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Abstract Book

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INVITED TALKS

When Michel's favorite tiny electrons fool the big atomic nuclei in the skies

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The atomic physics playground of Michel broadly pervades many fields of astrophysics. My talk illustrates this statement through the example of "bound-state beta-decay". Stellar conditions are especially favourable for the development of this mechanism that is highly marginal in normal laboratory conditions. It is indeed extremely sensitive to the ionisation state of the ions, which is in turn highly dependent on the temperatures attained in stellar situations. In particular, high, and even full, ionisation can be obtained in hot stellar interiors, which allows bound-state beta-decay to fully operate.

An introductory presentation of the relevant astrophysical context will help the non-expert to have some grips on the briefly discussed implications of bound-state beta-decay for nucleosynthesis, cosmochronology and cosmochemistry.

Precision Stellar Spectroscopy

Martin Asplund
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Stellar spectroscopy is firmly in the precision era. High-resolution spectrographs, including multi-object facilities, ensure that high-quality observations are obtained across a wide wavelength range. Accurate measurements and calculations of key atomic physics data are now available for most elements and molecules of astronomical significance, including transition probabilities, opacities, and radiative and collisional cross-sections for a wide range of atomic processes. Paralleling these important developments is major progress in modelling the stellar atmospheres and spectral line formation by means of 3D hydrodynamical stellar models and 3D non-LTE radiative transfer.

In this review talk, I will highlight a few examples of precision stellar spectroscopy and their implications for the broader field of astronomy and cosmology. The focus will be on the stellar modelling aspects leaving the impressive progress in atomic physics to other speakers. In particular I will discuss the solar chemical composition and the ongoing conflict with solar interior modelling as evident from helioseismology. I will also present evidence that the Sun in fact has an unusual abundance pattern which likely stems from the formation of planets. The effects of 3D non-LTE spectrum formation compared with classical 1D LTE modelling is particularly pronounced in extremely metal-poor stars, although the long-standing cosmological Li problem cannot be traced to faults with the spectroscopic analysis. I will finish by discussing how it is now possible to exploit 3D non-LTE spectral line formation together with a multitude of auxiliary information (e.g. photometry, parallaxes, asteroseismology, stellar evolution models) in a Bayesian framework for large spectroscopic surveys containing millions of stars to put the results and interpretations on a secure theoretical foundation.

Advances in the Spectroscopy of Highly Charged Ions for Astrophysics, Plasma Science, and Fundamental Physics

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Spectroscopy has been the enabling tool for research in multiple branches of physics, and the application of new spectroscopic technology is leading the way for advances in x-ray astronomy, plasma physics, atomic physics, and fundamental science. For example, X-ray microcalorimeters are now providing unprecedented high-resolution spectral measurements over the entire x-ray region at once, leading to new insights into x rays from comets, atomic cross sections, and nuclear decay schemes. Compact, broadband EUV spectrometers allow easy coverage of plasma impurity species and the calibration of astrophysical density diagnostics. Advanced grating spectrometers have the resolution needed to test QED in highly charged ions at levels that go beyond those achieved with laser spectroscopy in atomic hydrogen and are now applied to the study of two-loop QED and QED in the presence of nuclear magnetic fields. New crystal geometries make possible imaging of plasmas of all sizes from the core of the ITER tokamak to short-pulse laser-heated microdot targets. This talk will highlight some of the technological advances and the resulting new physics during the past decade.

Precision calculations of atomic and ionic spectra and searches for new physics

Julian C. Berengut
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The spectral properties of atoms and ions with more than a few electrons cannot be calculated with extremely high accuracy. Therefore, despite the extraordinary accuracy of precision spectroscopy, it is difficult to test the Standard Model in atomic systems by direct comparison of theory and experiment. On the other hand, differential measurements - for which the theory can be made sufficiently accurate - can provide strong tests of new physics.

Differential measurements in atomic systems include: searches for parity-invariance and time-invariance violating amplitudes to probe the weak interaction [1]; changes in spectral energies over space and time to probe potential variations in fundamental constants [2] and violations of Lorentz invariance [3]; and precision isotope-shift measurements which could uncover new force-carrying particles [4]. In this talk I will discuss some recent developments in these searches. In particular I will discuss emerging precision studies in highly charged ions, where the effects of new physics can be strongly enhanced [5].

A promising route to calculations in complicated atoms is the particle-hole configuration interaction with many-body perturbation theory (CI+MBPT) method [6]. This extends the CI+MBPT method [7] to non-perturbatively include configurations with electron holes below the designated Fermi level. The method has been implemented in AMBiT [8], a software package for fully relativistic, ab initio atomic structure calculations. The software is written in modern C++11, 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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[8] E. V. Kahl and J. C. Berengut, CPC 238, 232 (2019); https://github.com/drjuls/AMBiT.

Perspectives for laser spectroscopy of the heaviest elements

M. Block[1,2,3]

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The heaviest elements with $Z \geq 100$ owe their existence to nuclear shell effects in a subtle balance of the strong interaction and the Coulomb repulsion. Their nuclei may thus exhibit phenomena not present in lighter nuclei. For example, a central depression of about ten percent of the proton distribution has been predicted to occur in the heaviest nuclei by different mdoels. At the same time, the atomic structure of the heaviest elements is strongly influenced by relativistic effects, quantum electrodynamics and electron correlations. A powerful experimental approach to study atomic and nuclear properties of these exotic nuclides is through laser spectroscopy. The investigation of the heaviest elements is experimentally challenging due to lowest production rates, rather short half-lives and their production at relatively high energy. Recently, tailored methods of highest sensitivity have been developed to tackle these challenges. Guided by accurate theoretical predictions atomic transitions in No isotopes have been identified in pioneering laser spectroscopy experiments at the GSI in Darmstadt, Germany in the framework of the FAIR Phase-0 program [1-3]. These experiments have recently been complemented by data for long-lived actinides such as Es and Fm taken at Mainz university. In the near future the main task will be to further improve the sensitivity, the efficiency, and the resolution of laser spectroscopy to extend its reach towards the realm of superheavy elements. In my presentation I will summarize the recent experimental progress and discuss the perspectives for future experiments beyond nobelium.

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[1] M. Laatiaoui, Nature 538 (2016) 495
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Atomic calculations for the determination of magnetic fields in the solar corona and to support laser cooling of negative ions

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We will discuss two examples of projects where atomic structure theory is essential to solve important problems in both astrophysics and fundamental physics.

In the first example, we discuss the use of transitions induced in ions by an external magnetic field. These are caused by a quantum mechanical interference between states with very different lifetimes in ions. In turn this interference is enhanced by a pseudo-degeneracy, that makes it possible to monitor fields that are weak compared to the enormous fields inside the atom. An important application is the monitoring of the magnetic fields in the active region of the solar corona, which has evaded measurement so far. This is important, since this could lead to an understanding of the heating of the corona and the origin and prediction of space weather.

The second example is laser-cooling to create ultra-cold, negative ions (e.g. anti-protons) for measurements of fundamental properties. So far, the cooling of neutral and positive ions are well-established, but no working scheme for a negative ion has been confirmed. This is due to the lack of bound states in these species and therefore so far, no possible cyclic transition for cooling. We will present a recent discovery of such a transition in a negative ion, and thereby a candidate for laser cooling of anions.

In the Beginning

Charlotte Froese Fischer
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Laser spectroscopy of radioactive and stable negative ions

Dag Hanstorp
University of Gothenburg, Sweden

The extra electron in a negative ion does not experience the Coulomb force from the nucleus at large distances. Instead, core polarization induced by the extra electron stabilizes the ion. This correlated motion of the electrons requires theoretical models that go beyond the independent particle approximation. Experimental investigations of the structure and dynamics of negative ions can hence lead to an increased understanding of many-electron systems.

In this presentation, the general properties of negative ions and various experimental techniques to study these fragile quantum systems will be discussed. First, I will give an overview the basic concept of laser photo detachment spectroscopy, which yields information about bound as well as continuum structures of negative ions. Second, an experiment where a femtosecond laser and a velocity map imaging (VMI) spectrometer is used to visualize the electronic motion in the ground state of the carbon atom will be discussed. Thereafter, investigations of life-times of long-lived excited states of negative ions using the cryogenic electrostatic double storage ring DESIREE at Stockholm University, will be presented. Finally, I will discuss results from studies of radioactive isotopes of negative ions conducted at ISOLDE at CERN. The very first experimental investigation of the electron affinity of astatine, the least abundant element on earth, will be presented and future plans for studies of isotope shifts in electron affinities will be discussed.

Core-Collapse Supernovae and Nucleosynthesis

Hans-Thomas Janka
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The talk will review recent progress in our understanding of explosions of massive stars, focusing on theoretical work and computational modeling. The corresponding evolution of our picture of chemical element formation in supernovae will direct the presentation.

New developments in relativistic Multiconfiguration Calculations

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There is an increasing demand for accurate atomic data due to advancements in experimental techniques and investments in large scale research facilities. In astrophysics the quality and resolution of solar and stellar spectra has so improved that the accuracy of atomic data is frequently a limiting factor in the interpretation. Accurate atomic data are also required in plasma physics and in other emerging areas such as laser spectroscopy on isotope separators, X-ray lithography, and lighting research. The needs include accurate transition energies, fine- and hyperfine structures, mass- and field shifts as well as parameters related to interaction with external magnetic fields. Also, there is a constant need for transition rates of different multi- polarities between excited states. Data are needed for a wide range of elements and ionization stages.

To meet the demands for accurate atomic data the COMPutational Atomic Structure (COMPAS) group has been formed. The group is involved in developing state of the art computer codes for atomic structure calculations in the non-relativistic scheme with relativistic corrections in the Breit-Pauli approximation [1] as well as in the fully relativistic domain. Here we describe new developments of the GRASP relativistic atomic structure code [2]. We present results for a number of systems and properties to illustrate the potential and restriction of modern computational atomic structure. Among the properties are transition rates, hyperfine- and magnetically induced rates, energy structure, and isotope shifts. We also discuss current code developments and plans for future work.

The codes developed by the COMPAS group, along with detailed user manuals, are freely available at http://ddwap.mah.se/tsjoek/compas/.

