

MS 3: Mass Spectrometry - Posters

Time: Tuesday 16:30–18:15

Location: S Fobau Physik

MS 3.1 Tue 16:30 S Fobau Physik

MOCCA: a 4k-pixel molecule camera for the position and energy resolved detection of neutral molecule fragments —

•DENNIS SCHULZ¹, STEFFEN ALLGEIER¹, CHRISTIAN ENSS¹, ANDREAS FLEISCHMANN¹, LISA GAMER¹, LOREDANA GASTALDO¹, JULIA HAUER¹, SEBASTIAN KEMPF¹, SEBASTIAN SPANIOL², OLDŘICH NOVOTNÝ², and ANDREAS WOLF² — ¹Heidelberg University — ²Max Planck Institute for Nuclear Physics, Heidelberg

The MOCCA detector is a 4k-pixel high-resolution molecule camera based on metallic magnetic calorimeters and read out with SQUIDS that is able to detect low-energy neutral molecule fragments. It will be deployed at the Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg, a storage ring built to prepare and store molecular ions in their rotational and vibrational ground states, enabling studies on electron-ion interactions. To reconstruct the reaction kinematics, MOCCA measures the energy and position of incident particles on the detector, even with multiple particles hitting the detector simultaneously. Using different read-out techniques, MOCCAs 4096 pixel can be read out by using only 32 SQUID channels in total.

We present the most recent data from measurements of the MOCCA detector at 10 mK with a 6 keV photon source, demonstrating low cross-talk between rows and columns of the detector, the read-out principle and the energy resolution measured to be below 200 eV.

MS 3.2 Tue 16:30 S Fobau Physik

Recent developments at the Greifswald MR-ToF device —

•PAUL FISCHER, GERRIT MARX, and LUTZ SCHWEIKHARD — Institut für Physik, Universität Greifswald, 17489 Greifswald, Germany

The multi-reflection time-of-flight mass spectrometer (MR-ToF MS) at the University of Greifswald is further employed to develop and refine related techniques. In particular, metal cluster ions are produced in a laser ablation source and stored between electrostatic mirrors for several hundreds of milliseconds, leading to high mass resolving powers and the possibility to study ion properties as well as the storage characteristics of the trap itself.

Recently, the behavior of short-term ToF fluctuations between measurements have been studied with respect to comparability when the ion species of interest and the species used for a subsequent offline correction exhibit large mass differences [1]. Furthermore, the system's capabilities for the capture and selection of ions with large mass differences has been refined by employing multiple in-trap lift capture pulses and an in-trap deflection scheme allowing the retention of multiple ion species [2].

[1] P. Fischer et al., *Int. J. Mass Spectrom.* 432:44-51(2018)

[2] P. Fischer et al., *Int. J. Mass Spectrom.* (in print)

MS 3.3 Tue 16:30 S Fobau Physik

Photoexcitation of size-selected ions in an electrostatic storage device —

•PAUL FISCHER, GERRIT MARX, and LUTZ SCHWEIKHARD — Institut für Physik, Universität Greifswald, 17489 Greifswald, Germany

An electrostatic ion beam trap (EIBT) [1] (or multi-reflection time-of-flight mass spectrometer (MR-ToF MS) [2]) has been utilized for systematic investigations of molecular photofragmentation. To this end, bismuth clusters have been produced by a laser ablation source and subsequently stored and mass-selected [3] in the trap. A pulsed laser beam ($\lambda = 532\text{nm}$) is guided through the trap axially, the pulse timing of which is chosen to interact with the stored ion bunch at its turn-around point in the trap's mirror potential. Simultaneously, the trap is opened to release the clusters towards an ion detector. Thus, the fragment ions leave the EIBT as individual bunches and their masses can be determined via ToF mass spectrometry. In cases where higher resolving power is needed, the opening of the mirror can be delayed to allow MR-ToF operation. This marks a novel form of use for an MR-ToF MS in the sense that the device is used both to preselect an ion species of interest and investigate its reaction products in a single measurement cycle.

