cowan's HFR. It can also use non-unique orbitals so that different charge-states can be described by the appropriate physical potentials, e.g. for autoionization. The potentials themselves are optimized by the minimization of an energy functional (a feature found also in HULLAC). The goal here is to accelerate the convergence of the configuration interaction expansion for increasingly low-charge ions. In principle, AS can generate a single unique potential corresponding to that used by FAC and LANL and obtain essentially the same results. (The situation with HULLAC is complicated by the need to choose the same optimization strategy, but in principle it can be mimicked by AS as well.)

FAC is a very popular code within the atomic physics user community. But, as discussed above, it actually uses a rather restricted and simple approach to atomic structure. However, it is difficult to cross compare it with other codes in general since users tend to be expert in one code base. To this end, we have incorporated the current FAC potential within AS. We have applied it to a study of the dielectronic recombination of Be-like Ar using an extensive configuration interaction expansion so as to describe the so called trielectronic recombination seen in measurements on CSR[9]. We will present results obtained from FAC itself, AS using the FAC potential and AS using its standard Thomas-Fermi potential.

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ORTHOGONAL OPERATORS: EXTENSION TO HYPERFINE STRUCTURE

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Orthogonal operators are a next step in the semi-empirical description of complex spectra. Orthogonality yields optimal independence and thus least correlation between the operators. The increased stability of the fitting process is used to include higher order many-body as well as fully relativistic effects. The calculated eigenvalues are frequently an order of magnitude more accurate with respect to a conventional semi-empirical approach. The resulting eigenvectors may not only be put to use to calculate transition probabilities and g-factors, but also to calculate hyperfine structure constants. We illustrate our first steps in this field with some examples of first and second spectra of the iron group elements. The results are compared to current experimental A-values while strong and weak points of the method are discussed.

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IT 13

Electron-Impact Excitation Data for Astrophysical Plasma Diagnostics

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Plasma models built on extensive atomic data are essential to interpret the observed astrophysical spectra. Improving the accuracy and completeness of atomic data are particularly relevant in the era of the next generation of high-resolution spectroscopic instruments (e.g., XRISM, Athena, HUBS, and Arcus). Electron-impact excitation is one of the fundamental atomic processes in astrophysical plasmas. In this talk, I will focus on some recent R-matrix intermediate-coupling frame transformation (ICFT) calculations of electron-impact excitation data of cosmic abundant elements [1-4]. I will illustrate the importance of data with improved accuracy in the context of a wide range of astrophysical plasmas, including solar corona, dwarf nova, ionized winds driven away from black holes, hot plasmas in individual galaxies and galaxy assemblies.

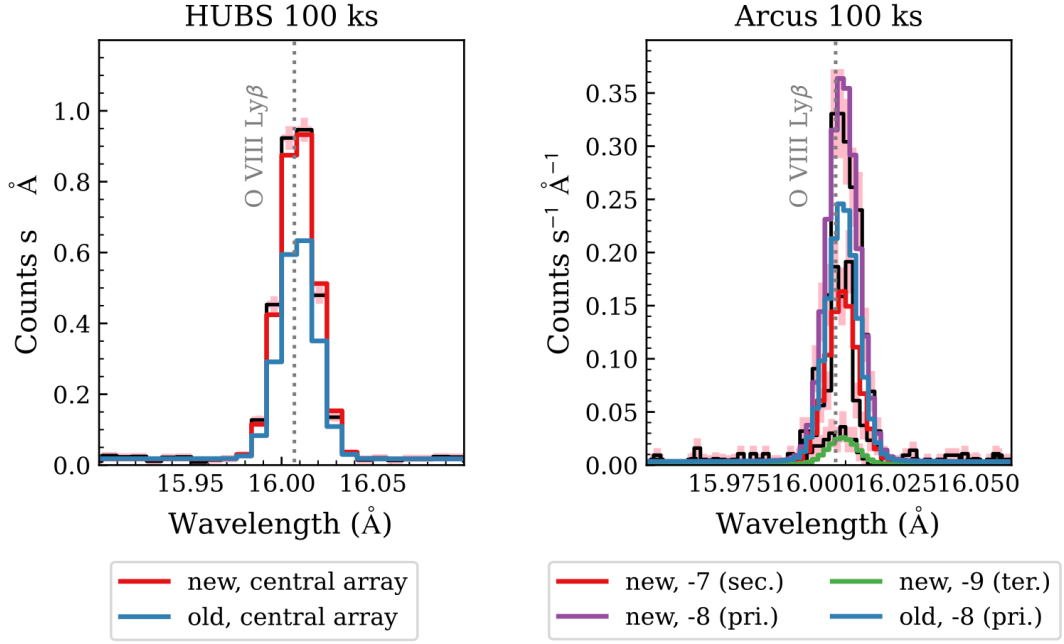

Figure 1: Simulated HUBS (left) and Arcus (right) spectra in the O VIII Ly beta neighborhood using old and new electron-impact excitation data.

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Atomic Structure Calculations for New Physics Searches

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Precision laboratory and astronomical measurements of atomic spectra can be used to search for new physics including dark matter, dark energy, new forces, variations of fundamental constants, and violations of fundamental symmetries. Accurate atomic calculations are required for planning and supporting experiments, understanding and removing systematics, and interpreting the results as limits on new physics. However, open-shell systems still pose a challenge for atomic structure theory.

As an example, comparison of astronomical and laboratory spectra can be used to constrain variations in the fine-structure constant (see, e.g. review [1]). This dimensionless constant, which measures the strength of the electromagnetic interaction, might change of time and space as suggested by some unification theories, or could couple to dark matter and hence vary according to the local dark matter density. Atomic calculations are used to determine how the spectra depend on the value of the fine-structure constant.

Measured atomic spectra also depend on the isotope abundances via the isotope shift. This is a significant potential systematic effect for astrophysical studies of fundamental constant variation, but it is also an opportunity to extract the isotope abundances, with implications for stellar evolution models [2]. In the laboratory, precise measurement of isotope shift has been used to place limits on hypothetical force-carrying bosons that couple electrons and neutrons [3]. Calculations of isotope shift in complex atoms are based on precise *ab initio* atomic structure methods and finite-field formulation of the relativistic isotope shift operators.