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Theory of polyvalent atoms

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At present atoms and ions are often used as precision instruments to study fundamental physics and to search for “new physics” beyond the Standard model. For this purpose, we need calculations of atomic properties which cannot be directly tested experimentally. Therefore, we need to develop reliable, accurate, and sufficiently general methods for atomic calculations. Experimental techniques are rapidly developing allowing for precision experiments with more and more complex atomic particles including highly charged ions and polyvalent atoms with dense spectra. Such systems may be very sensitive to the new physics, but are very difficult to calculate. In this talk I will discuss how atomic theory can meet these challenges.

Dense Matter Equation of State from Compact Object Mergers

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Stony Brook University

The recent detection of gravitational waves and electromagnetic emissions from the binary neutron star merger GW170817 resulted in stringent limits concerning the masses and radii of the coalescing stars and also the neutron star maximum mass. These estimates complement ongoing measurements from pulsar timing and X-ray observations as well as theoretical limits stemming from neutron matter theory and condensed matter and nuclear experiments. There are important ramifications for the dense matter equation of state. Additional gravitational wave events together with new results from the NICER X-ray mission will continue the excitement in this topic.

Laser spectroscopy as a probe for the size and shape of exotic nuclei

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High-resolution optical measurements of the atomic level structure readily yield fundamental and model-independent data on nuclear ground and isomeric states, namely changes in the size and shape of the nucleus, as well as the nuclear spin and electromagnetic moments. Laser spectroscopy combined with on-line isotope separators and novel ion manipulation techniques provides the only mechanism for such studies in exotic nuclear systems.

Atomic nuclei exhibit a rich array of quantum phenomena, with nucleonic shell structure somewhat similar to that of electronic structure in atoms and magic nuclei at specific numbers of neutrons and protons. Single-particle structure and the evolution of the traditional quantum shells as one moves away from stable nuclei is of long-standing interest both from an experimental and theoretical viewpoint. Away from the magic numbers, nuclei start to exhibit collective effects, in other words deformation, driven by an increase in nucleon-nucleon correlations. Even more strikingly is the observation that nuclei can exhibit more than one shape within the same isotope, and this effect has created a plethora of studies in different areas of the nuclear chart.

This contribution will provide a brief overview to some of the traditional methods used in the field of laser spectroscopy of exotic nuclei, highlighting the benefits and limitations of the different approaches. As will be shown, optical spectroscopy is an incredibly sensitive probe to sudden changes in nuclear shape, which can be driven simply by the addition or removal of a single neutron along an isotopic chain. I will show how the nuclear shape has provided one of the greatest motivations for optical spectroscopy of the nucleus, and therefore a critical and complementary connection to the general field of nuclear spectroscopy, which often relies on other methods, for example gamma-ray spectroscopy.

I will present regions of the nuclear chart of current active interest to the study of shapes, shape coexistence and more generally, changes in the nuclear size. This will include the region around mass A=100 which has been well studied in Jyväskylä using high-resolution spectroscopy, as well as the region below doubly-magic lead, extensively probed at ISOLDE using sensitive (yet lower resolution) in-source spectroscopy. The possibility to access higher order deformations, for example octupole (pear-shaped) nuclei will be discussed in connection to future avenues of research, in particularly accessing actinide elements. I will also highlight the very close connection between experiment and theory, required in order to gain a more intuitive understanding of the complexity of nuclei as many-body quantum systems.

Where are the limits of the periodic table?

Witold Nazarewicz
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This year marks the 150th anniversary of the formulation of the periodic table created by Dmitry Mendeleev. Accordingly, the United Nations proclaimed 2019 as the International Year of the Periodic Table of Chemical Elements. At 150 years old, the table is still growing. In 2016, four new elements were added: nihonium, moscovium, tennessine and oganesson. These elements define the current upper limits of mass and atomic numbers. As such, they carry the potential to transform the way we currently understand nuclear and atomic physics, and chemistry.

All elements with more than 103 protons are labeled as “superheavy". The speaker will discuss questions motivating the search for these systems: What are the heaviest nuclei and atoms that can exist? Are superheavy systems different from lighter nuclear species? Is there an island of very long-lived nuclei? Can superheavy nuclei be produced in stellar explosions? Questions such as these provide formidable challenges for science.

Further reading:
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Rev. Mod. Phys. 91, 011001 (2019).

Electrons spy the Nucleus: Laser Spectroscopic Determination of Nuclear Charge Radii

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Laser spectroscopy provides a unique tool to address nuclear ground-state properties, particularly the spin, the charge radius and nuclear moments. The technique can provide nuclear-model independent values for these observables, extracted from isotope shift and hyperfine structure measurements. It is especially versatile for short-lived isotope since even isotopes with lifetimes on the 1-ms scale can be addressed. This talk will concentrate on the determination of nuclear charge radii from light to medium-mass elements and their comparison with predictions from nuclear structure theory. In light nuclei, charge radii provide information on the cluster and halo structure, which are very prominent features in this region and recent work on boron isotopes will be presented [1]. In the medium-mass region recent efforts have concentrated on tests of nuclear charge radii predictions by ab-initio calculations based on chiral effective field theory as well as by density functional theory for example in [2,3,4,5,6].

Finally, our current aims to work towards the determination of all-optical charge radii for light systems that do not rely anymore on the combination with charge radii extracted from elastic electron scattering will be discussed.

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Spectroscopy to Support Short Wavelength Light Source Development

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Laser produced plasmas (LPPs) are versatile sources of extreme ultraviolet (EUV) or soft x-ray (SXR) radiation. Depending on the choice of target they can generate continuum or line radiation and indeed one of the first reported applications was their use as continuum sources for studies of inner shell photoexcitation of atoms and ions. In plasmas of some medium and high Z elements the short wavelength emission spectrum is dominated by intense bands of emission arising from unresolved transition arrays (UTAs) that result from resonance 4*d*-4*f* and 4*p*-4*d* transitions in a range of ion stages that overlap within a narrow wavelength range and whose intensity and spectral profile is very sensitive to plasma opacity. Since the critical density of LPPs is approximately $10^{21}(\lambda_L^{-2})$ cm^3, where λ_L is the laser wavelength in μm, plasmas produced by solid state lasers with $\lambda_L \leq 1$ μm, are, in general, optically thick. However the opacity can be reduced by using longer wavelength lasers, low density or foam targets, dual pulse irradiation to produce a lower density plasma that can be reheated by the main laser pulse or by using sub nanosecond pulses since opacity also increases with laser pulse duration. These observations have been successfully exploited in EUV lithography sources where power outputs exceeding 200 W in a 2% bandwidth centred on 13.6 nm are generated using tin droplet sources irradiated by a 1.06 μm pre-pulse followed by a 10.6 μm main pulse. However the production of similar power levels at shorter wavelengths remains a major challenge since the conversion efficiency, which depends on the ion stage distribution in the plasma, decreases due to need to produce higher ion stages.

More recently the application of LPPs as sources for biomedical imaging in the water window (2.4 – 4.3 nm) has become a topic of considerable interest following on the development of optical components such as multilayer mirrors and zone plates that can be used in this spectral region. Traditionally such work has been performed at synchrotron sources and laboratory based 'table top' alternatives are attractive in order to meet researcher requirements. Here microscope systems based on resonance lines of nitrogen and carbon ions have been developed and research is ongoing on the potential using of UTA emission. This work has being largely based on studies of $n = 4 – n = 4$ emission in plasmas of very high Z elements and $n = 3 – n = 4$ transitions in intermediate Z elements. Since imaging requires a small plasma size, lasers with pulse durations of a few hundred picoseconds or less, sufficient to produce the ion stages required but short enough to limit plasma expansion are required. However more work needs to be done to establish the optimum laser irradiation conditions for particular promising target materials which in turn depend on the availability of suitable optics. Moreover, such imaging systems are not without competition and alternative strategies based on the use of high harmonics with coherent diffractive imaging are starting to emerge.

Atoms and Molecules in Stellar Atmospheres

Bertrand Plez
U. Montpellier, Montpellier, France

Atomic and molecular lines make a strong imprint on stellar spectra, and are ubiquitous at all wavelengths in cool star spectra. They also have a profound impact on the thermal structure of cool star atmospheres. Large efforts have been devoted in recent years to compute and assemble line lists for model atmosphere and spectra calculations. I will show a few illustrative examples, including CH where Michel Godefroid contributed to creating a line list which in particular solved the enigma of the Bond-Neff depression in Ba stars.

Nuclei and matter: From fundamental interactions to structure and stars

Achim Schwenk
Technische U. Darmstadt, Darmstadt, Germany

The strong interaction described by quantum chromodynamics gives rise to the formation of hadrons and nuclei that constitute the baryonic matter in the Universe and governs the densest matter in neutron stars and highest temperatures reached in compact object mergers. Combined with the electroweak interaction, it determines the structure and properties of all nuclei in the nuclear chart in a similar way as quantum electrodynamics shapes the periodic table of elements. However, big science problems of the strong interaction remain unsolved, especially regarding the structure of extreme neutron-rich matter in the laboratory and stars.

New facilities for rare isotopes will discover over a thousand new isotopes, getting as close as possible to the nuclei in the Universe's heavy-element nucleosynthesis pathway. On the theoretical side, there are impressive advances towards a unified description of all nuclei and matter based on effective field theories of the strong interaction combined with powerful many-body methods. In this talk, we will discuss the advances, status and challenges in understanding and predicting strongly interacting matter, with a focus on how the nuclear chart emerges from nuclear forces. In addition, we will discuss new opportunities in the exploration of electroweak interactions in nuclei, which provide unique insights to nuclear structure and are key for tests of fundamental symmetries as well as for nuclear and particle astrophysics.

The Impact of improved Atomic Physics on the Chemical Compositions of Low Metallicity Stars

Chris Sneden
Department of Astronomy, University of Texas

Accurate stellar abundances are crucial inputs for progress toward understanding Galactic birth and chemical evolution with time. Determining trustworthy abundances requires excellence in all inputs: high-resolution stellar spectra, laboratory-based atomic and molecular line data, detailed model atmospheres, and radiative transfer analytical techniques. In this talk we will focus on the quiet revolution in laboratory atomic and molecular physics that has nearly solved the need for accurate line data in many small- and large-scale chemical composition studies of low metallicity Galactic halo stars. Examples of obvious successes will be shown, along with suggestions for future studies that will yield significant improvements in abundances of both metal-poor and metal-rich stellar populations.