[1] H. Wollnik et al., *J. Mass Spectrom.* Ion Processes 96(3):267-274(1990)

[2] D. Zajfman et al., *Phys. Rev. A* 55:R1577-R1580(1997)

[3] P. Fischer et al., *Rev. Sci. Instrum.* 89:015114(2018)

MS 3.4 Tue 16:30 S Fobau Physik

High-Precision Mass Measurements with PENTATRAP —

•RIMA X. SCHÜSSLER¹, JOSÉ R. CRESPO LÓPEZ-URRUTIA¹, MENNO DOOR¹, PAVEL FILIANIN¹, WENJIA HUANG¹, CHARLOTTE KÖNIG^{1,2}, KATHRIN KROMER^{1,2}, YURI. N. NOVIKOV^{1,3}, ALEXANDER RISCHKA¹, CHRISTOPH SCHWEIGER¹, SVEN STURM¹, STEFAN ULMER⁴, SERGEY ELISEEV¹, and KLAUS BLAUM¹ — ¹Max-Planck-Institut für Kernphysik, Heidelberg — ²Ruprecht-Karls-Universität Heidelberg — ³Petersburg Nuclear Physics Institute, Gatchina, Russia — ⁴RIKEN, Ulmer Fundamental Symmetries Laboratory, Saitama, Japan

The high-precision Penning-trap mass spectrometer PENTATRAP, situated at the Max-Planck-Institut für Kernphysik, Heidelberg has recently demonstrated a relative mass precision of 10^{-11} using highly-charged xenon ions. Mass-ratio measurements of single stable and long lived highly charged ions are performed by determining their respective cyclotron frequencies in the strong magnetic field of a Penning trap. A unique feature of the experimental setup is the use of five cylindrical Penning traps, making simultaneous storage and measurement of several ion species possible. At this precision level, PENTATRAP will, for example, contribute to electron-neutrino mass related measurements within the ECHO collaboration, which determines the de-excitation spectrum following the electron capture in ^{163}Ho .

The current status as well as the first measurements with PENTATRAP will be shown on the poster.

MS 3.5 Tue 16:30 S Fobau Physik

Development of an efficient high-current ion source for Accelerator Mass Spectrometry —

•DIMITAR YORDANOV¹, HANS HOFSSÄSS¹, GEORG RUGEL², SHAVKAT AKHMADALIEV², JOHANNES VON BORANY², and JENNY FEIGE³ — ¹Georg-August-Universität Göttingen — ²Helmholtz-Zentrum Dresden-Rossendorf — ³Technische Universität Berlin

A new concept for Caesium sputtering ion source is studied experimentally and theoretically regarding a development of a new high-efficient and high-current ion source for Accelerator Mass Spectrometry (AMS) to quantify the ratios of long-lived cosmogenic radionuclides in micrometeorites. The source design is modular providing ease of access and simplifying maintenance while having better mechanical stability at the same time. The results show: the geometry of the cathode and the ionizer, as well as the distance between them and the radius of the extraction hole, are factors influencing the ion-optics, the focus of the Cs beam on the sample, the sputtering of the sample and the extracted current of the ions. Moreover, for an additional increase of the sputtering process on the sample, the cathode bias is higher than usual – up to 20 kV. The experimental results at different configurations of the source are supported by 3D model of the source for the ion-optics and the particle trajectories, as well as Child Langmuir Law is included. The authors would like to thank the Federal Ministry of Education and Research of Germany for its financial support (project 05K2016), and the HZDR's Ion Beam Center for its essential contribution to the realization of this project.

MS 3.6 Tue 16:30 S Fobau Physik

Interaction of size-selected stored anionic tin clusters with electrons —

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At the ClusterTrap-setup [1] size-selected mono-anionic tin clusters Sn_n^{1-} , $n = 7 - 75$, are stored simultaneously with electrons in a Penning trap to produce poly-anionic clusters by electron attachment [2].