A promising route to calculations of spectra, isotope shifts, and other properties of complicated atoms is the particle-hole configuration interaction with many-body perturbation theory (CI+MBPT) method [4]. This extends the CI+MBPT method [5] to non-perturbatively include configurations with electron holes below the designated Fermi level. The method has been implemented in AMBiT [6], a software package for fully relativistic, *ab initio* atomic structure calculations. The software is written in modern C++, and can make use of both OpenMP and MPI to achieve demonstrated scalability from a personal notebook all the way up to state-of-the-art supercomputer clusters.

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Testing the Constancy of Electromagnetism's Strength with Dark Matter Density Using Stellar Twins

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The Standard Model of nature's laws provides no explanation for the fundamental constants, like electromagnetism's strength, alpha. It is therefore up to experiments to test whether fundamental constants are, indeed, constant and universal, or instead vary and depend on other physical parameters. I will describe a new probe of alpha's constancy within our Galaxy – stellar twins – and show our first results from solar twins which have an ensemble precision of 12 parts-per-billion. This is already the best astronomical measurement of any fundamental constant so far. I will also show that red clump stars also provide precise measurements with this approach. The results derive from archival high-resolution optical spectra (HARPS) from the ESO 3.6-m telescope, so there is considerable scope for extending them using larger facilities. Our goal is to map alpha across the Milky Way and, importantly, its widely-varying dark matter density field. This will be a completely new, direct test of physics beyond the Standard Model.

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Improvements in Oscillator Strengths and their Impact on Interstellaire Abundances and Depletions

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In this talk, I will discuss how recent improvements in the oscillator strengths of astrophysically-relevant atomic transitions have impacted our understanding of interstellar gas-phase abundances and dust-grain depletions. The abundances of neutral and ionized atomic species in interstellar clouds are typically derived by measuring the strengths of absorption lines that correspond to electronic transitions out of the ground state, using stars or quasars as background continuum sources. The absorption strength can be converted into a column density only if the oscillator strength of the transition is well determined. For atomic species that represent the dominant ionization stage of an element in neutral diffuse gas, such measurements yield the gas-phase abundance of the element. Many of the more highly refractory elements are found to be severely underabundant in interstellar gas (when their abundances are compared to those derived for the Sun or local B stars), indicating that large fractions of those elements are locked up in interstellar dust grains. Thus, accurate oscillator strengths are needed not only to understand gas-phase elemental abundances but also to correctly identify and characterize the depletion properties of different elements that yield clues to the formation and evolution of interstellar dust grains.

In recent years, new experimental oscillator strengths have been determined for commonly observed transitions in P II [1,2], Cl I [3], Cl II [4], Cu II [5], Ge II [6], and Pb II [7]. In these experiments, lifetimes and oscillator strengths are derived using beam foil techniques at the Toledo Heavy Ion Accelerator (THIA). I will discuss how the improvements in the oscillator strengths afforded by these measurements have given us new perspectives on the abundances and depletions of neutron-capture elements [8] and on the growth of dust grains in interstellar clouds [9]. I will also highlight cases where further experimental results may be needed to resolve discrepancies in existing determinations of oscillator strengths for astrophysically important atomic species.

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Atomic Data for 3D Non-LTE Solar and Stellar Spectroscopy

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Stars leave their signatures on the light they emit from their atmospheres, in the form of absorption and emission lines. By comparing with model stellar spectra, we can decode these signatures to reveal the physical properties of stars, in particular their chemical compositions. This information sheds light on the structure and evolution of the stars themselves, as well as their planets, and even the Galaxy as a whole... provided that the model spectra are sufficiently realistic [1].

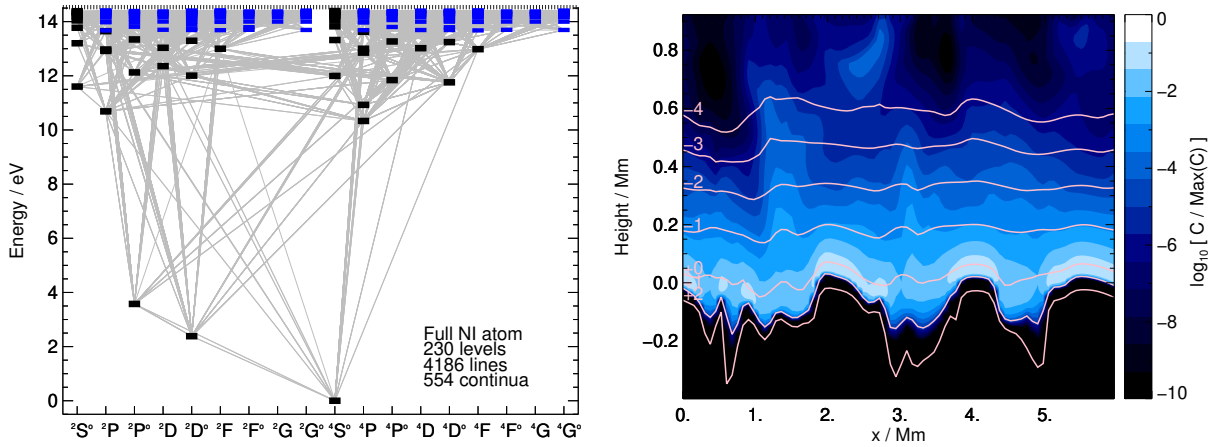

Figure 1: 3D non-LTE modelling of N I lines in the solar atmosphere [2]. *Left:* Term diagram illustrating the levels and transitions considered in statistical equilibrium. *Right:* Contribution function for the N I 868.34nm line in a vertical slice of a snapshot of the solar atmosphere.

