# Virtual workshop on the "Atomic Structure of Actinides & Related Topics"

Wednesday 26 May 2021 - Friday 28 May 2021


# Book of Abstracts

# Contents

# Wednesday events

**Wednesday 26, 2021 (09:05 – 09:40)**

## Laser Spectroscopy along the Series of Actinide Elements – A Rewarding Challenge

**Speaker:** Klaus Wendt for LARISSA Collaboration (JGU)
**Author(s):** Klaus Wendt for LARISSA Collaboration

Within the Periodic Table of the elements both, the series of 15 lanthanide elements with proton numbers $57 \leq Z \leq 71$ and, even much stronger pronounced, the iso-electronic sequence of 15 actinides with $89 \leq Z \leq 103$ exhibits very peculiar features representing their specific properties. Regarding the atomic structure these species stand out due to the enormous complexity of their level structure and the resulting richness of their optical spectra. Based upon the gradual but, on the other hand, not regular filling of the $nf$ shell, with $n = 4$ for the lanthanides and $n = 5$ for the actinides, and the possible inclusion of $(n+1)d$ electrons already the ground state exhibits up to 3 open valence shells while excited states easily exhibit 4 active electrons. Reliable assignment of electronic configurations and quantum numbers or even just the identification of regular patterns in the spectra, representing e.g., unperturbed series of Rydberg levels, which for $n \to \infty$ would converge towards the ionization level, are impossible in many cases. Even quantum chaos is observed due to strong quantum mechanical configuration interaction of near-by-levels, severely distorting the attractive Coulomb field of the nucleus[(1)]. While for the lanthanides only one element, promethium with $Z = 61$, is all-radioactive, the actinides in contrast only exhibit 2 elements with stable isotopes, thorium with $Z = 90$ and uranium with $Z = 92$. Fortunately, the lower 12 actinides can be studied off-line due to the existence of isotopes with sufficiently long half-lives. Nevertheless, most of these isotopes must be prepared in sophisticated machinery, e.g. using accelerator experiments or neutron breeding in nuclear high-flux reactors. Correspondingly the knowledge on fundamental properties of the atom and specifically the derivation of nuclear structure from high resolution laser spectroscopy is still very scarce and meaningful measurements are just carried out at the moment. We shall give an overview on the contributions of laser resonance ionization spectroscopy to the field of actinide analysis, covering as far as possible the full range of applications in ultra-trace analysis, in atomic spectroscopy and finally introducing those high-resolution approaches, which are needed for deduction of nuclear parameters.

**Wednesday 26, 2021 (09:40 – 10:15)**

# Accurate electronic structure calculations for heavy open-shell systems

**Speaker:** Julian Berengut (University of New South Wales)
**Author(s):** Julian Berengut

Due to extremely low production yields, experiments that seek to measure the spectra of superheavy elements require precise theoretical predictions of the spectral properties. Transition rates and lifetimes are needed to develop excitation schemes and quantify experimental requirements, while accurate wavelengths are needed to narrow the search window. Other properties such as isotope shifts and hyperfine structure are needed to extract nuclear parameters and assist in the search for the fabled Island of Stability.

A promising route to calculations in complicated atoms is the particle-hole configuration interaction with many-body perturbation theory (CI+MBPT) method[1]. This extends the CI+MBPT method[2] to non-perturbatively include configurations with electron holes below the designated Fermi level. The method has been implemented in AMBiT[3], 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.

We have also developed a method to reduce the size of the CI eigenproblem on hardware by neglecting the interactions between high-energy non-dominant configurations. This method, which we call emu CI after the flightless Australian ratite, allows us to saturate the CI space even in complex polyvalent atoms such as dubnium, which has five valence electrons[4]. Recently we have performed calculations of Lr [5] and $Lr^+$ [6], where we were able to compare our results with state-of-the-art Fock-space coupled cluster calculations.

[1] J. C. Berengut, Phys. Rev. A 94, 012502 (2016).
[2] V. A. Dzuba, V. V. Flambaum, M. G. Kozlov, Phys. Rev. A 54, 3948 (1996).
[3] E. V. Kahl and J. C. Berengut, Comput. Phys. Commun. 238, 232 (2019); https://github.com/drjuls/AMBiT.
[4] A. J. Geddes, D. A. Czapski, E. V. Kahl, J. C. Berengut, Phys. Rev. A 98, 042508 (2018)
[5] E. V. Kahl, S. Raeder, E. Eliav, A. Borschevsky, J. C. Berengut, arXiv:2103.11287 (2021)
[6] E. V. Kahl, J. C. Berengut, M. Laatiaoui, E. Eliav, A. Borschevsky, Phys. Rev. A 100, 062505 (2019)

**Wednesday 26, 2021 (10:15 – 10:45)**

# Current Status of Atomic/Chemical Studies of Heavy and Trans-Actinide Elements at JAEA

**Speaker:** Tetsuya K. Sato (JAEA)
**Author(s):** Tetsuya K. Sato

The heaviest actinide elements, whose atomic numbers are larger than 100, are, so to say, bridge elements from heavy elements to superheavy elements. To understand how the strong relativistic effects play a role in their atomic and/or chemical properties, various approaches have been conducted so far.

At Japan Atomic Energy Agency (JAEA), we have studied the nuclear properties of heavy actinide isotopes synthesized by the heavy-ion-induced nuclear reactions by the ISOL (Isotope Separator On-Line) setup. Recently, as an application of the technique to study atomic properties on a one-at-a-time scale, we successfully measured the first ionization potentials ($IP_1$) of heavy actinides, fermium (Fm, atomic number $Z = 100$), mendelevium (Md, $Z = 101$), nobelium (No, $Z = 102$), and lawrencium (Lr, $Z = 103$) by using a surface ion-source coupled to the aerosol gas-jet transport system[1,2]. The observed monotonic increase of $IP_1$ value with an increasing atomic number up to No would correspond to fill electrons to the $f$-orbital one by one. Besides, the atomic configuration of the Lr atom was proposed experimentally for the first time by a comparison between the experimental value and the theoretical ones.

In addition, we also investigated the adsorption properties of the Lr atom on a Ta surface, and volatile compounds of dubnium (Db, $Z = 105$) on a quartz surface. Though it has been pointed out that its volatility might be abnormally high, the observed adsorption behavior of Lr was similar to Lu's one[3]. In parallel, adsorption enthalpies of oxychlorides of group-5 elements have been measured[4]. The results showed that the volatility of Db oxychlorides could be almost similar to or lower than that of tantalum compounds.

At the presentation, recent activities about studies on atomic and chemical properties of the heaviest elements at JAEA will be introduced. Future experimental plans would be presented as well.

[1] T. K. Sato et al., NATURE, 520 (2015) 209.
[2] T. K. Sato et al., JACS, 140 (2018) 14609.
[3] B. Eichler & S. Hübener, Inorg. Chim. Acta, 146 (1988) 261-265.
[4] N. M. Chiera et al.,Angew. Chem. Int. Ed (submitted).

**Wednesday 26, 2021 (11:05 – 11:40)**

# Laser spectroscopy of trapped thorium ions

**Speaker:** Ekkehard Peik (PTB)
**Author(s):** Ekkehard Peik

Motivated by the prospect of developing an optical nuclear clock based on the radiative transition between the $^{229}$Th nuclear ground state and its 8-ev-isomer[1] we are performing experiments on laser spectroscopy of thorium ions in charge states 1+, 2+ and 3+, trapped in radiofrequency Paul traps. Characterized by 3, 2 and 1 valence electrons, respectively, the electronic structure of these ions shows vastly different level densities. This property becomes relevant for the study of the low-energy nuclear transition because resonant electronic bridge processes may strongly modify nuclear decay and excitation rates. We have observed 210 excited states of even parity in $Th^{+}$ in the energy range from 7.3 to 9.8 eV by two-step laser excitation from the ground state[2]. In $Th^{3+}$, by contrast, only two levels exist in the same energy range. Laser excitation of near-infrared resonance lines of $Th^{3+}$ can be used for laser cooling and the fluorescence detection of single trapped ions. Hyperfine spectroscopy of $^{229}$Th2+ has recently provided first experimental data on the nuclear moments of the isomer[3]. In a nuclear clock, the hyperfine structure will be used for efficient detection of the nuclear state. We are preparing an experimental setup for high-precision spectroscopy of sympathetically laser cooled $Th^{3+}$ in the ground and isomeric state.