In addition to doubly and triply charged clusters with the size of the precursors, fragments such as Sn_{n-7}^{1-} , Sn_{n-10}^{1-} or Sn_{n-15}^{1-} are observed [3]. The latter come along with the clusters Sn_{10}^{1-} and Sn_{15}^{1-} , probably due to fission as in the case of the group-14 neighbor element lead [4].

[1] F. Martinez et al., *Int. J. Mass Spectrom.* 365-366, 266 (2014)

[2] A. Herlert et al., *Phys. Scripta* T80, 200 (1999)

[3] S. König et al., *Eur. Phys. J. D* 72, 153 (2018)

[4] S. König et al., *Phys. Rev. Lett.* 120, 163001 (2018)

MS 3.7 Tue 16:30 S Fobau Physik

The Heidelberg compact EBIT as a source for highly charged holmium ions for high-precision mass spectrometry at PENTATRAP — ●CH. KÖNIG^{1,2}, J. R. CRESPO LÓPEZ-URRUTIA¹, M. DOOR¹, CH. E. DÜLLMANN³, P. FILIANIN¹, W. HUANG¹, K. KROMER^{1,2}, D. RENISCH³, A. RISCHKA¹, R. X. SCHÜSSLER¹, CH. SCHWEIGER¹, S. ELISEEV¹, and K. BLAUM¹ — ¹Max-Planck-Institut für Kernphysik, 69117 Heidelberg — ²Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg — ³Johannes Gutenberg-Universität Mainz, 55128 Mainz

The electron capture decay of ^{163}Ho to ^{163}Dy is a promising candidate for the determination of m_{ν_e} in the sub-eV range. For this purpose the ECHO collaboration [1] aims to perform a calorimetric measurement of the $^{163}\text{Dy}^*$ de-excitation spectrum. With its Penning-trap setup the PENTATRAP [2] experiment will contribute an independent Q -value as a consistency check acquired by a high-precision mass measurement of the mother and daughter nuclide with a relative mass ratio uncertainty of 10^{-11} . In order to achieve such an accuracy highly charged ions are necessary which can be produced in electron beam ion traps. Ions of various masses (40-165 amu) have been successfully produced, in particular charge states of up to 45+ have been achieved for ^{165}Ho using a sample size of about 10^{12} atoms. The injection of the atoms into a Heidelberg compact EBIT [3] is done via in-trap laser ablation. [1] Gastaldo, L. et al., Eur. Phys. J. Special Topics 226, 1623 (2017) [2] Repp, J. et al., Appl. Phys. B 107, 983 (2012) [3] Micke, P. et al., Rev. Sci. Instrum. 89, 063109 (2018)

MS 3.8 Tue 16:30 S Fobau Physik

Environmental influences on the high-precision mass measurements at PENTATRAP — ●K. KROMER^{1,2}, M. DOOR¹, A. RISCHKA¹, R.X. SCHÜSSLER¹, C. KÖNIG^{1,2}, CH. SCHWEIGER¹, W. HUANG¹, P. FILIANIN¹, S. ELISEEV¹, and K. BLAUM¹ — ¹Max-Planck-Institut für Kernphysik, 69117 Heidelberg — ²Ruprecht-Karls-Universität Heidelberg, 69120 Heidelberg

PENTATRAP [1] is a Penning-trap experiment consisting of five traps used to measure mass-ratios currently reaching a relative uncertainty of close to 10^{-11} . This allows for mass-ratio measurements of stable and long-lived highly charged ions with numerous applications, among others in neutrino physics [2] and tests of special relativity [3]. The systematic uncertainties stemming from environmental influences including the magnetic field, pressure and temperature fluctuations are being measured in order to find possible correlations to fluctuations in the cyclotron frequency of the trapped highly charged ions. This will determine if further stabilization, e.g. an active stabilization of the magnetic field with Helmholtz coils centered around the traps, will be necessary and to what extend.