I shall describe the state-of-the-art in modelling the spectra of late-type stars like our Sun. Such models are based on three-dimensional (3D) radiation-hydrodynamics and take into account departures from local thermodynamic equilibrium (non-LTE) [2,3]. I shall illustrate some of their successes, as well as their limitations, and thereby try to make the case for more reliable atomic data, in particular oscillator strengths, photoionisation cross-sections, and inelastic collision rates [4].

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Coronal Magnetic Field Measurements from EUV Wavelengths

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Coronal magnetic fields are at the heart of most of the unsolved problems in solar physics. The lack of precise measurements of coronal magnetic field has limited our investigation of many important topics in solar physics research including the driving mechanism of solar eruptions and the heating process of corona. In the past several decades, a number of techniques have been developed for coronal magnetic field diagnostics. Recently, a novel method by using unexpected transitions induced by external magnetic fields, so called magnetic-field-induced transitions (MITs) has been proposed for the magnetic field measurements in the solar and stellar coronae and subsequently received attention from the solar physics community. The most promising MIT candidate for coronal magnetic field measurements existed in EUV spectral lines of Fe X, in which the MIT is enhanced due to accidental close degeneracy between levels of short and long lifetimes [1-3]. It has been demonstrated that the Fe X MIT in EUV wavelength has great potential for solar and stellar coronal magnetic field diagnostics [4-9]. In this talk, I will report recent progress on the solar and stellar coronal magnetic field measurements from MIT method.

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The Athena X-ray Observatory Integral Field Unit (X-IFU): New Perspectives in the Study of the Universe Using High Resolution X-ray Spectroscopy

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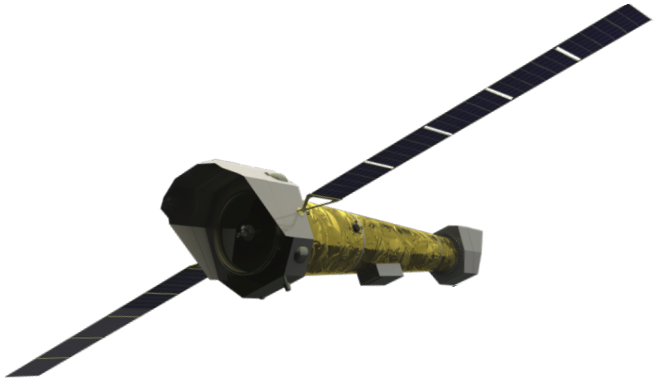
The Advanced Telescope for High ENergy Astrophysics (Athena) is the second large mission of the ESA Cosmic Vision science program. The X-ray Integral Field Unit (X-IFU), on board Athena, will provide spatially resolved high resolution spectroscopy from 0.2 to 12 keV with 5 arc second pixels over a nominal field of view of 4 arc minute equivalent diameter and a goal spectral resolution of 3 eV up to 7 keV, thanks to a ~1.5 kpixel array of microcalorimeters cooled down to 55 mK.

The core scientific objectives of Athena are defined in the science theme of the Hot and Energetic Universe:

- How does ordinary matter assemble into the large-scale structures we see today?
- How do black holes grow and shape the Universe?



Athena spacecraft artist's view (credit: IRAP, CNES, ESA).

Gas, heated to temperatures of tens of millions of degrees, resides in groups and clusters of galaxies. Stars in galaxies are collapsing at the end of their life, generating supernova explosions. These explosions generate heavy chemical elements, feeding galactic winds which, in turn, mix and push matter within and outside galaxies, triggering the birth of new stars.

X-IFU unique X-ray spectral images will give access to the nature of the emitting elements and their physical conditions such as temperature, speed and turbulence. The study of the associated astrophysical processes will require new model and laboratory data, as well as a careful calibration of the instrument and observational data.

The X-IFU will be provided by an international consortium led by France, The Netherlands and Italy, with ESA member state contributions from Belgium, Czech Republic, Finland, Germany, Poland, Spain, Switzerland, with additional contributions from the United States and Japan.

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Metallic Magnetic Calorimeters for High Precision of X-Ray Spectroscopy

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Metallic magnetic calorimeters (MMCs) are high energy resolution detectors operated at mK temperatures [1]. The achieved performance, like the energy resolution of 1.6 eV full width at half maximum (FWHM) at 6 keV and the reliable and stable energy calibration as well as the possibility to optimize the detector geometry for the particle/energy to be detected, motivated the use of MMCs for a large variety of applications. Figure 1 shows the energy spectrum acquired with a *maXs*-30 array while using an ^{241}Am calibration source. The photo of the 2D *maXs*-30 MMC array is shown in the inset of figure 1. The number of pixels is 64, covering an active area of 4 mm × 4 mm. The baseline resolution was determined to be 7.5 eV FWHM while at 60 keV the energy resolution was 9.8 eV FWHM indicating only a slight dependence of the energy resolution on the energy of the photon [2]. MMCs have also been optimized for measurements with radioactive sources fully contained in the absorber so that the emitted radiation can be detected with quantum efficiency close to unity. These measurements allow for the determination of the absolute intensities of different excitations. An example is the electron capture spectrum of ^{163}Ho whose interpretation has triggered several theoretical works [3].
After a short introduction on MMCs, a few key measurements will be presented with focus on the detector performance and the achieved results.