Solvay Colloquium

Galactic Palaeontology

Eline Tolstoy
University of Groningen, The Netherlands

I will talk about how observations of resolved stellar populations are being used to study the ancient fossil record of the formation and evolution of stars and the resulting chemical element production in nearby galaxies. This can only be done nearby, as it requires accurate colours, variability, chemical abundances and kinematic measurements of large samples of individual low mass stars from deep imaging and spectroscopy surveys. These studies provide detailed insights into galaxy evolution going back to the early Universe. I will concentrate on what we can learn from the smallest and simplest of galaxies, the so-called dwarf galaxies, but I will also make the link to our increasingly detailed understanding of our home galaxy, the Milky Way, and the role that chemical elements play in disentangling the story of all galaxies.

CONTRIBUTED TALKS

A new assessment of the solar s- and r- process components from a galactic chemical evolution with rotating massive stars yields

Carlos Abia et al.
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We present a new method for determining the s- and r- components of the Solar system abundances, fully consistent with our current understanding of stellar nucleosynthesis and galactic chemical evolution. The method is based on a study of the evolution of the solar neighborhood with a state-of-the-art 1-zone model, using recent yields of low and intermediate mass stars as well as of massive rotating stars. We compare our results with previous studies and we provide tables with the isotopic and elemental contributions of the s- and r-processes to the Solar system composition.

Precision big bang nucleosynthesis

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Big bang nucleosynthesis (BBN) is one of the three observational evidences for the big bang model. In the standard BBN model, the thermodynamic conditions can be calculated exactly, given the baryonic density of the universe. Hence, it is possible to accurately calculate the abundances of the "light elements" (^{4}He, D, ^{3}He and ^{7}Li) produced during BBN. There is indeed a good agreement between ^{4}He, D, and ^{3}He primordial abundances, either deduced from observation or from BBN calculations. In particular, precision on primordial abundances, deduced from observations, have now reached the percent level for ^{4}He and deuterium. To achieve the same level of precision in BBN predictions, the involved nuclear [1,2] and particle [3] physics need to be thoroughly investigated. (A state of the art code, including the, presently, most elaborate microphysics as recently been made freely available [3]). On the contrary, there is a tantalizing discrepancy of a factor of ≈3 between the primordial ^{7}Li abundance deduced from observations of halo stars, and the BBN calculations. Solutions to this problem have been proposed, involving stellar physics, non-standard BBN models, or nuclear physics, but none is fully satisfactory [1]. In spite of this lithium problem, BBN remains a valuable tool to probe the physics of the early universe, as it is, when we look back in time, the last milestone of known laboratory physics.

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New Frontiers in optical spectroscopy of radioactive nuclei: a case study on the silver isotopes

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Novel instrumentation developed for optical spectroscopy of radioactive nuclei has developed tremendously over the past years. I will explore some of the rich nuclear and atomic physics that we can extract with these new tools, using the silver isotope chain as a case study.

Recently, measurements on the silver isotopes were pushed to close to the $N=Z$ line using highly efficient in-source laser ionization spectroscopy, coupled to ultra-high mass resolving power penning trap purification techniques. Data has been collected to ^{96}Ag, thus crossing the N=50 neutron shell closure, with measurements aiming for ^{94}Ag planned soon. These measurements truly represent the *sensitivity frontier* for optical spectroscopy.

In addition to these lower resolution measurements, we also obtained new data with high-resolution collinear laser spectroscopy on neutron-rich isotopes, which trades in efficiency for two orders of magnitude better resolution. Using this precision, intriguing trends in the magnetic dipole moments of the $^{107\text{-}121}$Ag isotopes can be resolved. These patterns, also observed in the magnetic moments of indium, provide an interesting puzzle for the current state-of-the-art in nuclear theory.

These collinear laser spectroscopy measurements lead us to the *precision frontier* for nuclear structure studies. As an outlook to the future, I will discuss very recent measurements on stable silver and scandium, which combine laser resonance ionization with magnetic resonance methods, elevating the precision of optical spectroscopy by another two to three orders of magnitude. With this, higher-order effects (e.g. hyperfine anomalies, magnetic octupole moments, hyperfine mixing…) may be probed on exotic nuclei. The implications for future measurements on radioactive nuclei will be discussed.

Atomic data and solar spectral diagnostics, from the X-rays to the near infrared

Giulio Del Zanna and Roger P. Dufresne

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We provide an overview of recent atomic calculations and modeling that our group has recently carried out in collaborations with various other groups, and provide examples on the importance of accurate and complete atomic data and modeling for the analysis of solar spectra, in particular for measurements of electron densities, temperatures and chemical abundances. (cf. the review by Del Zanna & Mason[1].

Within the UK APAP team, we are providing to the astrophysical community cross-sections for electron-ion collisions. Within the CHIANTI team, we have provided a new accurate model of the satellite lines in the X-rays (CHIANTI v.9: Dere, Del Zanna et al. [2]). In collaboration with members of the COMPAS group, and thanks to large-scale atomic structure calculations (GRASP2K), we have improved/corrected the identifications of several levels of important Fe and Ni ions (cf. Wang et al [3]). In order to resolve long-standing problems in the modeling of lines formed in the transition region, we have developed a new collisional-radiative approach which produces ion charge state distributions that depend on the electron density. The simplified approach for Carbon (Dufresne & Del Zanna [4]) has been applied to Oxygen, and has recently been extended and applied to other cases.

Examples of diagnostic applications from past and near-future ground-based (e.g. DKIST, the first 4-meter solar telescope) and space-based (e.g. Solar Orbiter, the next major M-class ESA satellite) missions are provided.

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Atomic electronic structures at the edge of Periodic Table

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High-accuracy calculations of atomic properties of the heaviest elements, are reviewed (see ref.[1] for more details). The properties discussed include electronic structure and energetics (ionization potentials, electron affinities, excitation energies), which are associated with the spectroscopic and chemical behavior of these elements and are therefore of considerable interest. Accurate predictions of these quantities require high order inclusion of relativity, QED and electron correlation effects, as well as large, converged basis sets. The Dirac-Coulomb-Breit Hamiltonian, which includes all terms up to second order in the fine-structure constant, serves as the framework for the treatment; higher-order Lamb shift terms are considered in selected cases. Electron correlation is treated by the Fock-space coupled cluster method, enhanced by the intermediate Hamiltonian scheme, allowing the use of large, converged model (P) spaces.

The calculations on superheavy elements (SHE) are supported by the very good agreement with experiment obtained for the lighter homologues, usually within a few hundredths of an eV, and similar accuracy is expected for the SHEs, with Z>100, for which experimental values are scarce. Many of the properties predicted for these species differ significantly from what may be expected by straightforward extrapolation of lighter homologs, demonstrating that the structure and chemistry of SHEs are strongly affected by relativity and electron correlation.

The major scientific challenge of the calculations is to find the electronic structure and basic atomic properties of the SHE and assign its proper place in the periodic table. The extended Periodic Table up to E174 is presented on the base of our benchmark calculations. Different unusual inclinations and irregularities of the Periodic Law at the edge of extended Periodic System are discussed.

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High-resolution Laser Ionization Spectroscopy of Heavy Elements in Supersonic Gas Jets

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Resonant laser ionization and spectroscopy are widely used techniques at radioactive ion beam facilities to produce pure beams of exotic nuclei and measure the shape, size, spin and electromagnetic multipole moments of these nuclei. In such measurements, however, it is difficult to combine a high efficiency with a high spectral resolution. A significant improvement in the spectral resolution by more than one order of magnitude has recently been demonstrated without loss in efficiency [1] by performing laser ionization spectroscopy of actinium isotopes in a supersonic gas jet, a new spectroscopic method [2] that is suited for high-precision studies of the ground- and isomeric-state properties of nuclei located at the extremes of stability.

Spatial constraints and limitations of the pumping system in the present setup prevented a high-quality jet formation and, consequently, an optimal spatial and temporal laser-atom overlap. Offline characterization studies at the In-Gas Laser Ionization and Spectroscopy (IGLIS) laboratory at KU Leuven [3] are being carried out to overcome such limitations in future experiments when dedicated IGLIS setups are in operation at new generation radioactive beam facilities [4]. These studies also include the characterization by Planar Laser Induced Fluorescence (PLIF) and Resonance Ionization Spectroscopy (RIS) techniques of the flow dynamics and the formation of supersonic jets produced by different gas-cell exit nozzles [5], the test of new gas-cell designs with better transport and extraction characteristics and the characterization of a high-power, high-repetition rate laser systems of multi- and single-mode laser bandwidth. Extrapolation of the online results on the actinium isotopes show that the performance of the technique under optimum conditions can reach a final spectral resolution of about 150 MHz (FWHM) and an overall efficiency of 10 % when applied in the actinide region.

In this presentation, I will summarize the latest online results and mainly will focus on the characterization studies and future prospects of the in-gas-jet resonance ionization method applied to very-heavy elements.

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Kilonovae and the origin of the r-process elements: Atomistic non-LTE spectral modelling

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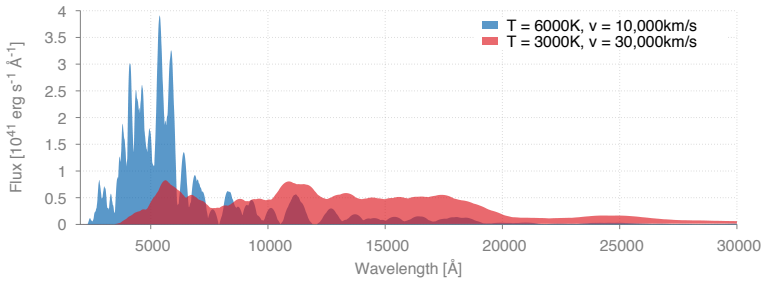
The cosmic origin of elements beyond iron in the periodic table is a long-standing puzzle. One of the main astrophysical highlights of the last decade is thus without doubt the indication of rapid neutron-capture (r-process) nucleosynthesis of heavy elements in the kilonova (KN) ejecta following the neutron-star (NS) merger gravitational-wave event detected in 2017 [1, 2].

The indications that the late-time light is dominated by high-opacity, r-process-element-rich ejecta introduces new demands on fundamental atomic data as input to the collisional-radiative spectral modelling, particularly of the infrared spectral region in largely uncharted territories of the periodic table. We also have to evaluate the radiative transfer models, since it is now for the first time possible to compare with an actual KN observation, and with hopefully more to come soon.