[1] Repp, J. et al., Appl. Phys. B 107, 983, (2012)
[2] Gastaldo, L. et al., Eur. Phys. J. ST 226, 1623 (2017)
[3] Rainville, S. et al., Nature 438, 1096, (2005)

MS 3.9 Tue 16:30 S Fobau Physik

Activity determination of reference nuclides in the nuclear waste management — ●C. MÜLLER-GATERMANN¹, S. HEINZE¹, M. SCHIFFER¹, A. STOLZ¹, G. HACKENBERG¹, S. HERB¹, L. BUSSMANN¹, R. SPANIER¹, A. DEWALD¹, R. MAGREITER², E. STRUB², M. MICHEL², K. EBERHARDT³, M. DEWALD⁴, and B. DITTMANN⁴ — ¹Institut für Kernphysik, Köln, Deutschland — ²Abteilung Nuklearchemie, Köln, Deutschland — ³Institut für Kernchemie, Mainz, Deutschland — ⁴Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) GmbH

In the field of nuclear waste management liquid scintillation technique (LS) plays an important role among others, but complex chemistry is needed to reach low detection limits. We explored the possibility to replace LS by AMS techniques for specific isotopes. For the test we used reactor concrete material originating from KNK and MZFR research reactors from Karlsruhe, in addition we irradiated concrete samples with thermal as well as with epithermal neutrons with different doses at the Mainz TRIGA reactor. In order to verify the AMS results we measured the concentration of γ -emitters also activated in the sample material. This data can be used for consistency check. In this contribution we describe the experimental setups and discuss the results obtained so far.

MS 3.10 Tue 16:30 S Fobau Physik

Investigation of formate and halide adducts on coinage metal phosphine complexes in isolation — ●BJÖRN KWASIGROCH, SEBASTIAN V. KRUPPA, MICHAEL BORCHERS, CHRISTOPH

RIEHN, and GEREON NIEDNER-SCHATTEBURG — Fachbereich Chemie und Forschungszentrum OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 52, 67633 Kaiserslautern, Germany

Coinage metal complexes are of interest for potential application, e.g. in photocatalysis [1]. Here, we use the phosphine complexes $[\text{M}_1\text{M}_2(\text{L}^{\text{C}y})_2]^{2+}$ ($\text{M}=\text{Cu}, \text{Ag}, \text{Au}$, $\text{L}^{\text{C}y}=\text{bis}(\text{dicyclohexylphosphino})\text{methane}$) and his anionic adducts as a model system in order to investigate metallic $d^{10}\text{-}d^{10}$ interactions [2,3]. To this end, we utilized quadrupole ion trap tandem mass spectrometry. Formate adducts $[\text{M}_1\text{M}_2(\text{L}^{\text{C}y})_2(\text{CHOO})]^+$ were investigated via collision-induced dissociation (CID) and infrared multiphoton dissociation (IRMPD) spectroscopy in the C-O- and C-H-stretching region, supported by density functional theory (DFT) calculations. We observed branching ratios of CO_2/CHOO fragmentation in CID and a shift in the antisymmetric C-O- and C-H-stretching modes by IRMPD which depend on the coinage metal, respectively. The influence of halide anions X (Cl, Br, I) in $[\text{M}_1\text{M}_2(\text{L}^{\text{C}y})_2\text{X}]^+$ complexes are explored systematically with respect to their CID fragmentation. We found metal/halide dependent fragmentation pathways.

References: [1]V. W.-W. Yam et al., Chem. Rev. 2015, 115, 7589-7728; [2]S. V. Kruppa et al., Phys. Chem. Chem. Phys. 2017, 19, 22785-22800; [3]S. V. Kruppa et al, J. Phys. Chem. Lett. 2018, 9, 804-810.