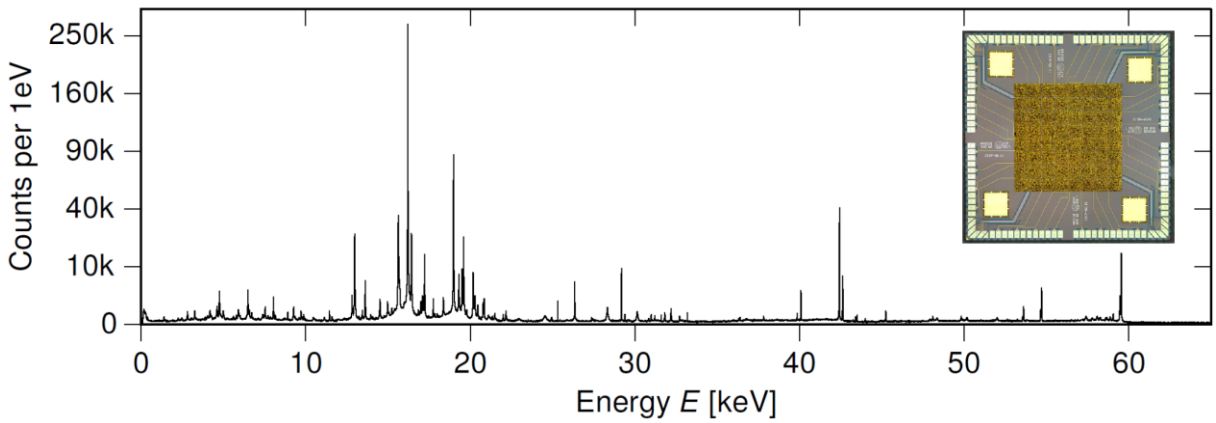

Figure 1: ^{241}Am spectrum acquired with the 2D *maXs*-30 MMC array showed in the inset of the spectrum. The chip size is 8 mm × 8 mm while the detection area in the middle, formed by 64 MMC pixels, has size 4 mm × 4 mm [2].

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Laboratory Atomic Astrophysics at Malmö University with Emphasis on the Infrared Spectral Region

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The infrared wavelength region continues to be the main focus of spectroscopic investigations of astrophysical plasmas. For example, the ESO ELT will have an echelle spectrograph (ANDES) with resolution of R≈100,000 and a simultaneous spectral range of 0.4 – 1.8 μm [1]. The infrared wavelength region is of particular interest due to the low scattering by particles, making it possible to observe stars in dust rich environments e.g., close to the Galactic center.

The important parameters needed for spectral analysis are wavelengths, energy levels, transition probabilities and line structures like hyperfine structure and isotopic shifts. However, atomic data in the infrared wavelength region is still scarce [2]. I will discuss laboratory measurements of wavelengths, energy levels, hyperfine structure and isotopic shifts in atoms and ions, with emphasis on the infrared spectral region. Furthermore, I will report recent and ongoing work at

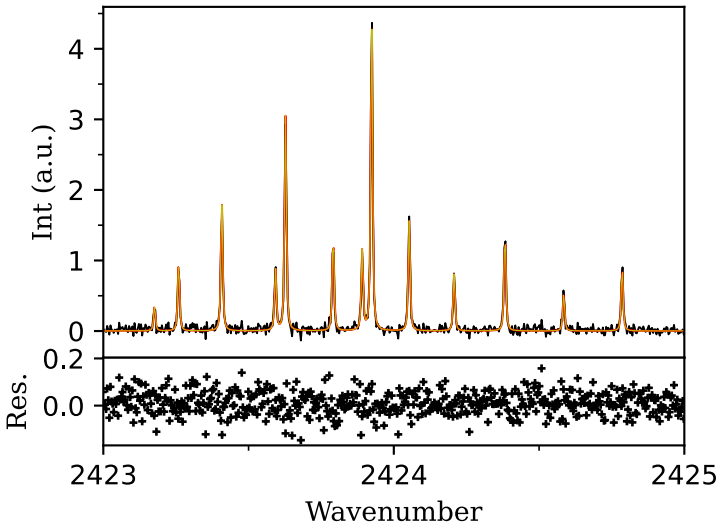

Figure 1: Infrared spectral line of In II showing large hyperfine structurer. The black spectrum is recorded with a Bruker 125HR IR FTS, and the red spectrum is a fitted spectrum. Bottom panel shows the residual between the recorded and fitted spectra.

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Spectroscopy Studies of Moderately Charged Tungsten, Sulfur, and Chlorine Ions at the SH-HTSCEBIT

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In this talk, we present the spectroscopy studies of moderately charged tungsten, sulfur, and chlorine ions during the past several years. To provide atomic data needed for magnetically confined fusion plasma diagnostics, the visible spectra of W^{7+} - W^{12+} have been measured using the Shanghai high-temperature superconducting electron beam ion trap (SH-HtscEBIT[1]) at Fudan University. The atomic structures of tungsten ions are given by our large-scale FAC[2] and GRASP[3] calculations. We utilize two methods to calculate the energy levels and the transition rates: the relativistic configuration interaction method with the FAC code and the multi-configuration Dirac-Hartree-Fock method with the GRASP package. To simulate spectra under different plasma conditions, a collisional-radiative model implemented in FAC is adopted. The calculated FAC and GRASP wavelengths agree with the experimental ones, except for a few lines. We hope that in the future, more theoretical studies will be conducted to address this discrepancy. To test the QED effects, the fine-structure splittings in S^{7+}, Cl^{8+}, S^{11+}, and Cl^{12+} have been measured with high precision at the SH-HtscEBIT. Their M1 transition energies are evaluated within the ab initio QED framework. The present experimental results agree with the theoretical calculations and provide a possibility to test QED effects and correlation effects with high accuracy in few-electron highly charged ions.

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Modeling for Spectroscopic Diagnostics of CCP-ICP and PBIF Plasmas in KAERI

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We report optical emission spectroscopy and collisional-radiative modeling (CRM) for diagnostics of He ICP (inductively coupled plasma) [1] and KPBIF (KAERI plasma beam irradiation facility) H/D plasmas [2], together with a Langmuir probe measurement, in low electron temperature regime (T_e ~ 5 eV). The CRM solves non-linear steady state balance equations including processes such as radiation rapping and heavy particle collisions self-consistently. The sensitivities of line spectra intensities and densities of particles to used atomic and molecular (AM) data [3] in the CRM was investigated (Fig. 1).

