

## MO 9: Posters 1: Dichroism, VUV and Xray, Clusters, and Cold Molecules

Time: Tuesday 17:00–19:00

Location: P OGs

MO 9.1 Tue 17:00 P OGs

**Theoretical study of photoelectron circular dichroism in the multiphoton ionization of bicyclic ketones** — ●ANNE DOROTHEE MÜLLER, ANTON N. ARTEMYEV, and PHILIPP V. DEMEKHIN — Institut für Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

Recently [1-3], it was demonstrated experimentally that absorption of several circularly polarized photons in the multiphoton ionization spectra of randomly oriented chiral molecules by femtosecond laser pulses may result in a considerable photoelectron circular dichroism (PECD) effect. So far, a reliable quantitative theoretical interpretation of these experimental results is missing. Here, we perform a systematic investigation of PECD in the resonance enhanced multiphoton ionization and above threshold ionization spectra of camphor and fenchone, by numerically solving the time-dependent Schrödinger equation for the single-active-electron wave-packet in a chiral molecular potential in the presence of intense circular polarized laser pulses [4]. Theoretical results obtained for randomly oriented and fixed-in space molecules are presented and compared with experiments [1].

[1] C. Lux et al., *Angew. Chem. Int. Ed.* **51**, 5001 (2012); *ChemPhysChem* **16**, 115 (2015); *J. Phys. B* **49**, 02LT01 (2016).

[2] M. H. M. Janssen and I. Powis, *Phys. Chem. Chem. Phys.* **16**, 856 (2014).

[3] S. Beaulieu et al., *New J. Phys.* **18**, 102002 (2016).

[4] A.N. Artemyev, A.D. Müller, D. Hochstuhl, and Ph.V. Demekhin, *J. Chem. Phys.* **142**, 244105 (2015).

MO 9.2 Tue 17:00 P OGs

**Broadband Time-resolved Circular Dichroism Spectroscopy of Hemoglobin** — ●HEIKO HILDENBRAND, ANDREAS STEINBACHER, FEDERICO KOCH, MARCO SCHMID, and TOBIAS BRIXNER — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Circular dichroism (CD) is a common technique for analyzing chiral samples by their difference in absorption of left and right circularly polarized light. However, chiral signals are small and the typically utilized long optical path lengths, high concentrations, and long integration times in steady-state measurements are not suitable for ultrafast spectroscopy. Hence, only few chirality-sensitive ultrafast time-resolved spectroscopic approaches in the liquid phase have been reported [1,2].

Here we present broadband time-resolved CD spectroscopy which is based on a setup capable of mirroring an arbitrary polarization state of an ultrashort laser pulse. Hence, by passing a circularly polarized broadband probe pulse through this setup we can switch between opposite handedness on a shot-to-shot basis to detect transient CD changes. To demonstrate the capabilities of this approach we investigate the early photochemistry of oxygenated hemoglobin and myoglobin by time-resolved circular dichroism and transient absorption spectroscopy in the visible spectral region, since the spectrometer is capable of acquiring both signals simultaneously.

[1] Meyer-Ilse et al., *Laser Photon. Rev.* **7**, 495 (2013)

[2] Hiramatsu et al., *J. Chem. Phys.* **143**, 121102 (2015)

MO 9.3 Tue 17:00 P OGs

**Broadband Photoelectron Circular Dichroism** — ●TOM RING, ALEXANDER KASTNER, PHILIPP HILLMANN, HENDRIKE BRAUN, ARNE SENFTLEBEN, and THOMAS BAUMERT — Universität Kassel, Institut für Physik und CINSaT, D-34132 Kassel

Photoelectron circular dichroism (PECD) describes the asymmetry in the photoelectron angular distribution (PAD) with regard to the light propagation direction after ionization with circularly polarized light. First investigated by one photon synchrotron ionization,<sup>1</sup> we demonstrated that PECD on isotropically distributed chiral molecules is accessible via 2+1 resonance enhanced multi photon ionization (REMPI) using femtosecond laser pulses and established PECD as a highly sensitive and robust analytical tool.<sup>2</sup> A different excitation scheme is addressed within PECD studies of electrons from above threshold ionization (ATI).<sup>3</sup>

In this contribution we present an ultra-broadband approach to PECD using white light generated by an argon filled hollow-core fiber. This way the excitation scheme changes due to the combination of different wavelengths with regard to the temporal structure of the pulses

and a wide range of excess energies in the PADs can be accessed simultaneously.