MS 3.11 Tue 16:30 S Fobau Physik

Temperature dependent magnetic studies of an isolated Fe - spin crossover complex by X-ray Magnetic Circular Dichroism (XMCD) spectroscopy — ●MICHAEL LEMBACH¹, MATTHIAS P. KLEIN¹, JOACHIM HEWER¹, VICENTE ZAMUDIO-BAYER², MARTIN TIMM², CHRISTINE BÜLOW², JULIUS A. WOLNY¹, TOBIAS J. LAU², VOLKER SCHÜNEMANN¹, and GEREON NIEDNER-SCHATTEBURG¹ — ¹Fachbereich Chemie, Biophysik und Forschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — ²Helmholtz-Zentrum für Materialien und Energie BESSY II, 14109 Berlin, Germany

Magnetic properties of isolated molecular ions have become an interesting research field since the last decade. One field of interest are so called spin crossover complexes. They are able to reversibly change their spin multiplicity from its electronic ground state to a energetically higher electronic state by change of temperature or pressure^[1]. We explore the difference between bulk and gas phase spin crossover temperatures. Here, the monometallic complex $[\text{Fe}(\text{btpa})]^{2+}$ ($\text{btpa} = \text{N,N,N',N'}$ -tetrakis(2-pyridylmethyl)-6,6'-bis-(aminomethyl)-2,2'-bipyridine)^[2] was investigated with regard to the temperature dependent spinmagnetic behavior by X-ray Magnetic Circular Dichroism (XMCD) spectroscopy. We found a decreasing dichroic effect with an increase of the temperature from 4.5 K to 25.0 K. We successfully fit the obtained temperature dependent magnetization data of the $[\text{Fe}(\text{btpa})]^{2+}$ complex to a Brillouin function.

MS 3.12 Tue 16:30 S Fobau Physik

A graphene-based neutral particle detector — ●JESSICA WARBINEK¹, DAVID LEIMBACH¹, DI LU², DAG HANSTORP², DAVID PEGG³, JAKOB WELANDER², AVGUST YURGENS⁴, and KLAUS WENDT¹ — ¹Johannes Gutenberg-Universität Mainz — ²University of Gothenburg — ³University of Tennessee — ⁴Chalmers University of Technology Gothenburg

A transparent neutral particle detector for applications in the fields of atomic and molecular physics as well as mass spectrometry is presented, which is operational for particle energies in the range of few hundreds eV to a maximum of some tens of keV. The traditionally used target material for the initial conversion electrode, indium tin oxide (ITO), which has to combine good optical transparency with reasonable electric conductivity, has been replaced by a graphene layer. This substitution leads to a transmission of significantly shorter wavelengths of light down to 230 nm compared to ITO-based detectors, which are limited at about 335 nm. In this way collinear laser - ion beam interactions on atoms, molecules and clusters of ions, used e.g. for photodetachment measurements, are enabled throughout the whole visible spectral range down to the far UV. Moreover, the background signal from the photoelectric effect is drastically reduced when using graphene. The application of this new detector type will enable studies on electron affinities of rare radioisotopes and was already successfully used for the first ever determination of this quantity in astatine at ISOLDE/CERN.

MS 3.13 Tue 16:30 S Fobau Physik

Towards parts per trillion mass measurements on light nuclei at LIONTRAP — SASCHA RAU¹, FABIAN HEISSE^{1,2}, FLORIAN KÖHLER-LANGES¹, WOLFGANG QUINT², SVEN STURM¹, and KLAUS BLAUM¹ — ¹Max-Planck-Institut für Kernphysik, Heidelberg, Germany — ²GSI-Helmholtzzentrum für Schwerionenforschung Darmstadt, Germany

The precise knowledge of the atomic masses of various light nuclei, e.g. of the proton, deuteron, helium and triton, is of great importance for several tests of fundamental physics. For example, the mass of the proton is an important input parameter for hydrogen spectroscopy. Furthermore, an essential consistency check of the KATRIN experiment will require an ultra-precise measurement of the mass difference of triton and helium on a so far unrivalled level of precision of 6 meV/c². However, five sigma discrepancies between high-precision measurements of these light nuclear masses question their current literature values [1] and give strong motivation for a new and independent experiment, the LIONTRAP (Light ION TRAP) apparatus, aiming for relative uncertainties of a few parts per trillion. The results of the first measurement campaign on the proton mass [2] and the complete setup will be presented, which includes several new developments, e.g. a doubly compensated Penning trap, an in-situ B2 shim coil, various precisely tuned detection systems and a simultaneous phase-sensitive measurement technique with two neighbouring ion traps.