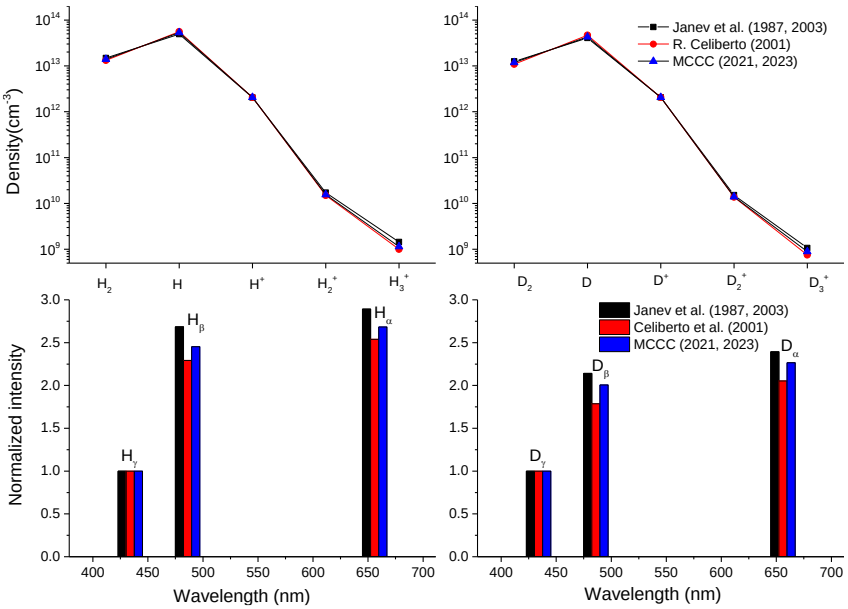

Figure 1: Population densities and line spectra intensities depending on various AM data.

In addition, measurements of S/XB ratios to determine sputtered flux of W I in KPBIF and the calculations by modeling using various atomic data on electron impact ionization/excitation and radiative decay are presented.

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Probing Strong Field Quantum Electrodynamics Through Precision Spectroscopy of Highly Charged Ions and Exotic Atoms

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Despite decades of effort, quantum electrodynamics (QED), the field theory that describes the interaction between light and charged particles, is poorly tested in the regime of strong coulomb fields. This is due to a confluence of difficulties linked to experimental limitations in highly-charged ion spectroscopy and nuclear uncertainties. I will show recent results from the Paris Double Crystal Spectrometer for He-like S [1] and Li-like Ar and S [2] for QED tests and astrophysics applications. The unique role of Bayesian analysis methods in untangling hidden contributions will be highlighted with a dedicated study of the influence of the atomic form factors on the response function of the Paris Double Crystal Spectrometer. I will then present a new paradigm for probing higher-order QED effects using spectroscopy of Rydberg states in exotic atoms, where orders of magnitude stronger field strengths can be achieved while nuclear uncertainties may be neglected [3]. Such tests are now possible due to the advent of quantum sensing detectors and new facilities providing low-energy intense beams of exotic particles for precision physics. I will present first results from experiments with muonic atoms at J-PARC within the context of the HEATES collaboration [4], and discuss a new project for antiprotonic atom spectroscopy at CERN.

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Hyperfine Resolved Laser Spectroscopy of Highly Charged I^{7+} Ions

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The study of hyperfine structures in many-electron highly charged ions (HCIs) can provide a deeper under- standing of strongly correlated electrons and serve as a benchmark for advanced theoretical calculations. Additionally, the possibility of using HCIs as atomic clock candidates emphasize the importance of hyperfine structures in many-electron HCIs [1]. However, there has been limited progress in hyperfine spectroscopy of many-electron HCIs due to experimental challenges. We successfully performed hyperfine-structure resolved laser spectroscopy of HCIs in an electron beam ion trap plasma. Here, we present laser-induced fluorescence (LIF) spectra of palladium-like I^{7+} in an electron beam ion trap (EBIT) plasma [2]. The electric quadrupole (E2) emissions ($(4d3/2^{-1}5s)J=2 \rightarrow (4d^{10})J=0$) induced by a pulse laser excitation via the magnetic dipole (M1) transition ($(4d5/2^{-1}5s)J=3 \rightarrow (4d3/2^{-1}5s)J=2$) were observed by a time-resolving extreme ultraviolet spectrometer directly coupled to the EBIT chamber. The collisional and radiative processes in the EBIT plasma provide a high population in the long-lived metastable state $(4d^{-1}5s)J=3$ and make it possible to continuously induce the E2 emission with the pulse laser irradiation. The small natural width of the transition between the metastable states without electric dipole (E1) decay paths enables to perform the high-precision wavelength measurement and reveals the hyperfine structure. Hyperfine structures were confirmed by theoretical calculations of hyperfine splittings and transition probabilities for $(4d5/2^{-1}5s)J=3$ and $(4d3/2^{-1}5s)J=2$ using the GRASP2018 [3].

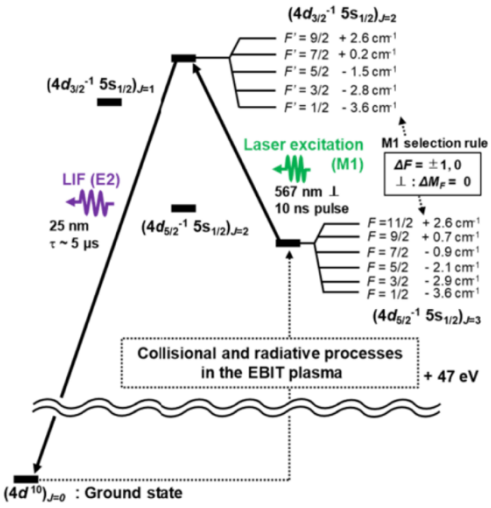

Figure 1. Schematic energy level diagram of $^{127}I^{7+}$ with the laser-induced transition.