[1] K. Beeks, T. Sikorsky, T. Schumm, J. Thielking, M. V. Okhapkin, E. Peik, Nat. Rev. Phys. (2021) https://doi.org/10.1038/s42254-021-00286-6
[2] D.-M. Meier, J. Thielking, P. Glowacki, M. Okhapkin, R. A. Müller, A. Surzhykov, E. Peik, Phys. Rev. A 99, 052514 (2019)
[3] J. Thielking, M. V. Okhapkin, P. Glowacki, D. M. Meier, L. v. d. Wense, B. Seiferle, C. E. Düllmann, P. G. Thirolf, E. Peik, Nature 556, 321 (2018)

**Wednesday 26, 2021 (11:40 – 12:10)**

# Extending our knowledge about the $^{229}$Th nuclear isomer

**Speaker:** Benedict Seiferle (LMU München)
**Author(s):** Benedict Seiferle

$^{229}$Th possesses a nuclear excited state ($^{229m}$Th) with the lowest excitation energy among all known nuclear states. The mean value of two independent measurements of the excitation energy[1,2] results in $8.11 \pm 0.12$ eV which is energetically accessible with today's laser technology. The low excitation energy allows to use this nuclear excited state as a basis for a nuclear optical clock[3] that can be employed in the search for new physics[4]. In this talk I will give an overview of the progress that has been achieved over the last years and present experiments that are currently conducted at LMU Munich to further extend our knowledge about $^{229m}$Th.

[1] B. Seiferle et al., Energy of the Th-229 nuclear clock transition, Nature 573, 243-246, 2019.
[2] T. Sikorsky et al., Measurement of the Th-229 Isomer Energy with a Magnetic Microcalorimeter, Physical Review Letters 125, 142503, 2020.
[3] E. Peik und C. Tamm, Nuclear Laser Spectroscopy of the 3.5 eV Transition in Th-229, Europhysics Letters, Bd. 61, Nr. 2, 181-186, 2003.
[4] E. Peik et al., Nuclear clocks for testing fundamental physics, Quantum Sci. Technol. 6 034002, 2021.

**Wednesday 26, 2021 (12:10 – 12:35)**

# Investigation of the low-energy isomer $^{229m}$Th using the beta decay of $^{229}$Ac

**Speaker:** Sandro Kraemer (KU Leuven)
**Author(s):** Sandro Kraemer, Silvia Bara, Lino Da Costa Pereira, Hilde De Witte, Rafael Ferrer, Janni Moens, Simon Sels, Thibo Van Doninck, Piet Van Duppen, Paul Van den Bergh, Andre Vantomme, Matthias Verlinde

A unique feature of thorium-229 is its isomer with an exceptionally low excitation energy, proposed as a candidate for future optical clocks[1]. The small decay width is expected to outperform the accuracy of current state-of-the-art atomic clocks by an order of magnitude[2]. The current best measurement of the excitation energy results in a value of $8.28(17)$ eV [3], whereby the isomer is populated in the alpha decay of uranium-233. The development of an optical clock requires however knowledge of the excitation energy by an order of magnitude more precise. Spectroscopic experiments searching for a direct signature of the radiative decay have to-date been unsuccessful, partially due to the background induced during the population of the isomer.

A new approach using the beta decay of actinium-229 is studied as a novel method to populate the isomer with high efficiency and in low background conditions[4]. Produced online at the ISOLDE facility, actinium is laser-ionized and implanted into a high-bandgap crystal in specific lattice positions, inhibiting the converted decay of the isomer. A favourable feeding pattern significantly increasing the population of the isomer compared to uranium-233 and the higher degree of control over the lattice position due to the low recoil energy of the beta decay of actinium-229 are expected to increase the signal-to-noise ratio of spectroscopic measurements of the radiative decay.

Preparatory measurements studying the extraction of actinium-229 using laser-ionisation and the ISOL technique, its beta decay, and the implantation behaviour inside the bulk of the lattice using emission channeling have been performed. A setup including a vacuum-ultraviolet spectrometer for the direct detection of the radiative decay of the low-energy isomer has been developed and is currently in the commissioning phase, paving the way to a more precise determination of the excitation energy.

[1] E. Peik et al., Europhys. Lett. 61, 2 (2003)
[2] C. Campbell et al., PRL 108, 120802 (2012)
[3] B. Seiferle et al., Nature 573, 243-246 (2019)
[4] M. Verlinde et al., Physical Review C, 100 (2), 024315-024315

**Wednesday 26, 2021 (14:00 – 14:30)**

# New developments in theory of actinides and online data portal

**Speaker:** Marianna Safronova (University of Delaware)
**Author(s):** Marianna Safronova

I will report on the recent methodology developments and resulting capabilities of the state-of-the-art atomic methods to compute atomic properties of actinides. We significantly accelerated the computation of the valence triple excitations and included for the first time core triple excitations in the framework of the coupled-cluster approach[1]. Using a new approach, we computed energies and hyperfine constants of $Th^{3+}$, proposed for a nuclear clock, for an improved determination of $^{229}$Th nuclear magnetic dipole and electric quadrupole moments. The possibility of developing optical clocks using transitions between the ground and a low-lying excited state in $Cf^{15+}$ and $Cf^{17+}$ ions was investigated in detail in [2]. In another project, we develop a broadly applicable approach based on a parallel (MPI) configuration interaction code that drastically increases the ability to predict the properties of complex atoms accurately[3]. We recently used this approach to evaluate the electronic bridge process in $^{229}Th^{35+}$ for a laser excitation of a nuclear transition[4]. These methods are applicable to a broad range of atoms and ions, including superheavy elements. The approaches to evaluate the accuracy of theoretical predictions are also discussed.
I will also report a release of the first version of a new online portal for high-precision atomic data and computation[5]. Future plans to add actinides and other data as well as to release computer codes are discussed.

[1] S.G. Porsev and M.S. Safronova, in preparation.
[2] S. G. Porsev, U. I. Safronova, M. S. Safronova, P. O. Schmidt, A. I. Bondarev, M. G. Kozlov, I. I. Tupitsyn, Phys. Rev. A 102, 012802 (2020).
[3] C. Cheung, M. S. Safronova, S. G. Porsev, M. G. Kozlov, I. I. Tupitsyn, and A. I. Bondarev Phys. Rev. Lett. 124, 163001 (2020).
[4] S. G. Porsev, C. Cheung, M. S. Safronova, arXiv:2105.00512, submitted to Quantum Science and Technology (2021).
[5] Parinaz Barakhshan, Adam Marrs, Bindiya Arora, Rudolf Eigenmann, Marianna S. Safronova, Portal for High-Precision Atomic Data and Computation (version 1.0). University of Delaware, Newark, DE, USA. URL: https://www.udel.edu/atom.

**Wednesday 26, 2021 (14:30 – 15:00)**

## A community platform for just atomic computations

**Speaker:** Stephan Fritzsche (Helmholtz Institut, Jena & Friedrich-Schiller-Universität, Jena)
**Author(s):** Stephan Fritzsche

Electronic structure calculations of atoms and ions have a long tradition in physics with applications in basic research and spectroscopy. With the Jena Atomic Calculator (JAC), I here present a new implementation of a (relativistic) electronic structure code for the computation of atomic amplitudes, properties as well as a large number of excitation and decay processes for open-shell atoms and ions across the periodic table. JAC[(1)] is based on Julia, a new programming language for scientific computing, and provides an easy-to-use but powerful platform to extent atomic theory towards new applications. 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 spectroscopists, 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)].

[1] S. Fritzsche, Comp. Phys. Commun. 240, 1(2019); https://github.com/OpenJAC/JAC.jl
[2] Fritzsche, User Guide & Compendium to JAC (unpublished, 2019).