The seemingly high abundance of r-process elements in the ejecta have initiated much activity in the atomic astrophysics community, with many approaches being developed to deal with the lack of fundamental data required to determine reasonable opacities (see [3a, b, c] for three of the most important results so far) – a task which probably will require significant computational and experimental efforts for decades to come. Well established atomic data for these species is crucial, not only to allow for their first direct identification in KN spectra, but also to determine fundamental parameters - such as temperature and expansion velocity - of the ejecta itself, and ultimately of the progenitor binary NS system. The figure below presents an example of a simplistic single-element (Ce I) spectral model of a typical early and late stage ejecta based on atomic data determined with GRASP2018 [4] and non-LTE radiative transfer using the supernova code SUMO [6] which we are currently adopting for KNe conditions.

In this contribution I will discuss the complexity of the most challenging r-process elements, and present preliminary results, based on new atomic data for all the neutrals up to triply ionized elements for all r-process elements (Z = 41 to 92), calculated with state-of-the-art atomic structure methods [4, 5], as well as opacities determined with our radiative transfer KNe model.



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Laboratory Atomic Spectroscopy for Near-infrared Astrophysics

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Analyses of astronomical spectra rely on detailed knowledge of the structure of the atomic species involved. Furthermore, the line strengths must be accurately known in order to use astronomical spectra for quantitative analyses, such as determination of stellar and nebular temperature, density or ultimately the chemical composition. The near-infrared wavelength region, 1–5 □m, is becoming more important thanks to its smaller interstellar extinction, and several spectrographs are coming online matching these needs, e.g. the CRIRES+ at VLT and the APOGEE survey. The planned E-ELT will also observe predominantly in the infrared domain, and the lack of data will be a limitation also in this case.

Our research program on Laboratory Atomic Astrophysics focuses on meeting the needs for infrared atomic data, both line identification and measurements of intrinsic line strengths, the oscillator strengths.

We use the branching fraction and lifetime technique to measure line strengths, using the high-resolution Fourier spectrometer at the Edlen Laboratory at Lund Observatory, in combination with radiative lifetimes. The measurements are combined with calculations using the GRASP and ATSP2k codes, providing a high-accuracy data sets for astrophysical analysis. We participate in observational programs to define the interesting problems and priorities in the need for atomic data.

In the present contribution, we will discuss infrared transitions from an atomic structure point of view and as a base for the astronomical analysis as well as for laboratory and theoretical priorities. We will also discuss the effect of hyperfine structure. Examples are given from recent and ongoing studies on e.g. Sc I, Mg I, Si I and La I.

Nuclear reaction ingredients based on the Gogny interaction

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Within the framework of a global microscopic approach, all the nuclear input required for nuclear reaction predictions are being, step by step, derived from a sole nucleon-nucleon effective interaction, namely the D1M Gogny force [1]. Nuclear masses [1], deformations, radial densities and level densities [2] have already been obtained and have shown a rather good agreement with experimental data either directly or when used, for instance, to derive optical models [3]. More recently, efforts have been devoted to obtain radiative strength functions within the Gogny-QRPA approach whose predictive power has been established with respect to photoabsorption experimental data up to heavy actinide targets [4]. The current status of this project will be discussed and illustrated with a few examples.

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Testing Bound-state Quantum electrodynamics with muonic and antiprotonic atoms

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Traditional tests of bound state QED (BSQED) are based on the spectroscopy of highly-charged ions (HCI). Because of the *Z*-dependence of BSQED corrections with respect to the transition energy, such tests are most sensitive at medium and high-*Z*. However, the production method for high-Z HCI requires fast beams, leading to large Doppler effects, which limits experimental accuracy together with uncertainties in nuclear properties [1]

Up to now, exotic atoms (atoms in which an electron is replaced by another particle like a muon or antiproton) have been used to measure nuclear properties like the nuclear size, as they are much closer to the nucleus and thus more sensitive to nuclear properties than normal atoms (distances reduced by a factor m_μ/m_e=207 for the muon for example). In this talk I will present new results showing that in fact there exists levels in exotic atoms which are much more favorable for BSQED tests than high-*Z* ions. I have identified several transitions in muonic and antiprotonic atoms in which the ratio of the total BSQED corrections to the transition energy is large, while the ratio of the finite-size correction to the total BSQED correction are small, making them the ideal candidates for next-generation precision BSQED tests. In these systems, the vacuum polarization dominates the BSQED corrections, while in normal atoms they are dominated by the self-energy, thus measurements of such transitions would be highly complementary to existing HCI studies and open the possibility of exploring in more detail the structure of the vacuum. I will show some examples and make a first comparison with some existing data on antiprotonic noble gases[2].

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The Belgian repository of fundamental atomic data and stellar spectra-brass

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BRASS is an international networking project for the development of a new public database providing accurate fundamental atomic data of vital importance for stellar spectroscopic research. We present an overview of research results obtained over the past years. The BRASS database offers atomic line data we thoroughly tested by comparing theoretical and observed stellar spectra. We perform extensive quality assessments of selected atomic input data using advanced radiative transfer spectrum synthesis calculations, which we compare to high- resolution Mercator-HERMES and ESO-VLT-UVES spectra of FGK benchmark stars observed with very high signal-to-noise ratios.

We have retrieved about half a million atomic lines required for our detailed spectrum synthesis calculations from the literature and online databases such as VAMDC, NIST ADS, VALD3, CHIANTI, Spectr-W^3, TIP/TOPBASE, SpectroWeb. The atomic datasets have been cross-matched based on-line electronic configuration information and organized in a new online repository at brass.sdf.org [1]. The validated atomic data, combined with the observed and theoretical spectra are also interactively offered in BRASS [2]. The combination of these datasets is a novel approach for its development providing 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, atomic data accuracy assessments including line log(*gf*)-values [3], and line equivalent width measurements.

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Rotating massive stars as sources of fluorine 19 through their winds

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I shall discuss the conditions needed for rotating massive stars to contribute to the synthesis and ejection of fluorine 19 through their winds. This discussion will be based on the recent grids of stellar models computed in Geneva and covering the metallicities from Z=0.0001 to 0.020 with and without rotation. The impact of different angular momentum transport processes will be discussed as well as the possible contribution of very fast rotators that follow during the Main-Sequence phase a nearly homogeneous evolution.

Short-live radioactive (RaF) molecules: a new perspective for fundamental symmetry studies

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High-precision laser spectroscopy on molecules containing Ra isotopes is predicted to be one of the most sensitive methods for searches of physics beyond the Standard Model at low energy [1]. Recent studies on a variety of molecules have revealed the superior sensitivity of molecules (as compared to atoms) to the electron EDM, due to their very large effective electric field [2]. This field is further enhanced in RaF molecules, due to the high Z of radium nuclei. Additionally, the sensitivity to P,T-symmetry violation effects is also increased by the static octupole deformation, which has recently been observed in ^{224,226}Ra [3].

Molecular spectroscopy on RaF with short-lived Ra nuclei requires the production of these isotopes and molecules at accelerator facilities. The first ever laser spectroscopy on a series of RaF molecules, containing radium isotopes with masses 223,224,225,226,228 has been performed at the ISOLDE radioactive ion beam facility at CERN. Numerous transitions in these systems were identified for the first time through collinear resonance ionization spectroscopy, providing important input to quantum chemistry. Properties of the observed transitions confirm that RaF is an ideal system for laser cooling, opening the door to high-precision studies [4].

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Quantitative Spectroscopy of Early B-Type Stars: the Impact of High-Quality Atomic Data

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The high luminosity of massive stars makes them accessible to high-resolution spectroscopy with large telescopes throughout the Milky Way and nearby galaxies. Early B-type main-sequence stars are the easiest targets for model atmosphere analyses among the massive stars. Hydrostatic atmospheres and non-LTE line-formation calculations suffice to interprete their spectra, which show lines of a variety of astrophysically important elements in their optical spectra. The choice of atomic data employed in the non-LTE calculations is decisive for achieving accuracy and precision in the analyses. An overview is given how the implementation of the available high-quality atomic data – mostly from *ab-initio* calculations, and in particular MCHF/MCDHF data for the spectrum synthesis – has facilitated these stars to be established as versatile present-day abundance indicators. Further data needs in order to improve the quality of analyses in the optical/near-IR and in particular with regard to the interpretation of their rich UV spectra are sketched.

Results from the analysis of a sample of early B-type stars in the solar neighbourhood [1,2, and so far unpublished work] are discussed in the context of stellar and Galactic chemical evolution. Conclusions of these for the birth place of the solar system within the Milky Way are drawn.

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POSTER PRESENTATIONS

Revised nuclear quadrupole moment for aluminum: Theoretical nuclear quadrupole coupling constants of aluminum compounds

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The nuclear quadrupole moment of aluminum (^{27}Al) has been re-evaluated[1] by determining the electric field gradients at this nucleus for AlF and AlCl using the coupled cluster method with single, double, and perturbative triple excitations [CCSD(T)]/aug-cc-pwCVXZ (X = T and Q) accounting for both vibrational averaging and core–core/core–valence electron correlation and then comparing to the experimentally measured nuclear quadrupole coupling constants (NQCCs). The new recommended value is Q(^{27}Al) = 148.2 ± 0.5 mb, which can be compared to the previous value of 146.6 ± 1 mb. Using the new value of the nuclear quadrupole moment, the accuracy is assessed for several computational approaches [i.e., Hartree–Fock, Møller–Plesset perturbation theory to the second order, quadratic configuration interaction with single and double excitations, CCSD, CCSD(T), and density functional theory (DFT) with the B3LYP, PBE0, and M06-2X functionals] and basis sets (the aug-cc-pVXZ and aug-cc-pwCVXZ families) for determining the nuclear quadrupole coupling constants for AlCN, AlNC, AlSH, AlOH, and AlCCH, where experimental measurements are available. From the results at equilibrium geometries of the polyatomic molecules, it has been determined that (i) the CCSD(T)/aug-cc-pwCVXZ approach is needed to obtain results within 4% of the experimental measurements, (ii) typical DFT values are only within 10%–15% of the experimental measurements, and (iii) the aug-cc-pVXZ family of basis sets is not recommended for computing the electric field gradients at aluminum. The present results also suggest that the NQCC for AlOH should be remeasured. Using the recommended CCSD(T)/aug-cc-pwCVXZ approach, the equilibrium geometries and corresponding NQCCs for $AlCH_3$ and AlCCCN were determined, and the NQCCs are in excellent agreement with previously reported experimental values.