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High-Resolution Laboratory Measurements of near Ar-like Fe EUV Line Emission using EBIT-I

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Ar-like Fe IX is formed over a broad range of solar temperatures, probing many solar structures. Its peak formation temperature, log[T(K)] = 5.9, is at the boundary between the transition region and the corona, making Fe IX a critical ion in understanding energy and mass flow into the corona. The Fe IX 241.74/244.91 Å intensity ratio is also predicted to be one of the best EUV density diagnostics for the solar corona. Despite this, the diagnostic is not commonly used, in part because previous observations by Orbiting Solar Observatory (OSO) 5, OSO 7, and Skylab, showed that the inferred electron densities differ significantly from those obtained from other ions. Uncertainties in the underlying atomic data have been proposed as one possible reason for the disagreement. Density diagnostics are very sensitive to uncertainties in the atomic data because they depend on many factors, such as collisional excitation and de-excitation rates, radiative transition rates, and cascade contributions from higher energy levels. Additionally, line blends, including those from other ions, can impact the accuracy of density diagnostics. In order to benchmark the density sensitive line ratio of the Fe IX line pair, we have measured the EUV line emission from Fe VII-Fe X in the wavelength range 238 to 258 Å at the Lawrence Livermore National Laboratory electron beam ion trap (EBIT-I). Here we report a new line survey of Fe VII-Fe X emission in this wavelength range and the implications for the 241.74/244.91 Å density diagnostic.

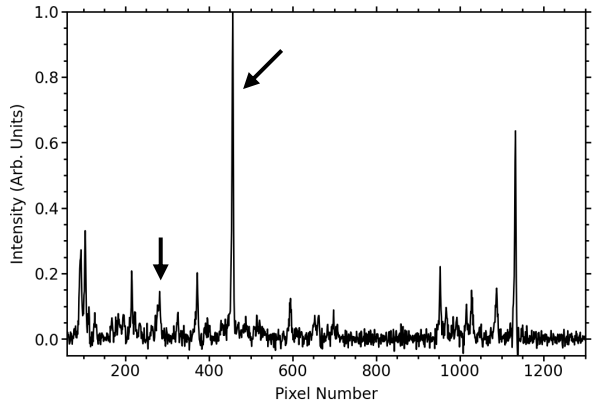

Figure 1: EBIT-I Fe VII-Fe X EUV line emission spectrum from 238 to 258 Å. The Fe IX 241.74 Å and 244.91 Å lines are indicated with arrows.

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Laboratory Measurements of Hyperfine Structure

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The theory of atomic hyperfine structure has been known for almost a hundred years and nearly 50 years ago, continuous-wave tunable single mode lasers heralded a new era in the study of atomic spectra. Since this time, a very large number of experimental and theoretical studies have been carried out. Despite these numerous studies, the data of hyperfine structure of almost all elements are still far from being fully known.

This lecture will give an overview of the current state of research and insight into recent studies on the hyperfine structure of atoms and atomic ions, which are carried out in recent years in collaboration with my cooperation partners at Istanbul University (Türkiye), Istanbul Technical University (Türkiye), University of Latvia (Latvia), Technical University Graz (Austria) and with other partners. Different spectroscopic methods and different spectral ranges were used in the different laboratories. By combining the experimental results of these different methods in different spectral ranges and by also include experimental and theoretical results from other research groups, new results could be obtained, which will be presented here by means of examples. A few examples of experimental atomic hyperfine structure spectra are already shown in Figure 1.

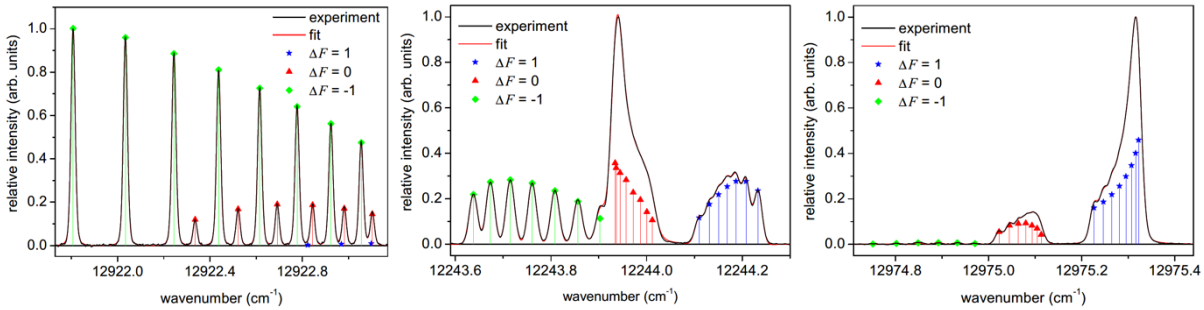

Figure 1: Examples of hyperfine structures of atomic Ho measured with laser-induced fluorescence spectroscopy [1]; experimental spectra together with the best fitted curves; the components are assigned by the difference F of the total angular momentum between the upper and lower hyperfine levels (for more details see [1])

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Storage Ring Measurements for Dielectronic Recombination of Na-like Fe^{15+}

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Dielectronic recombination (DR) is an impartant atomic process governing the charge balance in astrophysical and fusion plasmas, therefore, the accurate DR rate coefficients are required for interpretation of the plasma observations [1,2]. The absolute DR rate coefficients for sodium-like Fe^{15+} forming magnesium-like Fe^{14+} have been measured using the electron-ion merged-beam technique at the heavy ion storage ring CSRm at IMP, China. The measured DR rate coefficients, as shown in Figure 1, cover most of the DR resonances associated with the $3s \rightarrow 3p$ and $3s \rightarrow 3d$ core excitations ($\Delta N = 0$). In the range of 0-40 eV, our results agree very well with the previously DR measurement at the TSR [3]. Furthermore, we observed a clear signature in the range of 40-90 eV which belongs to $^2D_{3/2,5/2}\,nl$ resonances. We compare the experimental results with the calculations from AUTOSTRUCTURE and FAC and have a good agreement (comparison with JAC calculation is in progress). In addition, temperature dependent plasma recombination rate coefficients are derived from the measured DR rate coefficients and compared with the recommended atomic data from the literature [4].