**Wednesday 26, 2021 (15:00 – 15:25)**

## Studying the origin of actinides in the universe with radiative transfer simulations of neutron-star mergers

**Speaker:** Andreas Floers (GSI Darmstadt)
**Author(s):** Andreas Floers

It has long since been established that observable actinides in the universe originate from the r-process (rapid neutron capture process). In 2017, the electromagnetic counterpart to the gravitational wave detection of two merging neutron stars (GW170817) was observed. The light observed from the rapidly decaying material and the characteristic time scale of the fading kilonova confirmed that neutron star mergers are a viable r-process source. From the light curve alone it was possible to characterise two ejecta components: one that contains low-Ye material such as lanthanides and possibly actinides, and a high-Ye component with very low lanthanide abundances. The dividing characteristic between the two components is the opacity of the material: lanthanides have a $\sim 100$ times higher opacity than iron-group material. To identify specific elements from the lanthanide or actinide groups, spectroscopic information is required. However, so far no clear detection of individual lanthanides or actinides has been made in the only observed neutron star merger. A great challenge for spectroscopic modelling of kilonovae is the almost non-existent atomic data currently available for lanthanides and even more so, for actinides. I will present how we will be able to use radiative transfer simulations of kilonovae to learn about the proposed production site of r-process elements in kilonovae. This requires complex codes and precise knowledge of the atomic data. With the increased interest in neutron star mergers the available atomic data is likely going to improve in the coming years, finally making this study possible. The detection or non-detection of clear absorption or emission signatures in future kilonova observations will tell us which of our models is realised in nature. As a consequence, we will learn whether neutron-star mergers are indeed the origin of the present-day actinides in the universe.

**Wednesday 26, 2021 (15:25 – 15:50)**

## Atomic Structure Calculations in Lanthanide and Actinide ions relevant to kilonovae

**Speaker:** Ricardo F. Silva (Universidade de Lisboa)
**Author(s):** Ricardo F. Silva, Jorge Sampaio, Pedro Amaro, José P. Marques

The observation of the near-infrared emission from binary neutron-star merger events, often know as kilonova, has increased the confidence that these astrophysical sources are the potential sites of heavy r-process nucleosynthesis. This emission is present in the observations of the gravitational-wave signal (GW170817) by LIGO/Virgo and is consistent with an electromagnetic transient emission of a kilonova. However, data of opacities, necessary for the interpretation of these observations, relies heavily on atomic structure calculations of both lanthanides and actinides, which is still very sparse. In this work we discuss the details of these calculations and some of the limitations imposed by the complexity of f-shell elements. Besides reviewing some previous results, we compare them with our present calculations based on the atomic structure codes FAC and MCDFGME. We study the combined effect of transition wavelengths and oscillator strengths on the opacities and how energy precision can be important at lower wavelengths. Finally, we discuss how that higher sensitivity of the opacity curve at higher energies can be exploited, looking for features of specific of lantanides and actinides present in kilonovae.

**Wednesday 26, 2021 (16:10 – 16:45)**

# The isotope program at ORNL for target material for superheavy element research

**Speaker:** Julie Ezold (Oak Ridge National Laboratory)
**Author(s):** Julie Ezold, Laetitia Delmau, Miting Du, Susan Hogle, Shelley Van Cleve

For more than 50 years, Oak Ridge National Laboratory's (ORNL) unique research facilities and staff have provided the research community with heavy actinides through fermium ($^{257}$Fm). These actinides have been used in the fabrication of targets for the discovery of nine superheavy elements, as identified in Table 1. The Radiochemical Engineering Development Center and the High Flux Isotope Reactor are truly one-of-a-kind facilities for the production and recovery of heavy actinides. All aspects of the reactor-produced heavy actinides will be addressed from fabrication of curium targets to the radiochemical separations and purification processing as depicted in Figure 1. Research activities for new production and separations techniques are being pursued at ORNL and will include novel irradiation schemes and radiochemical processing for berkelium and einsteinium production.

Table 1. Superheavy element discoveries enabled by ORNL-produced radioisotopes

| Element | Year Produced | Target |
|---|---|---|
| 104-Rutherfordium | 1964 | $^{242}$Pu, $^{249}$Cf |
| 105-Dubnium | 1970 | $^{249}$Bk, $^{249,250}$Cf |
| 106-Seaborgium | 1974 | $^{249}$Cf |
| 113-Nihonium | 2004 | $^{243}$Am (decay from 115) |
| 114-Flerovium | 2000 | $^{244}$Pu |
| 115-Moscovium | 2004 | $^{243}$Am |
| 116-Livermorium | 2005 | $^{245,248}$Cm |
| 117-Tennessine | 2010 | $^{249}$Bk |
| 118-Oganesson | 2006 | $^{249}$Cf |

**Wednesday 26, 2021 (16:45 – 17:15)**

# Proton-induced fusion-evaporation reactions for actinide production at IGISOL

**Speaker:** Andrea Raggio (UNIVERSITY OF JYVASKYLA)
**Author(s):** Andrea Raggio, Iain Moore, Ilkka Pohjalainen, Emmanuel Rey-Herme, Jan Saren, Marine Vandebrouck

In recent years, a program of research for the study of the nuclear structure of actinide isotopes has been implemented at the IGISOL facility, University of Jyväskylä. Initially, this work focused on producing low-energy beams of plutonium and thorium via gas cell-based laser ionization of atoms released from filament dispensers[1,2]. This led to successful high-resolution collinear laser spectroscopy of several isotopes of plutonium allowing for a study of changes in mean-squared charge radii[3]. Radioactive $^{233}$U alpha recoil sources have also been considered and characterized via alpha and gamma spectroscopy of the decay radiation, aiming at maximizing the production of a thorium ion source for a future study of the low-energy isomer in $^{229}$Th [4].

More recently, we have initiated an exploration of the production of a wider range of actinide isotopes online, using proton-induced fusion-evaporation reactions on a $^{232}$Th target. In order to prepare to expand the reach of the technique to more exotic targets, we have compared yields from a metallic $^{232}$Th target as well as novel drop-on-demand inkjet-printed targets[5]. The success of this preliminary work has led to an accepted proposal to perform yield studies using inkjet-printed $^{233}$U targets which we aim to run in 2022.

This contribution will focus on the current analysis of a successful online decay spectroscopy experiment performed in July 2020. Short-lived actinide isotopes were extracted from the gas cell, mass separated and transported to a dedicated implantation station. A close geometry setup of Ge, Si and Si(Li) detectors was implemented to measure the emitted $\gamma$ rays, $\alpha$ particles and conversion electrons. The aim of the experiment is to extract basic decay spectroscopy information including lifetimes, decay schemes and Q-values which are missing or incomplete in the region. The measured production yields will also be presented and discussed in the context of future mass measurements and optical spectroscopy using resonance ionization techniques.

[1] Pohjalainen, I. et al., Nucl. Instr. Meth. Phys. Res. Sect. B, 376 (2016): 233-239.
[2] Pohjalainen, I., et al., Nucl. Instr. Meth. Phys. Res. Sect. B, 484 (2020): 59-70.
[3] Voss, A., et al., Physical Review A, 95.3 (2017): 032506.
[4] Pohjalainen, et al., Nucl. Instr. Meth. Phys. Res. Sect. B, 463 (2020): 441-448.
[5] Haas, R., et al., Nucl. Instr. Meth. Phys. Res. Sect. A, 874 (2017): 43-49.

**Wednesday 26, 2021 (17:15 – 17:40)**

## The NEXT Project

**Speaker:** Xiangcheng Chen (University of Groningen)
**Author(s):** Julia Even, Xiangcheng Chen, Alexander Karpov, Maarten Mijland, Vyacheslav Saiko, Gawein Sala, Jan Sarén, Moritz Schlaich, Thomas Schlathölter, Lutz Schweikhard, Arif Soylu, Juha Uusitalo, Frank Wienholtz

The NEXT project, located at the University of Groningen, aims to study Neutron-rich EXotic nuclei produced in multinucleon Transfer reactions. In particular, we are interested in the transfermium region where the access to the neutron-rich side is very limited and hence the experimental data are still scarce. Precision mass and lifetime measurements of those nuclei can provide valuable insights into the neutron shell evolution in the heavy element region. Within the NEXT project, the heavy neutron-rich nuclei will be produced by bombarding actinide targets with projectiles at energies slightly above the Coulomb barrier, which are accelerated by the AGOR cyclotron in Groningen. The mechanism of multinucleon transfer reaction causes fragments flying out in very divergent angles. To efficiently collect the products of interest and reject contaminants in the meantime, a novel solenoid fragment separator will be developed to selectively focus the products to a downstream gas catcher. The thermalised ions will then be transported via a stacked-ring-based ion guide to a Multi-Reflection Time-of-Flight Mass Spectrometer (MR-ToF MS) for direct mass measurements, or for further purifications before lifetime measurements will be carried out. In this talk, I will present the experimental setup for the NEXT project, with emphasis on the current developmental status. Once it is completed, NEXT will provide a unique access to the neutron-rich side of the actinide nuclei and open up new possibilities for spectroscopic studies on heavy elements.