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MCDHF and RCI calculations of energy levels, lifetimes, and transition rates in Si III

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Extensive multiconfiguration Dirac-Hartree-Fock (MCDHF) and relativistic configuration interaction (RCI) calculations are performed for 106 states in doubly ionized silicon (Si III), which are important for astrophysical determination of plasma properties in different objects. Electron correlation effects are accounted for through large configuration state function expansions. The calculations are in good agreement with available experiments for excitation energies, transition properties, and lifetimes. Important deviations from the NIST-database for a selection of perturbed Rydberg series are discussed in detail.

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Molecular P,T-violation as a signature for physics beyond the standard model

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New physics beyond the standard model can imply simultaneous violations of discrete symmetries such as space parity (P), time-reversal (T) and charge conjugation (C). Different hypothetical sources of simultaneous violation of P- and T-symmetry can be introduced on the level of elementary particles, such as P,T-odd electroweak currents between quarks and electrons or permanent electric dipole moments (EDMs). These fundamental P,T-odd interactions can induce net P,T-odd moments in bound systems such as atoms and molecules[1]. Consequently, a successful measurement of a permanent EDM of an atom or a molecule is difficult to interpret due to possible interference of the various fundamental sources of P,T-violation. Nevertheless, due to enormous electronic structure enhancements of such P,T-odd effects in polar molecules, low-energy high-precision experiments on these molecules can give access to the TeV energy-regime [2, 3].

In this contribution different possible sources of discrete symmetry violation and their effects on molecular spectra are discussed. Requirements for molecular candidates in high-precision measurements that aim to find such symmetry violations are elucidated. Trends of P,T-violation within the periodic table of the elements as predicted by quasi- relativistic calculations[4] as well as measurement models for disentanglement of sources of P,T-violation in molecules are discussed[5,6]. Simple analytical models, which are gauged by ab initio calculations, help to identify molecules with large enhancement factors that are favourable for spectroscopic experiments.

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MultiConfiguration Dirac-Hartree-Fock calculations of electron-nucleus interactions

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We present past, present, and future developments in atomic ab initio calculations of atomic properties, using multiconfiguration Dirac–Hartree–Fock theory, implemented in GRASP [1-4] and MCDFGME [5] relativistic atomic structure codes. For neutral atoms, the deviations of properties calculated within the Dirac–Hartree–Fock (DHF) approach (based on independent particle model) are often dominated by electron correlation effects, i.e. the non-central interactions of individual electrons. We present the methods developed for accurate calculations of electron correlation effects in small [6], medium [7], heavy, and superheavy [8] neutral or nearly neutral atoms.

We present methods and tools, which are designed to develop the numerical calculations in a controlled, systematic manner, where multiconfiguration expansions account for all leading electron correlation effects. We describe methods of systematic development of multiconfiguration expansions leading to systematic, controlled improvement of the accuracy of the ab initio variational calculations. We show examples of applications of the codes to calculations of hyperfine structures, but both codes can handle a large variety of operators. Over the years the codes have been applied to calculations of atomic and ionic spectra (transition energies and rates), hyperfine structures, hyperfine anomalies, isotope shifts, to determinations of nuclear electromagnetic moments, as well as to calculations related to interactions of bound electrons with nuclear electromagnetic moments leading to violations of discrete symmetries.

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Isotope shifts of electron affinities: a frontier for theorists and experimentalists

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Negative ions, due to their sensitivity to electron correlations, have long been known as a special challenge for *ab initio* atomic calculations. In this respect, their detachment thresholds, as differences between binding energies that involve different numbers of electrons, are particularly sensitive to the intricacies of atomic structure.

Isotope shifts, through the specific mass shift, are also critical tests for the descriptions of many-electron shells. Isotope shifts of electron affinities thus combine all difficulties, as concerns the quantitative description of atomic shells. It is therefore remarkable that a recent experiment, carried out with the photodetachment microscope[1], led to a measurement of the isotope shift ^{13}C-^{12}C of the electron affinity of carbon[2] that perfectly matched the theoretical prediction[3].

Isotope shifts of electron affinities have also been measured for hydrogen[4], oxygen[5], sulfur[6], chlorine[7,8], bromine[9] and iodine[10-11] though, in some cases, with too low a precision to check the expectated values. Prospects, in the field, will be presented at the workshop.

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Spectroscopic investigation of Al I for astrophysical applications

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Recent advances in resolution and spectral range of ground-based and space-based astronomical spectrographs imply that accurate atomic data is greatly required for the reliable interpretation and modelling of astrophysical spectra. Correctly interpreted, stellar spectra allow for precise abundance analysis, making it possible to study the galactic formation and evolution. To meet this demand, we are performing studies on neutral aluminium, Al I. Aluminum is specifically found in young, massive stars and is thus a key element for tracing ongoing nucleosynthesis throughout the Galaxy [1]. The near-infrared (NIR) wavelength region is of particular importance, since the extinction is lager for optical wavelengths. This makes the NIR wavelength region a better probe for e.g. regions close to the galactic center.

In this study we aim to provide oscillator strengths (*f*-values) of improved accuracy for Al I lines in the NIR and optical regions (~300 – 4000 nm). The *f*-values are derived from experimental branching fractions (BFs), together with published radiative lifetimes. To meet the desired accuracy, measurements have been performed using a hollow cathode discharge lamp (HCL) as light source, and a Fourier transform spectrometer (FTS), to record high resolution spectra. The spectra covers lines with upper levels up to n=5.

In a recent study, Papoulia et al [2] performed calculations for Al I, and the combined dataset allows for improved transition data for Al I allowing for improved accuracy in the stellar analysis.

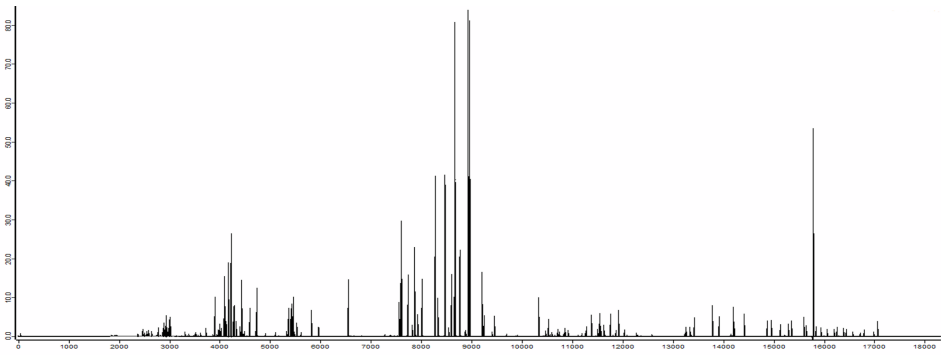

Figure 1: FTS spectrum including Al I lines, recorded with an InSb detector.

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Physics program in N=Z nuclei to be addressed at S3-LEB

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The Super Separator Spectrometer S3 is developed for SPIRAL2 and it will take advantage of the high intense stable beams to be produced by the LINAG at GANIL. These intensities will open new nuclear physics opportunities to study N=Z nuclei in the neighborhood of ^{100}Sn. The combination of S3 to the Low Energy Brunch (LEB) set-up and MR-TOF-MS device will be an unique tool to measure relevant observables in a model independent manner. In this talk, the physic program to be addressed will be presented.

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Unified equations of state of cold dense matter in neutron stars

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Formed in the aftermath of gravitational core-collapse supernova explosions, neutron stars are the most compact observed stars. Their average density exceeds than that found inside the heaviest atomic nuclei. Neutron stars are also endowed with the highest magnetic fields known, which can reach millions of billion times that of the Earth. According to our current understanding, a neutron star is stratified into distinct layers. The surface is probably covered by a metallic ocean. The solid layers beneath consist of a crystal lattice of pressure- ionized atoms embedded in a highly degenerate relativistic electron gas. With increasing density, nuclei become progressively more neutron rich until neutrons start to drip out of nuclei thus delimiting the boundary between the outer and inner regions of the crust, where neutron- proton clusters are immersed in a neutron liquid. At about half the density of heavy nuclei, the crust dissolves into a homogeneous liquid mixture of nucleons and leptons. We have developed a series of unified equations of state of dense matter in neutron stars[1,2]. Based on the nuclear energy-density functional theory, these equations of state provide a thermodynamically consistent treatment of all regions of the star and were calculated using functionals that were precision fitted to experimental and theoretical nuclear data[3,4]. These equations of state were specifically developed to assess the role of nuclear uncertainties on neutron-star properties. Recent applications to study the role of the symmetry energy on the tidal deformability[5] will be presented. Predictions will be compared to constraints inferred from the recent detection of the gravitational-wave signal GW170817 from a binary neutron-star merger and from observations of the electromagnetic counterparts.

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X-Ray Emission from High-Density Astrophysical Plasmas

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Iron X-ray K lines emitted by black hole accretion disks are very important lines for astrophysicists. Actually, they have observed widths and shifts that imply an origin very close to the central black hole [1]. Thus, they can be considered as natural probes of the regions very close to the compact object since the intensity and the shape of these lines can give information about the effects of special and general relativity in the emitting region. Moreover, some important properties of the black hole itself, such as its spin, can be inferred by modeling the distortion of the Fe K emission complex [2].

Plasma conditions in such accretion disks around black holes are thought to be characterized by electronic densities that can be as high as 10^{22} cm^{-3} [3]. Such high-density conditions may affect the atomic structure and processes corresponding to the ionic species present in the plasma. However, atomic data used in the standard programs to model astrophysical X-ray spectra are computed assuming an isolated ion approximation. Therefore, this shortcoming is thought to be the major reason for the inconsistencies observed in the results [4,5].

The main goal of the present work is to estimate the effects of high-density plasma environment on the atomic parameters involved in the K-line emissivities for iron ions, within the astrophysical context of accretion disks around black holes. For this purpose, relativistic atomic structure calculations have been carried out using the multiconfiguration Dirac-Fock (MCDF) method, in which a time averaged Debye-Hückel potential has been considered for both the electron-nucleus and electron-electron interactions in order to model the plasma environment, using a combination of the GRASP2K [6] and of the RATIP [7] codes. In this contribution, we present a sample of results concerning the influence of plasma environment on the atomic structure, and on the K-shell radiative, Auger and photoionization processes in highly-charged iron ions.