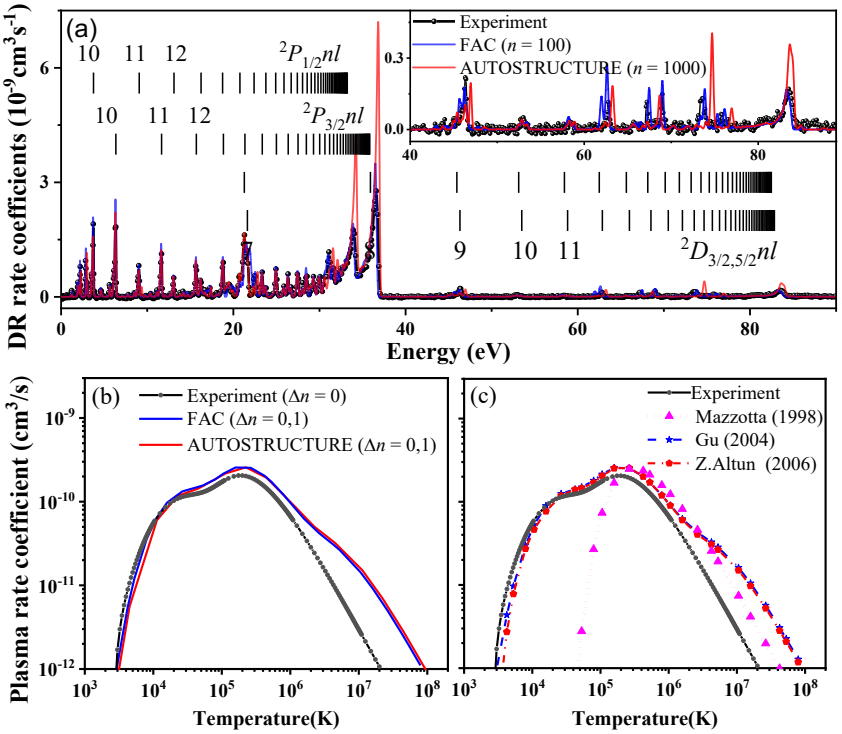

Figure 1. DR rate coefficients and plasma recombination rate coefficients of Na-like Fe^{15+}.

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Measuring Transition Probabilities of Rare-Earths: Experimental Requirements and Challenges

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Transition probabilities (Einstein coefficient for spontaneous emission, A_{ul}-values, $\log(g_i f_i)$) are essential atomic parameters that play a key role in a wide range of applications, from the lighting and laser development industry to the analysis of astrophysical spectra.

The Atomic Spectroscopy Laboratory at the University of Valladolid (Spain) has extensive experience in the measurement of transition probabilities using emission spectroscopy. After more than 30 years working on the noble gases, we have changed our focus to the measurement of transition probabilities of rare-earths given their current importance after the detection of the first kilonova [1]. As a light source, we use an in-house made water-cooled continuous hollow-cathode lamp under different conditions of carrier gas pressure and current (between 0.1 and 1 A). The radiation emitted by the lamp is analysed using a 1.5 m Jobin-Yvon monochromator with a 2400 lines/mm holographic diffraction grating (resolving power of 150 000 at 450 nm).

The determination of accurate spectral line intensities (area under the profile) is key to provide high-quality transition probabilities. We have conducted a detailed analysis of all the potential causes of uncertainty when measuring line intensities of rare-earth spectra with our experimental set-up. Key factors are: correct identification of lines, ability to resolve blends, stability of the hollow-cathode lamp, intensity calibration of the spectra and self-absorption correction for strong lines.

Due to the very crowded spectra of the rare-earths, knowledge of the intrinsic width of the spectral lines we want to observe (due to natural, Doppler and pressure broadening) is key to define our experimental requirements. The width of the monochromator´s entrance slit, the resolving power of the diffraction grating and the spatial resolution of the detector must work together to ensure that the total instrumental width is below the intrinsic width of the lines.

We have carried out a careful study of line widths for neodymium to define the minimum requirements our experimental set-up must meet to resolve these lines. We are currently using these findings to upgrade our laboratory for the measurement of the very rich rare-earth element spectra.

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Applications of Atomic Data to Studies of the Sun

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The wide range of temperature exhibited by the solar atmosphere, from 6000 K in the photosphere to over 20 MK in solar flares, makes it an important testing ground for atomic data of ionized ions. High signal-to-noise coupled with the ability to spatially discriminate a wide range of plasma structures has been valuable for identifying new atomic transitions and for assessing the accuracy of atomic data. The extreme ultraviolet (EUV: 10-91 nm) is of particular interest as it is very rich in emission lines but is mostly absorbed by the interstellar medium for other stars in the Milky Way. In this talk I summarize current and upcoming Solar Physics instrumentation and identify atomic data needs. Techniques for analyzing solar spectra are described, with a particular focus on how the CHIANTI atomic database is used by Solar Physicists. CHIANTI is an open-source database and software package for modeling emission line spectra and continuum emission.

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Evaluating Atomic Data Needs for X-Ray Astrophysics with the AtomDB Atomic Database

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The AtomDB project (www.atomdb.org) is a combination of a large atomic database and several spectral models designed for modeling emission from optically thin, X-ray emitting plasmas. The code and database are optimized in the EUV and X-ray ranges ($1 < \lambda < 1240$Å), although the models cover a wider range of spectra.

The upcoming launch of high resolution X-ray calorimeter on the NASA XRISM mission, which will have unprecedented spectral resolution in the $2<E_{phot}<10$ keV range, creates a new impetus for updating and interpreting X-ray spectra. In addition, other proposed instruments in the soft X-ray and EUV will place tighter requirements on the accuracy of atomic data to enable accurate interpretation of results.

We present here a general outline of the AtomDB project, including the range of plasmas which it is designed to model including equilibrium, non-equilibrium, charge exchange and non-Maxwellian plasmas. We then discuss ways to identify the limitations to diagnostic accuracy imposed by the current knowledge of atomic data using our *variableapec* software. Finally, we outline ways of estimating the uncertainties on atomic data and resulting line diagnostics from first principles, enabling us to identify which diagnostics may only be effective with improved experimental measurements.