**Wednesday 26, 2021 (17:40 – 18:05)**

## Solution combustion synthesis of thin actinide targets for nuclear science measurements

**Speaker:** Khachatur Manukyan (University of Notre Dame)
**Author(s):** Khachatur Manukyan, Ashabari Majumdar, Dede Stefania, Jordan Roach, Peter Burns, Ani Aprahamian

Several research areas in nuclear science rely on experiments on various projectile and target combinations to extract key nuclear cross-section and structure information. Typically, thin uniform films of radionuclides with thicknesses in the range of from few to several hundreds of nanometers are deposited on a backing for support. Current target preparation techniques are based on decades-old approaches that do not take advantage of the most recent developments in materials science. Solution combustion synthesis (SCS) is a novel and highly efficient method for the deposition of thin actinide oxide targets on different backings. The basis of this method relies on the use of rapid exothermic chemical reactions between actinide metal nitrates with various organic compounds. SCS of thin-film targets involves the deposition of reactant solutions on backings using spin coating or spraying followed by short heating periods on a hot plate or in a furnace. The heat generated during SCS considerably reduces the duration and temperature of the process compared with other methods. This talk will present recent results and achievements on the preparation of actinide targets using SCS. It will discuss the relationships between process conditions, structure, and morphology of the resulting actinide films. Selected examples of UO2 thin-film target tests with charged particles or neutrons will also be highlighted. The results on target characterization by X-ray fluorescence (XRF), X-ray photoelectron spectroscopy (XPS), alpha-particle emission spectroscopy, Raman spectroscopy, and high-resolution transmission electron microscopy (TEM) before and after irradiation tests will also be presented. The significant relationship between the structure of targets and their stability will be discussed.

# Thursday events

**Thursday 27, 2021 (09:05 – 09:40)**

## In-gas-jet laser spectroscopy studies of actinides: A quest for $^{229m}Th^{+}$

**Speaker:** Rafael Ferrer (KU Leuven - IKS)
**Author(s):** Rafael Ferrer, Arno Claessens, Sandro Kraemer, Yuri Kudryavtsev, Vaila Leask, Sheila Roelens, Jekabs Romans, Simon Sels, Paul Van den Bergh, Piet Van Duppen, Elise Verstraelen, Matthias Verlinde

In the IGLIS laboratory at KU Leuven ongoing studies are devoted to designing, producing and characterizing the flow properties of convergent-divergent (de Laval) hypersonic nozzles, as well as to find optimal experimental conditions. Such conditions will enable laser spectroscopy studies of short-lived isotopes, from e.g. the hardly-accessible actinide and transactinide elements, with an unprecedented spectral resolution and a high efficiency at radioactive beam facilities such as SHIP (GSI) and S3-LEB (GANIL).
Along with a new 10 kHz pulse-repetition-rate dye laser system, combining a single-mode tunable laser for spectroscopy applications with high power ionization lasers, we plan to produce pure ion beams of $^{229m}Th^{+}$ and to determine its lifetime and excitation energy at the IGLIS laboratory and at ISOLDE (CERN).
In this talk I will summarize the characterization studies of new nozzles with the established PLIFS technique and with a novel flow mapping methods based on Resonance Ionization Spectroscopy. Furthermore, I will report on the first results of the production and investigation of $^{229m}Th$ and on the future plans.

**Thursday 27, 2021 (09:40 – 10:10)**

## Calculation of electronic structure of Fm, Md and No

**Speaker:** Vladimir Dzuba (UNSW Sydney)
**Author(s):** Vladimir Dzuba, Victor Flambaum, Saleh Alehabi, Jiguang Li, Anatoli Afanasjev

A combination of the configuration interaction and perturbation theory methods is used to calculate electronic structure and spectroscopic properties of atoms with open shells, including fermium (Fm), mendelevium (Md), and nobelium (No) atoms. We calculate energy levels, transition rates, ionization potentials, electron affinities, polarizabilities, hyperfine structure and isotope shift. The role of correlation and relativistic effects is studied. We argue in particular, that the isotope shift can be used to study nuclear structure beyond nuclear rms radius. Accurate measurements and corresponding calculations for at least two atomic transitions are needed to do this. In contrast to the hyperfine structure, the isotope shift can be used for both, odd and even nuclei.

**Thursday 27, 2021 (10:10 – 10:35)**

# Developments of the In-Gas-Jet Laser Ionization Spectroscopy technique: towards laser ionisation spectroscopy of $^{229}$Th$^{+}$

**Speaker:** Arno Claessens (KU Leuven)
**Author(s):** Arno Claessens, Rafael Ferrer, Sandro Kraemer, Yuri Kudryavtsev, Vaila Leask, Sheila Roelens, Jekabs Romans, Simon Sels, Piet Van Duppen, Paul Van den Bergh, Matthias Verlinde, Elise Verstraelen

At KU Leuven, efforts are undertaken to develop the in-gas-jet-laser ionization and spectroscopy technique for medium-heavy and heavy elements. Recent efforts have focussed on preparing the technique for the study of the low-lying $^{229}$Th isomer. Progress has been made in three key areas: production and laser ionisation of thorium ions, suppression of molecular sidebands and characterization of a new de Laval nozzle. Producing $^{229m}$Th was realized using $^{233}$U sources in a fast gas cell and laser ionisation of Th II was achieved by producing ions with laser-assisted ablation of a $^{232}$Th target. The presence of oxides and water adducts hampered initial progress and was counteracted to produce a pure $^{229}$Th ion beam. Lastly, a new de Laval nozzle was designed, manufactured and characterised to provide a cold ($\sim$ 15K) and collimated gas jet at low stagnation pressure conditions, which are required for producing isomeric thorium as well as for spectroscopy studies of (trans)actinides in the gas jet apparatus of the RADRIS experiment at GSI[(1)].

[1] S. Raeder et al., Nucl. Instrum. Methods Phys. Res. B, 463:272-276, 2020.

**Thursday 27, 2021 (10:35 – 11:00)**

# Commissioning tests of the S3-Low Energy Branch at SPIRAL2-GANIL

**Speaker:** Jekabs Romans (KU Leuven)
**Author(s):** Jekabs Romans, Anjali Ajayakumar, Martial Authier, Michael Block, Frederic Boumard, Lucia Caceres, Jean-Francois Cam, Samuel Damoy, Pierre Delahaye, Philippe Desrues, Antoine Drouart, Patrice Duchesne, Rafael Ferrer, Xavier Flechard, Patrice Gangnant, Thomas Goigoux, Sandro Kraemer, NATHALIE LECESNE, Mustapha Laatiaoui, Renan Leroy, Julien Lory, Franck Lutton, Vladimir Manea, Yvan Merrer, Iain Moore, Alejandro Ortiz-Cortes, Benoit Osmond, Julien Piot, Olivier Pochon, Sebastian Raeder, Blaise-Mael Retailleau, Herve Savajols, Simon Sels, Emil Traykov, Juha Uusitalo, Piet Van Duppen, Paul Van den Bergh, Christophe Vandamme, Marine Vandebrouck, Matthias Verlinde, Elise Verstraelen, Klaus Wendt, Ruben de Groote, serge franchoo

At GANIL[(1)] and LPC Caen[(2)], a cutting-edge project is under development to study exotic nuclei by the In-Gas Laser Ionization Spectroscopy (IGLIS)[(3)] technique. The underlying motivation is to extract nuclear ground- and isomer-state properties, such as nuclear mean-square charge radii $\delta r^2$, magnetic dipole $\mu$ and electrical quadrupole $Q$ moments, and nuclear spins $I$ from medium-heavy and heavy elements. In Spiral2-GANIL facility nuclides will be created by fusion-evaporation reactions, and in-flight separated from the primary accelerator beam and contaminants by the Super Separator Spectrometer (S3)[(4)]. The nuclides of interest will enter the S3-Low Energy Branch (S3-LEB)[(5)] at S3 focal plane via a thin window, separating the beamline and a gas cell. Here, under a constant gas flow, nuclide thermalization, neutralization and extraction will take place. At the gas cell exit a hypersonic gas jet will be created by a de Laval nozzle. The nozzle is designed to have a high Mach number at the necessary gas cell pressures, resulting in a collimated low-temperature and low-density environment, where laser ionization will be subsequently performed. The resulting photo ions will be guided and further mass-filtered by electric fields towards the detection stage[(6)]. The IGLIS method will combine high efficiency and high spectral resolution[(7)] due to minimized broadening mechanisms.
The research perspectives of the S3-LEB, providing access to refractory elements, $N = Z$ and proton drip line nuclei, as well as heavy actinides, will be presented. Furthermore, the results of commissioning tests of the setup will be summarized.