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Community Platform for Just Atomic Computations

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JAC [1], the Jena Atomic Calculator, has been developed for performing (relativistic) atomic structure calculations of different kind and complexity. In particular, this code has been designed and worked out to compute not only atomic state functions and properties but also the (many-electron transition) amplitudes for a large number of atomic processes, including the associated cross sections, rates, angular distributions and various other parameters. While the present focus in developing JAC has been placed upon the (automatic) generation of self-con-sistent fields, atomic properties and processes, this code will support with some further work also simulations of atomic cascades, the time-evolution of statistical tensors as well as a few semi-empirical estimates of selected atomic properties.

A primary guiding philosophy in designing JAC was to develop a general and easy-to-use toolbox for the atomic physics community, including an interface that is equally accessible for working spectroscopiest, theoreticians and code developers. In addition, I also wish to provide a modern code design, a reasonable detailed documentation of the code and features for integrated testing [2]. In particular, most typical atomic calculations and the handling of (atomic) data should appear within the code similar to how they would occur in spoken or written language. Shortly speaking, therefore, JAC aims to provide a powerful platform for daily use and to extent atomic theory towards new applications. In this contribution, I shall explain by simple examples the use of JAC and how the code is distributed via Github [3].

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Theoretical Calculations of Oscillator Strengths for Radiative Transitions of Cosmochronological Interest in Singly Ionized Thorium (Th II)

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Up to now, there are very few available calculations of radiative data for singly ionized thorium (Th II). This is mainly due to the complexity of its electronic configurations and to the fragmentary knowledge of its experimental spectrum.

Transitions probabilities and oscillator strengths for Th II radiative transitions are important in astrophysics [1]. Indeed, Th II, as well as U II, is used as a cosmochronometer in order to determine the age of stars. More specifically, the ^{232}Th isotope, with a half-life of 14 Gyr, is used to date galactic stars [2-6]. Goriely and Clerbaux [7] pointed out that new accurate data on heavy radioactive elements could improve the accuracy of cosmochronometric analyses.

For the particular use in cosmochronology, knowing the Th II abundances in stars is of high importance. Indeed, in order to date a star, we use [8]:

$$R\frac{U}{Th} = P\frac{U}{Th}\ exp\left(\frac{T}{\tau_U} - \frac{T}{\tau_{Th}}\right)$$

where R is the Uranium/Thorium abundances ratio, P is the production rate, τ is the half-life and T the studied star's age. Therefore, in order to precisely determine R, a better knowledge of Th II's spectrum is necessary.

The accuracy of this dating technique is still hampered by the lack of available radiative parameters for Th II spectral lines. Some oscillator strengths were obtained experimentally by combining branching fraction measurements with laboratory lifetimes determined using laser spectroscopy [9-10], but these data only concern a restricted number of strong lines. In order to partly fill this gap, we carried out extensive calculations of oscillator strengths for the most intense Th II lines of potential cosmochronological interest using the pseudo-relativistic Hartree-Fock [11] theoretical approach. Some preliminary results will be presented at the conference.

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Precision theory of the *g* factor of highly charged ions[1]

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Quantum electrodynamic (QED) effects in strong Coulomb fields have been scrutinized in high-precision Penning trap *g* factor measurements [1], also hinting towards the possibility of determining nuclear properties with such experiments. The uncertainty of the atomic mass of the electron has been largely decreased via measurements with the hydrogenlike $^{12}C^{5+}$ ion, and by using the theoretical value of the *g* factor [2]. In order to further reduce uncertainties in the theoretical description, we calculate further higher-order corrections, such as two-loop Feynman diagrams in nonperturbative nuclear fields [3-5], i.e. applying an all-order method in terms of the nuclear coupling strength parameter $Z\alpha$, with Z being the atomic number and α the fine-structure constant.

In future, an independent determination of the fine-structure constant may also be possible by employing a specific weighted difference of the *g* factors of the hydrogen- and lithiumlike (or, alternatively, boronlike) ions of the same element. This weighted difference in chosen to cancel uncertainties due to nuclear effects. It is shown that this method can be used in future to extract a value for α from bound-electron *g*-factor experiments with an accuracy competitive with or better than the present literature value [6,7]. In a very recent experiment, the *g* factor of the boronlike $^{40}Ar^{13+}$ ion has been measured with an uncertainty on the 10^{-9} level, in agreement with the most recent theoretical predictions [8], including our value obtained using the relativistic configuration interaction method, together with screened QED corrections. This represents a significant step towards the determination of α from the bound-electron *g* factor.

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Homemade instrument to study ions by high-resolution photodissociation spectroscopy

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This instrument is dedicated to the study of molecular ions and ionic complexes by high-resolution photodissociation spectroscopy. It is essentially com- posed of (i) a pulsed supersonic expansion plasma source, to produce the ionic species at low rotational temperature, (ii) a time of flight mass spectrometer which includes a single unit able to perform acceleration, bunching and gating[1] and (iii) a second mass selection of the fragmented ions produced by the resonant interaction with a nanosecond laser. We will present in this poster, (i) the first mass spectra of cationic and anionic clusters, formed from different gas mixtures and (ii) the first high-resolution photodissociation spectrum of N_2O^+ obtained with this instrument using a pulsed dye laser.

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Constraining atomic oscillator strengths using FGK-type stellar spectra

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Accurate atomic transition data are crucial input parameters for the modelling of stars. Fundamental atomic data, such as oscillator strengths and rest wavelengths, governs our very understanding and interpretation of the internal structures, atmospheres, and evolution of stars and stellar environments. As such, any errors and uncertainties in the adopted atomic data run the risk of systematically propagating throughout the entire field of astronomy.

A small number of databases offer compilations of both experimental and theoretical atomic data, often containing data that are complementary to one another. Unfortunately, despite the tremendous ongoing efforts of atomic data producers and atomic data providers information is often not sufficient or available on the accuracy of the data, complicating the interpretation of results for astronomy and other fields.

The poster summarises the work of my PhD thesis: to constrain oscillator strengths for over a thousand atomic transitions, relevant for stellar spectroscopy in FGK-type stars, as accurately and precisely as possible. The work employs extremely high-quality stellar spectra of benchmark FGK-type stars, including the Sun, taken at a resolution of R~85,000 and with signal-noise ratios of S/N~1000.

1091 theoretically deep and unblended spectral lines, in the wavelength range 4200-6800 Å, were systematically and homogeneously selected using constraints on the degree of theoretical line blending in our detailed transfer calculations. Astrophysical log(gf) values were then determined for the 1091 transitions using two complementary methods: the curve-of-growth and equivalent width approach, and by using iterative radiative-transfer modelling. We pay particular attention to reducing systematics and producing realistic uncertainty estimates.

The agreement between the two methods was used to select 845 well-behaved spectral lines, including a subset of 408 spectral lines that are robust against any systematic differences in the adopted methodologies. We quantify the systematic impact of line blending treatment, often neglected in the literature, revealing that even small blends contributing as little as 5% of the total equivalent width impact log(gf) and abundance determinations by on average ~0.10 dex.

We provide literature recommendations on atomic data based upon their agreement with our 845 and 408 reliable and robust spectral lines. We found that around 53% of the 845 lines had at least one literature log(gf) value in agreement with our derived values, though the remaining values could disagree by as much as 0.5 dex. Only ~38% of Fe I lines were found to have sufficiently accurate log(gf)values, increasing to~70-75% for the remaining Fe-group lines. We finish by highlighting how our log(gf) values can be used as benchmark values to determine fruitful techniques for producing accurate atomic data.

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Optical pumping schemes for nuclear spin polarization of argon 35

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Quantum state preparation has a wide range of applications ranging from quantum optics to quantum metrology to fundamental physics precision measurements. In the context of nuclear □-decay correlation experiments using for instance ^{35}Ar, one needs to prepare a sample of atoms with a high degree of spin polarization. Creating such a polarized sample amounts to generating a so-called stretched state (i.e. a state with the maximal projection of the total angular momentum along the quantization axis), which is typically achieved through optical pumping. We propose and compare various schemes which we have been investigated numerically in the case of the multilevel structure of ^{35}Ar. Our model uses the density matrix formalism, which makes it possible to study effects such as coherent population trapping, a phenomenon which can affect both the efficiency of the optical pumping process and the polarization signal [1,2].

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Deduction of model-independent nuclear moments by atomic hyperfine structures

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The electromagnetic interaction between nuclear multipole moments and atomic electrons brings about hyperfine structures. High-precision determination on the atomic factors of hyperfine structures paves the way for deducing model-independent nuclear moments from experimental hyperfine splittings. However, it is a knotty problem to estimate the uncertainties of atomic structure calculations due to complicated electron correlations, especially for neutral or near-neutral atomic systems. In the framework of the multi-configuration Dirac-Hartree-Fock method, the active space approach has been developed in order to capture electron correlations efficiently [1]. Recently, we also show in the case of Al^+ [2] and Sr [3] that higher-order electron correlation must be taken into account for reducing computational uncertainties, although their effect is minor and cancel out the first-order correlations among the electrons in the core to a large extent. Towards heavy elements, a new project was just started to reevaluate the nuclear quadrupole moment of bismuth by using various atomic-structure computational strategies [4].

With the advent of high-precision measurements of atomic properties (e.g., laser spectroscopy and atomic clocks), the determination of the magnetic octupole hyperfine interaction becomes feasible. Therefore, we have developed the rhfs module in the GRASP2018 package [5] to include a treatment of the diagonal magnetic octupole hyperfine interaction constant [6]. The first application of this module is to estimate the octupole hfs of the $^3P_2$ state for ^{87}Sr [7].

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HFSZEEMAN95 -- A program for computing weak and intermediate magnetic-field- and hyperfine-induced transition rates

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Hyperfine-induced (HIT) and magnetic-field-induced (MIT) transitions have been theoretically and experimentally studied for various atomic systems due to their potential applications in plasma diagnostics, e.g. the determination of electron densities, isotope compositions, and magnetic fields [1, 2]. The development of programs for computing the rates of the corresponding transitions along with synthetic spectra is essential for utilizing their diagnostic potential.