[1] L. Nahon et al.: *J. El. Spectr. Rel. Phen.*, **204**, 322 (2015)

[2] C. Lux et al.: *Chem. Phys. Chem* **16**, 115 (2015)

[3] C. Lux et al.: *J. Phys. B* **49**, (2016)

MO 9.4 Tue 17:00 P OGs

**Towards continuous-wave cavity-enhanced polarimetry for highly sensitive chirality measurements** — ●OLEG TRETIAK<sup>1</sup>, LYKOURGOS BOUGAS<sup>1</sup>, DIONYSIS ANTYPAS<sup>2</sup>, and DMITRY BUDKER<sup>1,2</sup> — <sup>1</sup>Johannes Gutenberg Universität Mainz, 55128 Mainz, Germany — <sup>2</sup>Helmholtz Institut Mainz, 55128 Mainz, Germany

We present our work towards the construction of a cavity-enhanced polarimeter for highly sensitive, continuous-wave, measurements of chirality in the gas, liquid, and solid phase. The developed polarimeter employs an optical cavity that allows for the enhancement of the chiral (optical-rotation) signals by the number of cavity passes, and, for the introduction of crucial signal reversals that enable absolute chirality measurements with high sensitivity. The presented technique has applications in different science fields ranging from fundamental physics, to atmospheric chemistry and medical research. We present our newly constructed chiral-polarimeter here in Mainz, and discuss its current sensitivity and our efforts towards shot-noise limited optical rotation measurements.

MO 9.5 Tue 17:00 P OGs

**Transient absorption and VCD spectroscopy of two azobenzene derivatives with chiral sidegroups** — ●KEVIN ARTMANN<sup>1</sup>, KAROLINE BUENNEMANN<sup>2</sup>, JOHANNES KNORR<sup>1</sup>, CHRISTIAN MERTEN<sup>2</sup>, and PATRICK NUERNBERGER<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum — <sup>2</sup>Organische Chemie II, Ruhr-Universität Bochum, 44780 Bochum

Azobenzenes are a widely-studied class of photochromic molecular switches with versatile applicability. Their photoswitching is based on a *trans/cis* isomerization, with the exact isomerization mechanism still under debate and subject of many recent investigations [1]. We examine two azobenzene derivatives with chiral sidegroups: the one substituted in para position, whose *cis* isomer is observable for >48 h after photoswitching, shows ultrafast dynamics similar to unsubstituted azobenzene [2]. Global analysis yields three time constants for accurately describing the experimental data. The second azobenzene derivative, with two substituents in *ortho* position, behaves differently: the *cis* isomer is absent in stationary absorption spectra, yet transient absorption discloses that it is formed. Hence, a fast thermal back-isomerization occurs, caused by electronic and/or steric effects of the sidegroups. The experiments are complemented with IR and vibrational circular dichroism (VCD) studies: switching is observed in vibrational spectra for the *para* compound, whereas the fast back-reaction prevents the observation of VCD changes for the *ortho* compound.

\*[1] H.M.D. Bandara, S.C. Burdette, *Chem. Soc. Rev.* **41**, 1809 (2012).

\*[2] I.K. Lednev *et al.*, *Chem. Phys. Lett.* **290**, 68 (1998).

MO 9.6 Tue 17:00 P OGs

**Angle-resolved spectroscopy of electron emission by chiral molecules** — ●DANIEL ROMAN PAUL, JAN DREISMANN, and STEFAN SCHIPPERS — I. Physikalisches Institut, Justus-Liebig-Universität Gießen

Elementary particle physics chirality is of great importance, in particular for the weak interaction. According to the Vester-Ulbricht-hypothesis a symmetry breaking by the weak interaction might be a reason for homochirality of molecules of life. While chemical properties of chiral molecules are already well observed, the physical basis is still a topic of current research. In this context collision experiments can give insight into the electronic structure and electron dynamics of chiral molecules.

We use an ESA22 [1,2] electron spectrometer for angle- and energy-resolved electron spectroscopy. Electrons produced by the collision of spin-polarized electrons as well as circular polarized photons on a gas target are separated by energy via a combination of electrostatic fields and detected by 22 channel electron detectors.

We here report on electron collisions on methyl lactate ( $C_4H_8O_3$ ).

The resulting Auger spectra are compared with Auger spectra for oxygen and carbon dioxide, measured under similar conditions.