**Thursday 27, 2021 (11:00 – 11:25)**

## A diode-pumped, continuous-wave Ti:sapphire laser and its application to high resolution laser spectroscopy of actinides

**Speaker:** Volker Sonnenschein (University of Nagoya)
**Author(s):** Volker Sonnenschein, Gyo Itsubo, Nina Kneip, Dominik Studer, Matou Stemmler, Felix Weber, Hideki Tomita, Klaus Wendt

We recently developed a single-frequency Ti:sapphire oscillator using a multimode InGaN diode pumping system[(1)] as a cost-effective master laser source for an injection-locked amplifier[(2)]. The system so far has demonstrated a tunable wavelength range of up to 200 nm, output power up to 500 mW and a linewidth below 1 MHz if locked to an external reference cavity.
A similar system was constructed at the LARISSA laboratory at Mainz university, here a first demonstration experiment aimed at hyperfine spectroscopy of actinides was carried out at the RISIKO mass separator, using perpendicular beam geometry to minimize Doppler-broadening. First spectroscopy on Americium and Curium samples was performed, resulting in resolved hyperfine spectra of several atomic lines. Though the first experiments were interrupted and delayed by the pandemic, measurements have now resumed, and additional results are expected soon.

[1] V. Sonnenschein, H. Tomita et al., Hyper. Interact 241, 32, 2020, DOI: 10.1007/s10751-020-1706-4
[2] V. Sonnenschein et al., Laser Phys. 27 085701, 2017, DOI: 10.1088/1555-6611/aa7834

**Thursday 27, 2021 (11:45 – 12:10)**

# Calculations of the Electron Affinity of Polonium at the CCSD(T) level

**Speaker:** Raphaël Crosa-Rossa (RUG - University of Groningen)
**Author(s):** Raphaël Crosa-Rossa, Anastasia Borschevsky

The electron affinity (EA) is a fundamental atomic property which, together with the ionization potential (IP), allows to predict the physico-chemical behaviour of an element such as the electronegativity and the basicity, among others[1]. In the periodic table, polonium is the only element of the 6th row whose EA remains unknown. It will be measured in the near future at ISOLDE (CERN) by means of photodetachment spectroscopy, with an experimental set-up similar to the one recently used for measuring the EA of Astatine[2]. Herein, we aim to predict the value of the EA of polonium with state-of-the-art single reference CCSD(T) calculations in order to support the experiment and help in the interpretation of the resulting spectra. To do so, we provide a large exploration of the computational parameters (cardinality, augmentation, number of correlated electrons, etc.) to reach a meV accuracy within a reasonable computation cost. This approach, which allows to set an uncertainty on the prediction, is assessed by the calculations of the IP of Po and the EA and IP of Te, its lighter homologue, where experimental data is available and allows for comparison. Finally, the results are compared to previous theoretical work, where various methods such as MCDHF, CASPT2 or RECP-ccaCA among others, were used to predict the value of the electron affinity of Po [3–7].

[1] Leimbach, David, et al. "The electron affinity of astatine." Nature communications 11.1 (2020): 1-9.
[2] Nichols, Miranda. Preparation of negative ion beams for the determination of the electron affinity of polonium by laser photodetachment. No. CERN-INTC-2021-011. 2021.
[3] Borschevsky, Anastasia, et al. "Ionization potentials and electron affinities of the superheavy elements 115–117 and their sixth-row homologues Bi, Po, and At." Physical Review A 91.2 (2015): 020501.
[4] Laury, Marie L., and Angela K. Wilson. "Examining the heavy p-block with a pseudopotential-based composite method: Atomic and molecular applications of rp-ccCA." The Journal of chemical physics 137.21 (2012): 214111.
[5] Zeng, Tao, Dmitri G. Fedorov, and Mariusz Klobukowski. "Multireference study of spin-orbit coupling in the hydrides of the 6p-block elements using the model core potential method." The Journal of chemical physics 132.7 (2010): 074102.
[6] Roos, Björn O., et al. "Main group atoms and dimers studied with a new relativistic ANO basis set." The Journal of Physical Chemistry A 108.15 (2004): 2851-2858.
[7] Li, Junqin, et al. "Theoretical study for the electron affinities of negative ions with the MCDHF method." Journal of Physics B: Atomic, Molecular and Optical Physics 45.16 (2012): 165004.

**Thursday 27, 2021 (12:10 – 12:35)**

## Ionisation potentials and electron affinity of oganesson with relativistic coupled cluster method

**Speaker:** Yangyang Guo (University of Groningen)
**Author(s):** Yangyang Guo, Anastasia Borschevsky, Lukáš Pašteka, Ephraim Eliav

We present high accuracy relativistic coupled cluster calculations of the first and second ionisation potentials and the electron affinity of the heaviest element in the Periodic Table, Og. The results were extrapolated to the basis set limit and augmented with the higher order excitations (up to perturbative quadruples), the Breit contribution, and the QED self energy and vacuum polarisation corrections. We have performed an extensive investigation of the effect of the various computational parameters on the calculated properties, which allowed us to assign realistic uncertainties on our predictions. Similar study on the lighter homologue of Og, Rn, yields excellent agreement with experiment for the first ionisation potential and a reliable prediction for the second ionisation potential.

**Thursday 27, 2021 (12:35 – 13:00)**

## Direct laser spectroscopy of a short-lived, heavy molecule

**Speaker:** Shane Wilkins (Massachusetts Institute of Technology)
**Author(s):** S. G Wilkins, R. F. Garcia Ruiz, R. Berger, M. L. Bissell, A. A. Breier, A. J. Brinson, K. Chrysalidis, T. E. Cocolios, R. P. de Groote, K. T. Flanagan, S. Franchoo, T. F. Giesen, F. P. Gustafsson, T. A. Isaev, J. Karthein1, A. Koszorus, G. Neyens, C. M. Ricketts, S. Rothe, H. A. Perrett, S. M. Udrescu, A R. Vernon, X. F. Yang

Molecules that are composed of at least one unstable isotope offer a versatile platform upon which a diverse range of physical phenomena can be explored. In fundamental physics studies, subtle effects resulting from the violation of fundamental symmetries can be dramatically amplified in certain classes of molecules[(1−4)]. These additional dimensions enable a particular molecule to be engineered to possess an unparalleled sensitivity to a particular symmetry-violating effect that far exceeds the systems that currently set the strictest limits on new physics beyond the Standard Model. In addition to being of marked interest for fundamental physics, these molecules are of significance in other areas of research encompassing nuclear structure[(5)], chemistry[(6)] and astrophysics[(7)].
This contribution outlines results from the first laser spectroscopy study of a short-lived molecule performed at the Collinear Resonance Ionization Spectroscopy (CRIS) experiment at ISOLDE-CERN[(8)]. An outlook on extending laboratory studies to other molecular systems, in particular those containing actinide elements, will be given.