HFSZEEMAN95 is an updated and extended Fortran 95 version of the HFSZEEMAN program [3]. Given relativistic atomic state functions generated by the Grasp2018 package [4], HFSZEEMAN95 together with the accompanying Matlab/GNU Octave program MITHIT allows for: (1) the computation and plotting of Zeeman energy splittings of magnetic fine- and hyperfine structure substates as functions of the strength of an external magnetic field, (2) the computation of transition rates between different magnetic fine- and hyperfine structure substates in the presence of an external magnetic field and the rates of hyperfine-induced transitions in the field free limit, (3) the synthesization of spectral profiles for transitions obtained from (2). With the new features, HFSZEEMAN95 and the accompanying Matlab/GNU Octave program MITHIT are useful for the analysis of observational spectra and to resolve the complex features due to the splitting of the fine and hyperfine levels.

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Contribution of charge-exchange in H/D(nl) + He^+ collisions to the diagnostics of fusion plasmas following helium thermal beam injection

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We present a study of the emission contributions from charge-exchange of excited hydrogen or deuterium (n = 2, 3) with He^+ ions in fusion plasmas. We employ a 1-D kinetic collisional radiative model in order to analyze their effects on the Thermal Helium Beam (THB) line-ratio diagnostic on ASDEX Upgrade and Laser Induced Fluorescence (LIF) He I density measurements in ITER. Recent charge-exchange calculations [1, 2] show that cross sections from excited deuterium (n = 2, 3) with He^+ are over four orders of magnitude higher than those from the ground state (n = 1) and occur at very low energies where they are more likely to interact with the thermal He^+ ions introduced by ionization of the diagnostic helium gas-puff injection. Higher densities of excited deuterium are typically present in the scrape-off layer, divertor, and edge regions of tokamaks, where the LIF and THB helium diagnostics are typically used for the simultaneous determination of electron temperatures and densities and where contributions from charge-exchange emission may offset these values if not taken into account. Despite this, we show that the dominant contribution to the helium emissions comes from electron-impact excitation [3].

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Mutual neutralization in Li^+ – H^-/D^- collisions: a combined experimental and theoretical study

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Mutual neutralization processes in ion-pair collisions play an important role in the analysis of the chemical composition of astronomical objects such as stellar atmospheres or the early universe due to their large cross section. In this work, we present a combined experimental and theoretical study of the mutual neutralization process in collisions of lithium ions (Li^+) with deuterium anions (D^-) at collision energies from 1 eV down to 3 meV. We employ a merged-beam apparatus to determine total and state-to-state mutual neutralization cross sections. We perform nuclear dynamics calculations using the multi-channel Landau- Zener model based on accurate *ab initio* molecular data. We obtain an excellent agreement between the experimental and theoretical results over the energy range covered in this work. We show that the basis sets used in the *ab initio* calculations have a limited influence on the total cross section, but strongly impacts the results obtained for the partial cross sections or the reaction branching ratios. This demonstrates the important role of high-precision measurements to validate the theoretical approaches used to study gas-phase reactive processes. Finally, we compute state-to-state mutual neutralization rate coefficients for $Li^+ + H^-$ and $Li^+ + D^-$, and discuss their significance for astrochemistry models [1].

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R-matrix electron impact excitation data for the C-like iso-electronic sequence

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Emission and absorption features from C-like ions are served as temperature and density diagnostics of astrophysical plasmas [1,2,3]. R-matrix electron-impact excitation data for C-like ions in literature merely cover a few ions and often only for the ground levels.

We performed a systematic R-matrix calculation of level-resolved effective collision strength over a wide temperature range for C-like ions from N II to Kr XXXI (i.e., N^{+} to Kr^{30+}).

For each ion, we include a total of 590 fine-structure levels in both the configuration interaction target and close-coupling collision expansion. These levels arise from 27 configurations. The AUTOSTRUCTURE code [4] is used to calculate the target structure and the R-matrix intermediate coupling frame transformation method [5] is used to calculate the collision strength.

We compare the present results of selected ions with archival database and results in the literature [6,7,8,9,10,11]. The comparison covers energy levels, transition rates, and effective collision strengths. The electron-impact excitation data is archived according to the Atomic Data and Analysis Structure (ADAS) data class adf04 and will be available in OPEN-ADAS.

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Photodetachment of C^- in the ground state

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Negative ions, in particular those of carbon and oxygen, are of fundamental interest for the understanding of electron correlation and also play an important role in domains such as astrophysics and atmospheric physics. In the case of O^-, there was a long-standing discrepancy between theory and experiment, which was recently resolved by new measurements using an animated-crossed-beam technique to determine absolute total cross sections [1]. The new experimental cross sections are about 20% larger than the earlier values, and are in very good agreement with new theoretical results presented in the same publication. For C^- , the only experimental values near the photodetachment threshold date back more than 40 years [2, 3]. The measurements however were not absolute, and were normalized using the older O^- cross sections. Since the latter have now been superseded, it appears necessary to revise the experimental values for C^- by measuring them directly.

Here we report results for the photodetachment of C^-, determined using the same experimental techniques as in [1]. These are in good agreement with results of a new R-matrix calculation, which employs a basis set with polarized pseudostates to reproduce the polarizability of the carbon ground state. These give a polarizability of 11.58 a_0^3, which compares well with the value of 11.67 a_0^3 from an extensive coupled cluster calculation [4]. The electron affinity of the ground state is 1.258 eV, very close to the experimental value of 1.262 eV [5].

As shown in Figure 1, the agreement between the new theoretical and absolute experimental cross sections is very good. There is no sign of the small bump just above threshold (dashed line) present in the results of a previous R-matrix calculation [6]. Below 2.2 eV, the results are similar to those of earlier experiments (diamonds [2] and crosses [7]), but differences of the order of 15% to 25% appear at higher energies.

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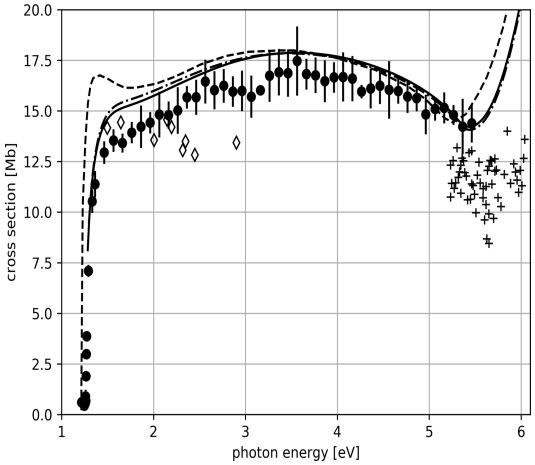

Figure 1. Experimental (circle: present work, diamonds: [2], crosses: [7]) and theoretical (solid: length form, dash-dot: velocity form) total cross sections for photodetachment of C^- ($^4S^o$).

New C12+C12 reaction rate with STELLA and its impact on the advanced stages of Massive stars

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New C12+C12 reaction rates found with STELLA seems to lead to a trend confirming the hypothesis of fusion suppression. This leads at lower temperature to much lower reaction rates, up to a few order of magnitude compare to Fowler models currently used in stellar evolution. We present here new results combining whole new STELLA's C12+C12 reaction rates and the state-of-the-art Geneva stellar evolution code. We show how changing the reaction rates of a few order of magnitudes will impact the more advanced phases of Massive Stars and their final fate.

Progress on Experimental and Theoretical Studies of Heavy Element Ion Spectra

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Spectra of moderately charged heavy element ions such as lanthanide and actinide ions have been attracting much attention these last years because of their applications in several astrophysical environments [1]. As example, one may mention the determination of abundances in stellar atmospheres, the calculations of opacity of the ejected matter of two neutron star mergers and the determination of the age of the Galaxy in cosmochronology. For modelling laboratory and astrophysical plasmas, a great amount of data on radiative and collisional properties on these elements is needed. The knowledge of experimental level energies is often a starting point, which can only be derived from term analyses of high-resolution spectra.

We will describe some current experimental and theoretical studies of emission spectra carried on by our collaboration team, mainly in the vacuum ultraviolet wavelength range. High- resolution spectra are recorded using vacuum spark sources and the 10.7 m vacuum spectrograph of the Meudon Observatory. Photographic plates are used for accurate wavelength measurements and image plates, for linear intensity measurements. Uncertainties between ±0.001Å and ±0.005Å are currently obtained on wavelengths in the range of 300Å-2900Å. Analyses of spectra are supported by parametric calculations of atomic configurations using the Cowan codes [2], including relativistic corrections and configuration interactions. A least-squares fit of energy parameters minimizing the differences between calculated and experimental energies allows a better description of wavefunctions leading to more reliable radiative transition probabilities. Furthermore, isoelectronic and isoionic regularities are of great help to unravel these complex spectra. After the U II spectrum [3], we are making progress on several other uranium ions (U IV-VI). Preliminary results will be reported.

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First stars in the Universe need Non-LTE radiative transfer and precision atomic data!

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The nature and formation of very first stars in the early Universe is of prime importance to understand the subsequent chemical enrichment of stars in galaxies. The abundance patterns of the most iron-poor stars in the Galaxy can be compared to the SNe explosion abundance yields of the first stars to infer the latter's properties (such as their masses, SNe energies, mixing factors, etc.). Fe-peak element high precision abundances are especially important, as they are able to place stringent constraints on the nature and geometries of the First star explosions. Characterizing the most iron-poor stars requires non-Local Thermodynamic Equilibrium (non-LTE) radiative transfer for a multiple key elements. We present here the build of new non-LTE iron-peak model atoms, with the first non-LTE model of Ni in late-type stars. Such elements shows UV lines detected in the HST spectra, with the recent discovery of a Zn line in the ultra metal-poor star HE 1327−2326. First order NLTE-abundance corrections will also be presented.

Weak Correlation and Strong Relativistic Effects on the Hyperfine Interaction in Fluorine

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In previous work devoted to *ab initio* calculations of hyperfine structures constants on nitrogen [1] and fluorine [2,3] atoms, we observed large relativistic effects, a priori unexpected for such light systems, that can even largely dominate electron correlation. In these cases where even a small relativistic term mixing may become crucial, we observed that the atomic wave function calculated in the Breit-Pauli approximation describe adequately the relevant atomic levels.

In the present work we identify new levels within the spectroscopic terms $2p^4 3d\ ^{2,4}(P,D,F)$ of fluorine atom for which correlation effects on the hyperfine structures are negligible but relativistic LS-admixtures and contamination, are decisive to correctly reproduce the experimental values [4].