[1] J. A. Smith et al., Phys. Rev. Lett. 120, 143002 (2018)

[2] F. Heiße et al., Phys. Rev. Lett. 119, 033001 (2017)

MS 3.14 Tue 16:30 S Fobau Physik

Metastable states of the silicon anion observed in a cryogenic storage ring — D. MÜLL¹, F. GRUSSIE¹, E. A. GUERIN¹, A. BECKER¹, K. BLAUM¹, C. BREITENFELDT^{1,2}, S. GEORGE^{1,2}, J. GÖCK¹, M. GRIESER¹, R. VON HAHN¹, P. HERWIG¹, J. HÖRL¹, Á. KÁLOSI³, J. KARTHEIN¹, C. KRANTZ¹, H. KRECKEL¹, S. LOHMANN¹, C. MEYER¹, P. M. MISHRA¹, O. NOVOTNÝ¹, A. P. O'CONNOR¹, D. PAUL¹, R. REPNOW¹, S. SAURABH¹, K. SPRUCK¹, S. SUNIL KUMAR¹, X. URBAIN⁴, S. VOGEL¹, P. WILHELM¹, and A. WOLF¹ — ¹Max-Planck Institut für Kernphysik, Heidelberg, Germany — ²Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, Germany — ³visitor from Charles University Prague, Czech Republic — ⁴Institute of Condensed Matter and Nanosciences, Université Catholique de Lou-

vain, Louvain-la-Neuve B-1348, Belgium

We have used the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics to study the metastable states of the silicon anion. To this end we have stored a fast (58 keV) Si⁻ beam in the near-perfect cryogenic vacuum of the CSR, using only electrostatic deflection elements. We used several continuous laser systems at 633 nm, 980 nm, 1064 nm and 1390 nm, as well as a tunable pulsed optical parametric oscillator, in order to obtain information about the decay of the metastable anionic states by selective photodetachment. As a result, we show evidence for the existence of an extremely long-lived metastable state with a lifetime of several hours. We also found indication of another metastable state with a lifetime on the order of 20 s, in agreement with theoretical predictions.

MS 3.15 Tue 16:30 S Fobau Physik

Construction of a new electrospray ionization time of flight mass spectrometer (ESI-TOF-MS) for femtosecond laser experiments — PETER KRÜGER and KARL-MICHAEL WEITZEL — Philipps-Universität Marburg, Germany

Femtosecond laser mass spectrometry (fs-LMS) is a versatile method with many different applications [1]. It not only offers great temporal and mass resolution, but also allows non-resonant excitation schemes due to high laser peak intensities.

However, the technique relies on the sample of interest being in the gas phase, which poses a challenge regarding high molecular masses. This limitation can be overcome by employing an electrospray ionization (ESI) source, which allows intact vaporization and soft ionization of heavy molecules, e.g. biopolymers or pharmaceuticals [2].

In the current work we present a new apparatus specifically designed to combine the advantages of ESI and fs-LMS. The experimental setup consists of an ESI source, an ion guide, and an interaction region where the ion beam and a fs-laser beam overlap. This interaction region constitutes the source of an ion time-of-flight mass spectrometer (ion TOF-MS) and an electron TOF-MS with spatially resolved detector. The setup is described and first experiments aimed at the photoionization/-dissociation of cations and photodetachment/-dissociation of anions by the femtosecond laser pulses will be discussed.

[1] K.W.D. Ledingham, R.P. Singhal, Int. J. Mass Spectrom. Ion Proc., 163, 149, (1997) [2] J.B. Fenn, Angew. Chemie, 42, 3871, (2003)