[1] Altuntaş, E. et al., Phys. Rev. Lett. 120, 142501 (2018)
[2] ACME Collaboration, Nature 562, 355–360 (2018)
[3] Flambaum, V. V. et al., Phys. Rev. Lett. 113, 103003 (2014)
[4] Berger, R. et al., WIREs Comput. Mol. Sci. 9, e1396 (2019)
[5] Rosiak, D. et al. Phys. Rev. Lett. 121, 252501 (2018)
[6] Formanuik, A. et al., Nat. Chem. 9, 578–583 (2017)
[7] Kamiński, T. et al., Nat. Ast. 2, 778–783 (2018)
[8] Garcia Ruiz, R. F. et al., Nature 581, 396–400 (2020)

**Thursday 27, 2021 (14:00 – 14:35)**

## Progress and prospects for Laser Ionization and Spectroscopy of Actinides within the LISA Innovative Training Network

**Speaker:** Bruce Marsh (CERN)
**Author(s):** Bruce Marsh

**Thursday 27, 2021 (14:35 – 15:05)**

## Development of Ultrasensitive Analytical Techniques to Detect Trace Elements

**Speaker:** Alfredo Galindo-Uribarri (ORNL)
**Author(s):** Alfredo Galindo-Uribarri

The monitoring and quantification of actinides at ultra-low levels is a challenge in many fields of physics: neutrino physics, dark matter searches, nuclear astrophysics and environmental sciences. These fields are pushing the limits of conventional techniques for ultra-trace analysis, demanding more sensitive and more efficient techniques. In this work, two approaches for ultra-trace analysis were investigated: using the negative-ion based Accelerator Mass Spectrometry (AMS) and positive-ion based Resonant Ionization Mass Spectrometry (RIMS) techniques. We demonstrated a method using AMS to detected traces of Th and U from ultrapure Cu made underground for the Majorana Demonstrator. Using RIMS we searched for more efficient three-step ionization paths for Pu, Th and U. We obtained efficiencies up to $51\%$ for Pu, $32\%$ for Th and $9\%$ for U. These results compare very favorably with the efficiencies obtained in AMS for actinides which are typically between $0.1\%$ to $1\%$. We also established a detection limit of $10^3$ atoms for Pu. In the spectroscopy studies for Pu we observed two Rydberg series. The convergence limits of these Rydberg series allowed us to measure the first ionization potential (IP) of Pu with the highest precision. In this talk I will report on results of these studies.

**Thursday 27, 2021 (15:05 – 15:30)**

# Towards efficient and reliable ISOL production of $^{225}$Ac: Placing an upper bound on collection efficiency

**Speaker:** Jake Johnson (KU Leuven)
**Author(s):** Jake Johnson, Thomas Elias Cocolios, Charlotte Duchemin, Reinhard Heinke, Frank Bruchertseifer, Wiktoria Wojtaczka, Michael Heines, Kristof Dockx, Sophie Hurier, Benji Leenders, Stephan Heinitz, Hanna Skliarova, Thierry Stora

In 2016, a landmark clinical study was reported, in which a $^{225}$Ac-labeled radiopharmaceutical was successfully used to treat metastatic prostate cancer[(1)]. In order to support further trials, an increased global effort to efficiently produce $^{225}$Ac has ensued. Even before the amazing results of this study were made available, a number of accelerator-based production routes were already being investigated. Out of these routes, the proton spallation of heavy metallic uranium or thorium ($^{nat}$U, $^{232}$Th (p, x) $^{225}$Ac) are amongst the most promising. It has been shown that $^{225}$Ac with activities high enough to support pre-clinical trials can be produced in-target, however there is still some discussion on how to optimally extract it in an isotopically pure form. Most efforts have so far focused on radiochemical separation of $^{225}$Ac from the irradiated target, but this method may not sufficiently suppress the troublesome $^{227}$Ac content in the final sample[(2,3)]. To get around this, the Isotope Separation On-Line (ISOL) method has been proposed for $^{225}$Ac extraction, as it is known to produce beams of unparalleled isotopic purity. However, the quantification and optimization of the collection efficiency of $^{225}$Ac using the ISOL technique still remains to be done. To inform this discussion, the results from two offline studies of $^{225}$Ac separation performed at the CERN-MEDICIS facility are presented.
The results that will be reported concern an upper bound on the ISOL collection efficiency of atomic $^{225}$Ac. This bound of order 10% quantifies the laser ionization efficiency of the scheme developed by the LARISSA group at Mainz and already employed at LISOL, TRIUMF and ISOLDE.
Alongside this, observations of the appropriate operating conditions for atomic $^{225}$Ac extraction in the case where oxidizing species are present in the target material (e.g $ThO_2$) are also discussed.
The results are finally rounded up in the context of on-line production prospects of $^{225}$Ac at CERN MEDICIS and beyond.

[1] Kratochwil, Clemens, et al., 225Ac-PSMA-617 for PSMA-targeted α-radiation therapy of metastatic castration-resistant prostate cancer, Journal of Nuclear Medicine 57.12 (2016): 1941-1944.
[2] Morgenstern, Alfred, et al., An overview of targeted alpha therapy with 225Actinium and 213Bismuth, Current radiopharmaceuticals 11.3 (2018): 200-208
[3] Joao Alberto Osso Junior et al., Report on joint IAEA-JRC Workshop Supply of Actinium-225, IAEA,Vienna, 2018.

**Thursday 27, 2021 (15:50 – 16:25)**

## Challenges in studies of actinide spectra: An example of the first three spectra of actinium

**Speaker:** Alexander Kramida (National Institute of Standards and Technology)
**Author(s):** Alexander Kramida

In 1957, Meggers et al. [J. Res. Natl. Bur. Stand. (U.S.) 58, 297] published the last comprehensive experimental study of the first three actinium spectra (Ac I-III), which was a result of several years of work. They produced many tens of high-resolution spectrograms recorded on photographic plates archived at the National Institute of Standards and Technology (NIST). Since then, only a few fragmentary observations were made using laser spectroscopy methods. Atomic theory also made very little progress in interpretation of these spectra. These new developments have recently been consolidated in the new actinium datasets of the NIST Atomic Spectroscopy Database (ASD). In this presentation, I will explain the problems encountered by both experimentalists and theorists in interpretation of these spectra.

**Thursday 27, 2021 (15:25 – 16:55)**

# Laser Spectroscopic Investigation of the heaviest actinides at GSI

**Speaker:** Premaditya Chhetri (HI Mainz, GSI)
**Author(s):** Premaditya Chhetri

Precision measurements of optical transitions of the heaviest elements is a versatile tool to probe the electronic shell structure which is strongly influenced by electron-electron correlations, relativistic, and QED effects. Optical studies of transfermium elements with $Z > 100$ are hampered by low production rates and the fact that any atomic information is initially available only from theoretical predictions. Using the sensitive RAdiation Detected Resonance Ionization Spectroscopy (RADRIS) technique coupled to the SHIP separator at GSI, a strong optical $^1S_0 \rightarrow {}^1P_1$ ground-state transition in the element nobelium ($Z = 102$) was identified and characterized[1]. Furthermore, the isotopes $^{252-255}$No were measured, revealing the isotope shift and a hyperfine splitting for the odd mass nucleus $^{253,255}$No [2]. From these measurements, nuclear information on the shapes and sizes was inferred. In addition, several high-lying Rydberg levels were observed, which enabled the extraction of the first ionization potential with high precision[3]. Recently, several isotopes of fermium (Fm, $Z = 100$) were also measured.

These results will be discussed as well as the prospects for future investigations involving the study of additional nobelium and fermium isotopes and the exploration of the atomic structure of the next heavier element, lawrencium ($Z = 103$).

[1] M. Laatiaoui et al., Nature 538, 495 (2016).
[2] S. Raeder et al., PRL 120, 232503 (2018).
[3] P. Chhetri et al., PRL 120, 263003 (2018).

**Thursday 27, 2021 (16:55 – 17:20)**

# Investigation of the atomic structure of curium and re-determination of its first ionization potential

**Speaker:** Nina Kneip (JGU)
**Author(s):** Nina Kneip, Felix Weber, Magdalena Anna Kaja, Christoph Düllmann, Sebastian Raeder, Dominik Studer, Klaus Wendt

Curium ($Z = 96$) is an actinide element, for which even the longest-lived isotope ($^{247}$Cm, $T_{1/2} = 15.6$ Ma) is entirely extinct. Cm isotopes are thus only artificially produced, e.g. as very minor share of spent nuclear fuel or by neutron capture of $^{238}$U during transmutation[(1)]. Located just in the middle of the actinide series, it exhibits a half-filled atomic $f$-shell with a ground state configuration [Rn] $5f^7 6d 7s^2$ coupling to $^9D_2^o$. As for any element its ionization potential IP, i.e., the energy required to remove a bound valence electron from the atomic shell, is of high relevance, e.g. for comparison to the isoelectronic lanthanide gadolinium as well as for predictions towards the superheavy elements via identification of trends in the binding energy along the series of actinides[(3)]. We report on an experiment, which we performed using resonance ionization spectroscopy (RIS), which is a very versatile method to study the atomic and nuclear structure of exotic isotopes. The high efficiency and selectivity of this method makes it particularly well suited for studies using only minute sample amounts. In the atomic spectrum of Cm three different initial excitation steps (FES) into the $5f^7 6d 7s 7p\ ^9D_3$, $5f^8 6d 7s\ ^9D_3$, and $45f^7 6d 7s 7p\ ^7D_2$ energy level were used. By scanning the second excitation step around the expected value of the IP numerous Rydberg levels and autoionizing levels were located. The IP was re-determined using both techniques of electric field ionization and Rydberg convergences for inter-comparison.