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α-decay energies of superheavy nuclei: systematic trends

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New superheavy nuclei are often identified through their characteristic α-decay energies, which requires accurate calculations of Q_α values. While many Q_α predictions are available, little is known about their uncertainties, and this makes it difficult to carry out extrapolations to as-yet-unknown systems. This work aimed to analyze several models, compare their predictions to available experimental data, and study their performance for the unobserved α-decay chains of $^{296}120$ and $^{298}120$, both of which are of current experimental interest.

Using nuclear density functional theory (DFT) with seven Skyrme energy density functionals (EDFs), we evaluated the Q_α values for even-even nuclei from Fm to Z = 120. For well-deformed nuclei between Fm and Ds, we find excellent consistency between different model predictions, and a good agreement with experimental results. For transitional nuclei beyond Ds, intermodel differences grow, resulting in an appreciable systematic error. In particular, our models underestimate Q_α for the heaviest nucleus ^{294}Og. These results will serve as a benchmark for future, more sophisticated statistical studies based on, for example, Bayesian machine learning techniques.

This abstract is for a poster presentation at the Solvay Workshop on "New Frontiers in Atomic, Nuclear, Plasma and Astrophysics" to be held in Brussels, Belgium from 25-27 November 2019.

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New QED operators and updated CI program in GRASP

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GRASP – the General Relativistic Atomic Structure Package – is a suite of Fortran programs for fully-relativistic 4-component Dirac-Hartree-Fock and configuration interaction (CI) calculations of many-electron atomic systems [1]. The CI portion of the software can also estimate corrections arising from the non-infinite mass of the nucleus (mass shifts), the non-instantaneous nature of the inter-electron interaction (the Breit operator) and quantum electrodynamics (QED; specifically, the QED self-energy and vacuum polarization corrections).

This work focuses on the QED self-energy operators. GRASP has been able to estimate the self-energy from early on by appropriately scaling self-energy values of hydrogen-like systems. In the meantime, however, alternative effective single-particle operators have been proposed for describing the self-energy correction. We have implemented into GRASP the approaches described by Shabaev et.al (QEDMOD) [2,3], Flambaum & Ginges [4], and Pyykkö & Zhao [5], as alternatives to the hydrogenic approach. With the implementation done, we are now able to benchmark the accuracy of these operators in large many-particle systems.

We have also added another program that can be used to estimate, as a first-order perturbative correction, all the contributions that were not included in the CI matrix in the original calculation. This program can be run after the CI calculation has finished and the CI coefficients have been determined. This way you can avoid having to run a separate full CI calculation when wishing to compare alternative implementations of the Hamiltonian terms.

As a consequence of the development effort, we have significantly reorganized the source code of the rci program. All new code has been written with modern software engineering practices in mind, including the use of CMake to manage the build process and the development of a unit and integration test suite. We aim to have rci as an example of how the GRASP source code could be organized to improve readability and maintainability.

The poster will briefly review the new QED operators and show a few benchmark calculations for Be-like and F-like system. It will also discuss modern coding and software engineering practices, as they have been applied in the refactoring of the code of the RCI program.

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Determination of the Sn electric field gradient

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The magnetic dipole hyperfine structure constants and electric field gradients of the [Kr]4d^{10}5p6s $^3P_1^o$ and [Kr]4d^{10}5p6s $^1P_1^o$ excited states of tin have been calculated using the relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) method. The nuclear electric quadrupole moment is extracted by combining the calculated value of the electric field gradient (EFG) with the experimental value of the electric quadrupole hyperfine constant *B* [1].

Three independent sets of calculations, all using the General Relativistic Atomic Structure Package computer codes, GRASP2K [2] and GRASP2018 [3], based on the same relativistic MCDHF theory and methodology [4, 5] but following different computational models, were performed to estimate the EFG. The final EFG-value, 706(50)MHz/b, results from the statistical mean over the different strategies [6]. The choice of the zero-order space is investigated using the single- and multi-reference pictures. The multireference strategy exploits the concept of the Layzer complex to capture most of the static correlation while the single reference strategy allows an easier treatment of triple excitations. Each strategy provides information about the influence of the electron correlation on the calculation of the dipole hyperfine structure constants *A* and the EFGs. A careful analysis of the convergence of the *A/g* and EFG electronic factors along the active space expansion is performed to assess the reliability of the results. The progressive introduction of new classes of electron substitutions from the reference to the active set of orbitals extends the active space until the required computational resources reach our clusters limits. In particular, the opening of shells deep in the krypton-like core to describe core correlation lead to a huge number of CSFs. However, since the hyperfine structure results from the interaction between the electromagnetic field of the nucleus and the electron cloud, electrons close to the nucleus play an important role and the opening of closed-shells core is necessary.

Further investigations were carried out to estimate the hyperfine anomaly. This was accomplished by considering for each isotope a Fermi charge distribution with adopted rms radius and a parametrized squared harmonic-oscillator wave function of the last unpaired neutron as magnetization distribution [7].

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Recent Theoretical and Experimental Studies on Negative Ions

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Negative ions represent a special niche of atomic physics and offer excellent opportunities for studies of atomic structure, dynamics and interactions in systems characterized by the binding of an extra electron to a neutral atom in a short-range potential.

One of the most important properties is electron affinity. We have systematically studied the electron affinities of the elements in groups VII, and achieved an improved accuracy by more than a factor of 10 compared to previous theoretical studies [1].

Most negative ions have only a few bound states, often with the same parity and within the same configuration. The radiative lifetimes for excites states are therefore dominated by magnetic dipole transitions. We will discuss the radiative lifetimes for excited states of negative O, S, Se, Te, Ni and Pt as determined by analytical [2] and ab initio relativistic methods [3]. The structure and radiative lifetimes of negative ions of group V are also investigated [4].

The negative ions with bound states of opposite parities are of special interests because of their rare existence and, more importantly, because they are candidates for laser cooling of negative ions. Our experimental and theoretical studies support negative Th as a new promising candidate for laser cooling. The measured and calculated electron affinities of Th are 0.607690(60) and 0.599 eV, respectively, almost a factor of two larger than the previous theoretical value of 0.368 eV. The negative Th has two bound configurations $6d^37s^2$ and $6d^27s^27p$, which provide several strong E1 transitions. The ground state belongs to $6d^37s^2\ {}^4F^e_{3/2}$. We propose the ${}^2S^o_{1/2}\leftrightarrow{}^4F^e_{3/2}$ transition with wavelength of 2.6 μm, and transition rate 1.17×10^4 s^{-1} is the potential candidate for laser-cooling [5].

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MCDHF calculations of the superheavy element Nihonium using GRASP2018

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Nihonium (Nh) is an extremely radioactive transactinide element obtained in synthetic way in two independent laboratories [1, 2]. Up to now eight isotopes has been identified including the most stable ^{286}Nh with the a quite long half-life of about 10 seconds, what may be sufficient to measure the frequencies of the most strong transitions and study its chemical properties in laboratories [3, 4]. This half-life duration is a sign of approaching the hypothetical island of stability [5]. The Nh nucleus with 113 protons and 173 neutrons is quite close to the one of doubly magic nuclei, which assuming its spherical shape should have 114 protons and 172 neutrons [6]. Optical lines of superheavy elements like Nh can be found in spectra of supernovas and from regions of colliding neutron stars. In order to do this sufficiently accurate calculation giving reliable basis for line identification are needed. Partially it concerns the most intensive lines of s-p resonance transitions. The electron structure and spectra of Nh were already calculated by means of the coupled cluster method, the all-order correlation potential technique, and the configuration interaction method [7, 8]. Nihonium can be considered as a heavier homologous of Thallium which above five closed shells possesses three electrons configured as $6s^2 6p$. Then the Nh atom above six closed shells has also three electrons configured as $7s^2 7p$.

We present our recent multiconfiguration Dirac-Hartree-Fock calculations of the energy levels, g-factors and polarizabilities for the lowest states of Nihonium, as well as for Thalium. Calculations were performed using GRASP2018 package [9]. In case of the polarizabilities, the influence of the continuum electron has been taken into account.

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Calculations of QED Corrections to Energy Levels of F-like Ions Using Model Lamb Shift Operator

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Ab initio Lamb shift calculations can be performed only for few-electron atomic systems. As to many-electron systems, the corresponding calculations are generally possible only for atoms with a few valence electrons. For this reason, the construction of simple approaches to account for the QED corrections is an important task of the relativistic quantum theory of atoms and molecules described by the Dirac-Breit-Coulomb (DCB) Hamiltonian. The one-particle model QED operator was introduced in our previous papers [1,2] and was tested in the calculations of many-electron atoms and ions [3].

In the present work, the model Lamb shift operator [1,2] is used to evaluate the QED effects on the $2P_{1/2} - 2P_{3/2}$ fine structure in F-like ions. This is done by incorporating this operator into the calculations based on the DCB equation employing different approaches. In [4] it was claimed that the model-potential computations of the Lamb shift on the fine structure in F-like uranium lead to a discrepancy between theory and experiment. Later [5], it was reported that the *ab initio* QED calculation yields the result which restores the agreement between theory and experiment and strongly disagrees with the model-potential values. In the present work, we demonstrate that three different methods, based on including the Lamb-shift operator into the Dirac-Fock equations, into the configuration-interaction Hamiltonian, or into the calculations by perturbation theory, lead to the theoretical results which are in good agreement with experiment and very close to the aforementioned *ab initio* QED results. It is also shown that the contribution of the negative-energy Dirac continuum can be important for the calculations of the QED corrections in heavy ions using the model operator.

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Accurate calculations of energy structures and radiation rates of L- and M-shell ions for astrophysics

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Employing two state-of-the-art methods, multiconfiguration Dirac-Hartree-Fock [1] and second-order many-body perturbation theory [2], level energies, wavelengths, electric dipole, magnetic dipole, electric quadrupole, and magnetic quadrupole transition rates, oscillator strengths, and line strengths are calculated for a number of L- and M-shell ions of iron group elements for astrophysics interest [3-11]. Extensive comparisons with experiments from the NIST [12] and CHIANTI [13] databases, and other recent benchmark calculations, show that the present results are highly accurate: for excitation energies, uncertainty is less than 0.1% for most states; for transition rates, uncertainty is better than 10% for the majority of transitions.

The excellent description of energy separations along the isoelectronic sequence makes it possible to point out a number of lines for which experimental identifications are questionable. A complete dataset should be helpful in analyzing new observations from the sun and other astrophysical sources, and is also likely to be useful for modeling and diagnosing astronomical and fusion plasmas.

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