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Larry J Curtis 1935-2020: A Brief History: His Revelations in Atomic Structure and Dynamics

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I will very briefly review the 40-year career of Larry Curtis and his discoveries both experimental and theoretical. The focus will be limited to three atomic physics areas in which he played a principal part: these include the first observations of light from oriented atoms; observations of light from doubly-excited states in light atoms (helium and lithium). These include the verification of the only light ever observed from a negative atomic ion; thirdly, his theoretical analysis multiple exponential decays, enhancing the precision of beam-foil measurements of atomic lifetimes. Finally, some reminiscences about his personal life, his Swedish honorary doctorate, his wife Maj Rosander, and other European adventures.

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EVALUATION OF UNCERTAINTIES IN ATOMIC DATA ON SPECTRAL LINES AND TRANSITION PROBABILITIES

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This talk will discuss some recent advances in methods of critical evaluation of experimental data on wavelengths of spectral lines and theoretical data on transition probabilities and oscillator strengths for atoms and atomic ions. In particular, recently developed new statistical approaches to estimation of uncertainties of weighted means of multiple measurements are described, and a numerical toolbox implementing these new approaches is presented. There are also some new developments in estimation of uncertainties of theoretical transition probabilities. A short review of literature implementing these new procedures is provided, including a description of the methodology.

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The XSTAR Atomic Database

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XSTAR [1] is a spectral modeling code of photoionized plasmas widely used in X-ray astronomy. It relies on an extensive atomic database for elements with atomic number $Z \leq 30$ [2, 3], which has taken over 20 years to compute in-house and collect from diverse sources. The XSTAR database emphasizes the descriptions of the recombination spectra of H- and He-like ions [4, 5] and the transition arrays associated with the K edge (namely, Kα and Kβ lines) due to their plasma diagnostic potential (see [3] and references therein), but the database also includes radiative and collisional rates for processes involving the valence shell. In this presentation, we bring to the fore the perspective of the atomic-data user and the adaptations that must be made to the atomic datasets, e.g., line positions and high-density effects, to be able to model astrophysical systems reliably [6, 7, 8]. We are particularly concerned with the modeling of the reflection spectrum of the high-density ($n_e > 10^{18}$ cm^{-3}) inner region of AGN accretion disks to deduce the black-hole spin. In this respect, the consistently high iron abundances currently obtained from the flagship Fe Kα lines are believed to be indicators of missing atomic processes [9].

We will also briefly discuss database maintenance difficulties that have led to the development of the Python module PyXstarDB to automate atomic data collecting from online databases (e.g., CHIANTI [10]. and NIST [11]) into an SQLite environment, which may also be of interest to prospective modelers.

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Assessment of the FAIRness of the Virtual Atomic and Molecular Data Centre following the Research Data Alliance Evaluation Framework

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We will present the result of the analysis [1] made on the Virtual Atomic and Molecular Data Centre infrastructure [1], following the FAIR Data Maturity Model framework defined by the Research Data Alliance [2]: after recalling the technical architecture of the VAMDC infrastructure, we will introduce the RDA FAIR evaluation framework and define the methodology we adopt to perform our analysis. After having presented the results, we will conclude with some lines of work aimed at improving the FAIRness of VAMDC, together with some ideas for further development of this work.

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Charge Exchange Recombination Spectroscopy of W Ions for ITER Neutral H-Beam Diagnostics

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Charge-exchange recombination spectroscopy (CXRS) remains one of the most important diagnostic methods for existing and future magnetic fusion devices. In particular, the CXRS with energetic neutral beams of hydrogen will be a key diagnostic tool for ITER where interactions with its important impurity, namely, tungsten, should result in new spectral features to be analyzed. The results of the present spectral synthesis are based on the new set of *nl*-resolved CX cross sections for recombination of the W^{q+} ions (q = 61-66) with atomic hydrogen calculated using the classical trajectory Monte Carlo method for the planned ITER neutral beams (diagnostic beam of 100 keV/u and heating beam of ~ 1 MeV/u). These calculated CX cross sections, along with the atomic data needed for other relevant physical processes, were used in a large-scale collisional-radiative model to study the population kinetics of atomic states of the tungsten ions and to generate the synthetic spectra across a wide range of photon energies. The simulations demonstrated that the CX-induced emission drastically modifies the observed spectrum in the visible and VUV ranges for the interaction with diagnostics neutral beam, which can provide important predictions for interpretation and evaluation of the CXRS diagnostics on ITER. Details of the theoretical calculations and results will be presented and discussed.

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Magnetically-Confined Nuclear Fusion and Atomic Data

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Atomic physics and spectroscopy are intertwined in the history of fusion. Unlike astrophysical plasmas, laboratory fusion experiments, such as tokamaks, have independent measurements of the local electron temperature and density. They are therefore less reliant on traditional line ratio methods for diagnosing the plasma environment but these plasmas cover a very wide parameter range and present demanding challenges to atomic physics. High magnetic fields, large gradients in electron temperature and density, fast fluctuations and non-Maxwellian electrons and conditions which favour both highly charged ions and un-dissociated molecules in the same plasma are some of the interesting situations which must be considered when using atomic physics to model the radiation properties of fusion plasmas and to interpret spectroscopic measurements as diagnostics of the plasma. Many of the atomic based measurements are needed in terms of engineering or operational parameters and are therefore the result of a synthesis and reduction of large amounts of fundamental atomic data via, primarily, collisional-radiative models. The uses for machine protection, operating scenario design, impurity content detection and understanding plasma transport places demands on the availability and precision of atomic data.

This talk will give an overview of the quality of atomic and molecular data used in magnetically confined fusion analysis. The basis for all calculated data is a good atomic structure and how this influences the many processes involved is explored. The choices, and comprises, made in calculating cooling curves for low, medium and high-Z elements is examined from the point of view of controlling the radiated power and spectroscopy. The specific challenges for the atomic data and models of tungsten in its journey from a neutral influx species to X-ray emitter in the core illustrates the successes of recent work but also highlights that significant and essential work is needed in fundamental atomic physics.

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