[1] Makarova, T. P., Bibichev, B. A., Domkin, V. D., Radiochem. 50(4), 414-426 (2008).
[2] Gorietti, D., Giardina, I., Arginelli, D., Battisti, P., J. Radioanal. Nucl. Chem. 314, 1785-1792 (2017).
[3] Wendt, K., Gottwald, T., Mattolat, C., Raeder, S., Hyperfine Interact. 227, 55-67 (2014).

**Thursday 27, 2021 (17:20 – 17:45)**

# Nuclear structure investigations on $^{253-255}$Es by laser resonance ionization spectroscopy

**Speaker:** Steven Nothhelfer (JGU, HIM, GSI)
**Author(s):** Steven Nothhelfer, Thomas E. Albrecht-Schönzart, Michael Block, Premaditya Chhetri, Christoph Düllmann, Klaus Eberhardt, Julie G. Ezold, Vadim Gadelshin, Alyssa Gaiser, Francesca Giacoppo, Reinhard Heinke, Tom Kieck, Nina Kneip, Mustapha Laatiaoui, Christoph Mokry, Sebastian Raeder, Jörg Runke, Fabian Schneider, Joseph Sperling, Dominik Studer, Petra Thörle-Pospiech, Norbert Trautmann, Felix Weber, Klaus Wendt

Experimental data on the hyperfine structure splittings and isotope shifts of spectral lines in rare elements reveal valuable information about the structure of their atomic nuclei. In this talk we will present results from resonance ionization laser spectroscopy performed on the rare isotopes $^{253-255}$Es at the RISIKO mass separator in Mainz. The Es isotopes were produced at the HFIR reactor and sample sizes of $\sim$ 0.2 pg ($^{253}$Es), $\sim$ 4 pg ($^{254}$Es) and $\sim$ 4 fg ($^{255}$Es) were used. The isotope shift of the 351.5 nm ground-state transition was measured in all three isotopes, while the hyperfine structure splitting for $^{254}$Es was resolved in four additional ground-state transitions at 364.4 nm, 408.3 nm, 410.9 nm, and 417.8 nm. The hyperfine structure analysis yielded a conclusive determination of the nuclear spins of $I(^{254}\text{Es}) = 7$ and $I(^{255}\text{Es}) = 7/2$, which were only tentatively assigned so far. In addition, the nuclear magnetic dipole moments as well as the spectroscopic electric quadrupole moments of $^{254,255}$Es were extracted from hyperfine structure coupling to $\mu(^{254}\text{Es}) = 3.42(7)\,\mu_N$, $Q_s(^{254}\text{Es}) = 9.9(1.6)\,\text{b}$, $\mu(^{255}\text{Es}) = 4.14(9)\,\mu_N$, and $Q_s(^{255}\text{Es}) = 5.3(1.8)\,\text{b}$. Our magnetic dipole moment value for $^{254}$Es deviates significantly from the previously reported literature value of $|\mu(^{254}\text{Es})| = 4.35(41)\,\mu_N$, which was extracted from the angular anisotropy of alpha radiation emitted by $^{254}$Es.

**Thursday 27, 2021 (17:45 – 18:10)**

## Laser spectroscopy of $^{248,249,250,254}$Fm

**Speaker:** Jessica Warbinek (GSI)
**Author(s):** Jessica Warbinek, Brankica Anđelić, Michael Block, Pierre Chauveau, Bradley Cheal, Premaditya Chhetri, Arno Claessens, Charlie Devlin, Christoph Düllmann, Rafael Ferrer, Francesca Giacoppo, Fritz P. Heßberger, Oliver Thomas Kaleja, EunKang Kim, Sandro Kraemer, Peter Kunz, Mustapha Laatiaoui, Jeremy Lantis, Werner Lauth, Nathalie Lecesne, Andrew Mistry, Danny Münzberg, Steven Nothhelfer, Sebastian Raeder, Emmanuel Rey-Herme, Elisabeth Rickert, Jekabs Romans, Elisa Romero Romero, Herve Savajols, Barbara Sulignano, Piet Van Duppen, Marine Vandebrouck, Thomas Walther, Alexander Yakushev

Laser spectroscopy of the heaviest elements reveals not only information on the atomic shell but also on their nuclear properties. This information is essential for the understanding of the enhanced nuclear stability in the region of the super-heavy elements. Also in the case of the heaviest actinides investigations by laser spectroscopy are hampered by the lack of availability of these nuclei as most of them have to be produced at accelerator facilities on-line. In this context first on-line laser spectroscopy measurements on $^{248,249,250,254}$Fm were performed with the Radiation Detected Resonance Ionization Spectroscopy (RADRIS) method at the SHIP separator at the GSI Helmholtz Centre. These isotopes were produced at a rate down to a few atoms per minute via the radioactive decay of nobelium nuclei produced in fusion-evaporation reactions. Laser spectroscopy was performed on the $5f^{12}7s^2\ ^3H^e_6$–$5f^{12}7s7p\ ^5G^o_5$ ground-state transition known from off-line measurements on the the longer-lived $^{255}$Fm. The isotope shift along the Fm isotope chain around $N = 152$ was measured at GHz precision. These experimental results in combination with atomic calculation give access to the nuclear mean-square charge radii. In combination with results from off-line measurements on the reactor-bred isotopes $^{255,257}$Fm at Mainz University, the investigated Fm isotopes span well across $N = 152$ allowing us to probe the effect of the neutron shell closure on the charge radii. Future studies on additional Fm isotopes are anticipated to also address the atomic structure of Fm.

# Friday events

**Friday 28, 2021 (09:05 – 09:35)**

## High accuracy predictions of properties of heavy atoms and evaluation of uncertainties

**Speaker:** Anastasia Borschevsky (University of Groningen)
**Author(s):** Anastasia Borschevsky

Theory can provide important support at all the stages of spectroscopic experiments, from planning the measurements, through extracting the properties of interest from the data, and to the interpretation of the results and their comparison to theoretically predicted values. To this end, highly accurate calculations of atomic properties are needed. In order to be reliable, such calculations must include both relativistic effects and electron correlation on the highest possible level.
Relativistic coupled cluster is considered one of the most powerful methods for accurate calculations of properties of heavy many-electron systems. This approach can be used to obtain ionization potentials, electron affinities, excitation energies, hyperfine structure parameters, and other atomic properties. It has been shown to be extremely reliable and to have very strong predictive power. Recently, we have developed a scheme that allows us to use extensive computational investigations to assign uncertainties on the theoretical predictions, facilitating the use of these predictions in experimental context.
A brief introduction to the relativistic coupled cluster method will be provided and the new development for estimation of uncertainties will be presented. The talk will focus on recent successful applications of the coupled cluster approach to atomic properties, in particular in connection to recent and planned experiments.

**Friday 28, 2021 (09:35 – 10:05)**

# Nuclear polarization and other enhanced effects in the heaviest elements

**Speaker:** Victor Flambaum (University of New South Wales)
**Author(s):** Victor Flambaum, Igor Samsonov, Hoang Bao Tran Tan, Anna Viatkina

In heavy atoms and ions, nuclear structure effects are significantly enhanced due to the overlap of the electron wave functions with the nucleus. This overlap rapidly increases with the nuclear charge $Z$. We study the energy level shifts induced by the electric dipole and electric quadrupole nuclear polarization effects in atoms and ions with $Z \geq 20$. The electric dipole polarization effect is enhanced by the nuclear giant dipole resonance. The electric quadrupole polarization effect is enhanced because the electrons in a heavy atom or ion move faster than the rotation of the deformed nucleus, thus experiencing significant corrections to the conventional approximation in which they 'see' an averaged nuclear charge density. The electric nuclear polarization effects are computed numerically for $1s$, $2s$, $2p_{1/2}$ and high $ns$ electrons. The results are fitted with elementary functions of nuclear parameters (nuclear charge, mass number, nuclear radius and deformation). We construct an effective potential which models the energy level shifts due to nuclear polarization. This effective potential, when added to the nuclear Coulomb interaction, may be used to find energy level shifts in multi-electron ions, atoms and molecules. The fitting functions and effective potentials of the nuclear polarization effects are important for the studies of isotope shifts and nonlinearity in the King plot which are now used to search for new interactions and particles.
Other effects include quantum chaos in actinide atoms and its manifestations, enhanced CP-violation effects in certain actinide nuclei and atoms, and high sensitivity of atomic spectra and isotope shifts to nuclear charge density distribution including different kinds of deformation and depletion in the centre.

**Friday 28, 2021 (10:05 – 10:30)**

# Hyperfine field calculations for electronic states in germanium using the relativistic Fock-space coupled-cluster method

**Speaker:** Martijn Reitsma (Van Swinderen Institute, University of Groningen)
**Author(s):** Martijn Reitsma, Anastasia Borschevsky

The hyperfine fields for the germanium $4p^2\ ^3\mathrm{P}_{1,2}$ and $4p5s\ ^3\mathrm{P}_1$ states were calculated using the relativistic Fock-space coupled-cluster (FSCC)[1] method in combination with the finite-field approach[2]. Nuclear dipole and quadrupole moments of germanium isotopes were determined by combining these calculations with hyperfine parameter measurements at ISOLDE-CERN[3]. The effects of different computational parameters were investigated and used to determine the uncertainty on the calculated values. Investigating the nuclear moments near the $Z = 28$ shell closure is needed to improve the understanding of the evolution of nuclear structure in that region.

[1] U. Kaldor and E. Eliav, Adv. Quantum Chem. 31, 313 (1998);
[2] H.J. Monkhorst, Int. J. Quantum Chem., 12, 421-432 (1977);
[3] A. Kanellakopoulos et al., Phys. Rev. C 102, (2020).

**Friday 28, 2021 (10:50 – 11:25)**

## Laser resonance chromatography: theoretical assessment for lanthanide and actinide ions

**Speaker:** Alexei Buchachenko (Skolkovo Institute of Science and Technology)
**Author(s):** Alexei Buchachenko, Giorgio Visentin, Mustapha Laatiaoui, Larry Viehland

The basic idea of the laser resonance chromatography (LRC) is the detection of the resonant electronic excitation of an ion by measuring its transport through a buffer gas. It has certain advantages over the spectral detection, particularly important for heavy and superheavy elements. Ions are better counted than the photons and their time of flight is better controlled than the radiative lifetime. Ion selection and drift velocity measurement are perfectly compatible with on-line heavy and superheavy element production. On the other hand, LRC imposes additional requirements to optical and collisional properties of the electronic states involved, which make the preliminary theoretical modeling indispensable for experimental realizations.
The fundamental concept behind LRC is the dependence of interaction potential between buffer gas particles and ion on the electronic configuration of the latter. It determines the difference in the ion-atom collision energy transfer and, in turn, in the ion drift velocities. Thus, the resonant laser population of the ions in the metastable state, relatively stable with respect to collisional quenching, leads to the appearance of ions at times not observed for the ground-state ions in the off-resonance pumping regime. The change in the temporal profile of the ion count signal firmly identifies the resonance pumping condition.
The ions of lanthanide and actinide families provide a convenient testbed for exploration of the LRC effect. Distinct populations of the outer $d$- and $s$-shells in the their ground state along the period allow one to estimate expected differences in the drift velocities, while known energy level schemes – to assess the optical routes to the metastable state pumping. We first overview the experimental and theoretical data on the ground-state lanthanide and actinide ions and then demonstrate how the theory can be used for the experimental-scale modeling of the LRC effect in the Lu ion. We also discuss the prospects for refinement of the theoretical approaches to interaction potentials and modeling of the macroscopic ion drift.

**Friday 28, 2021 (11:25 – 11:50)**

## Laser Resonance Chromatography (LRC): A Progress Report

**Speaker:** Elisa Romero Romero (Helmholtz Institut Mainz)
**Author(s):** Elisa Romero Romero, Michael Block, EunKang Kim, Steven Nothhelfer, Sebastian Raeder, Harry Ramanantoanina, Elisabeth Rickert, Mustapha Laatiaoui

The research of superheavy elements has been an exciting endeavor for scientists for many decades, as it enables probing the limits of nuclear existence and provides a fertile ground to advance our understanding of the atom's structure. However the experimental access to these atomic species is very challenging. A great leap forward in this research field was recently achieved with successful laser spectroscopy of the element nobelium[1,2]. Beyond nobelium, only very few predictions of the atom's structure exist, which in general are far from sufficient to reliably identify atoms from spectral lines. In this contribution I will present the Laser Resonance Chromatography (LRC) technique, which is conceived to enable atomic structure investigations beyond nobelium[3]. Subsequently, I will give a short update on the experimental progress and discuss prospects for LRC on $Rf^+$ ($Z = 104$).

[1] J. Reader A. Kramida, Yu. Ralchenko and NIST ASD Team (2018), 2019.
[2] M. Laatiaoui et al., Nature, 538 (2016) 495.
[3] M. Laatiaoui et al., Physical Review Letters, 125 (2020) 023002.

**Friday 28, 2021 (11:50 – 12:15)**

# Electronic structure of $Rf^+$ ($Z = 104$) from ab initio calculations

**Speaker:** Harry Ramanantoanina (Johannes Gutenberg-Universität Mainz)
**Author(s):** Harry Ramanantoanina, Anastasia Borschevsky, Michael Block, Mustapha Laatiaoui

In this presentation, We report calculation of the energy spectrum and the spectroscopic properties of the superheavy element ion: $Rf^+$. We use 4-component relativistic Dirac-Coulomb Hamiltonian and the multireference configuration interaction (MRCI) model to tackle the complex electronic structure problem that combines strong relativistic effects and electron correlation[(1)]. We determine the energies of the ground and the low-lying excited states of $Rf^+$, which originate from the $7s^2\ 6d^1$, $7s^1\ 6d^2$, $7s^2\ 7p^1$, and $7s^1\ 6d^1\ 7p^1$ configurations. The results are discussed vis-à-vis the lighter homologue, $Hf^+$ ion. We also assess the uncertainties of the predicted energy levels. The main purpose of the presented calculations is to provide a precise prediction of the energy levels and to identify suitable metastable excited states that are good candidates for the planned ion-mobility-assisted laser spectroscopy studies within the "Laser resonance Chromatography" (LRC) project[(2)].

[1] E. Eliav, U. Kaldor, and Y. Ishikawa, Phys. Rev. Lett. 74, 1079 (1995), https://link.aps.org/doi/10.1103/PhysRevLett.74.1079.
[2] M. Laatiaoui, A. A. Buchachenko, and L. A. Viehland, Phys. Rev. Lett. 125, 023002 (2020), https://link.aps.org/doi/10.1103/PhysRevLett.125.023002.

**Friday 28, 2021 (12:15 – 12:40)**

# Conceptual Design of an Ion Mobility Spectrometer for mobility measurement of actinides

**Speaker:** Elisabeth Ute Rickert (HIM, GSI, JGU)
**Author(s):** Elisabeth Ute Rickert, Hartmut Backe, Michael Block, Christoph Düllmann, Mustapha Laatiaoui, Werner Lauth, Sebastian Raeder

Relativistic effects strongly influence the chemical and physical properties of the heaviest elements, which can differ significantly from the periodicity predicted by the periodic table of elements. Previous systematic mobility measurements on monatomic lanthanide ions revealed the dependence of ion-atom interactions on the underlying electronic configuration and helped to investigate the aforementioned effects[(1)]. Presently, the measurements are being extended to the actinides, where larger deviations from periodicity are expected. Two-step photoionization will provide an element-selective ion production from a sample filament in argon gas and thus ensure an element-selective detection. In the talk, experimental approach, first results, and future plans are presented.

[1] M. Laatiaoui et al., EPJD 66, 232 (2012).