- [1] Ricz et al., *Phys. Rev. A* **65**, 042707 (2002)  
 [2] Ábrók et al. *Nucl. Instr. Meth. Phys. Res. B* **369** (2016) 24-28

MO 9.7 Tue 17:00 P OGS

**Electron-nuclear Coupling through Autoionizing States after Strong-field Excitation of H<sub>2</sub> Molecules** — ●YONGHAO MI, NICOLAS CAMUS, LUTZ FECHNER, MARTIN LAUX, ROBERT MOSHAMMER, and THOMAS PFEIFER — Max-Planck-Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg

Channel-selective electron emission from strong-field photo-ionization of H<sub>2</sub> molecules is experimentally investigated by using ultrashort laser pulses and a Reaction Microscope. The electron momenta and energy spectra in coincidence with bound and dissociative ionization channels are compared. Surprisingly, we observed an enhancement of the photoelectron yield in the low-energy region for the bound ionization channel. By further investigation of asymmetrical electron emission using two-color laser pulses, this enhancement is understood as the population of the autoionizing states of H<sub>2</sub> molecules in which vibrational energy is transferred to electronic energy.

MO 9.8 Tue 17:00 P OGS

**Imaging of the He<sub>2</sub> wave function using a free electron laser**

— ●STEFAN ZELLER<sup>1</sup>, MAKSIM KUNITSKI<sup>1</sup>, JÖRG VOIGTSBERGER<sup>1</sup>, ANTON KALININ<sup>1</sup>, ALEXANDER SCHOTTELIUS<sup>1</sup>, CARL SCHOBERT<sup>1</sup>, MARKUS WAITZ<sup>1</sup>, HENDRIK SANN<sup>1</sup>, ALEXANDER HARTUNG<sup>1</sup>, TOBIAS BAUER<sup>1</sup>, MARTIN PITZER<sup>1</sup>, FLORIAN TRINTER<sup>1</sup>, CHRISTOPH GOHL<sup>1</sup>, CHRISTIAN JANKE<sup>1</sup>, MARTIN RICHTER<sup>1</sup>, GREGOR KASTIRKE<sup>1</sup>, MIRIAM WELER<sup>1</sup>, ACHIM CZASCH<sup>1</sup>, MARKUS BRAUNE<sup>2</sup>, ROBERT E. GRISENT<sup>1,3</sup>, LOTHAR PH. H. SCHMIDT<sup>1</sup>, MARKUS S. SCHÖFFLER<sup>1</sup>, JOSHUA B. WILLIAMS<sup>4</sup>, TILL JAHNKE<sup>1</sup>, and REINHARD DÖRNER<sup>1</sup> — <sup>1</sup>Institut fuer Kernphysik, Goethe-Universitaet Frankfurt, 60438 Frankfurt, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — <sup>3</sup>GSI Helmholtz Centre for Heavy Ion Research, 64291 Darmstadt, Germany — <sup>4</sup>Department of Physics, University of Nevada, Reno, NV 89557, USA

We report on Coulomb explosion imaging of the wavefunction of the quantum halo system He<sub>2</sub>. Each atom of this system is ionized by tunnel ionization in a femto second laser pulse and in a second experiment by single photon ionization employing a free electron laser. We visualize the exponential decay of the probability density of the tunneling particle over distance for over two orders of magnitude up to an internuclear distance of 250 Å. By fitting the slope of the density in the tunneling regime we obtain a binding energy of 151.9 ± 13.3 neV, which is in agreement with most recent calculations [Przybytek et al., *PRL* **104**, 183003, 2010].

MO 9.9 Tue 17:00 P OGS

**Ultrafast photodissociation of small molecules studied by interferometric VUV-VUV pump-probe experiments** — OLIVER SCHEPP<sup>1</sup>, ARNE BAUMANN<sup>1</sup>, MAREK WIELAND<sup>1,2,3</sup>, and ●MARKUS DRESCHER<sup>1,2,3</sup>

— <sup>1</sup>Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg — <sup>2</sup>The Hamburg Centre for Ultrafast Imaging (CUI), Luruper Chaussee 149, 22761 Hamburg — <sup>3</sup>Centre for Free-Electron-Laser Science, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg

Ultrafast photoreaction dynamics of small molecules are studied in the time domain, using a single-color VUV-pump/ VUV-probe scheme [1]. 17-fs VUV-pulses, centered at 161 nm with pulse energies up to 1.1 μJ created with high harmonic generation are split by two moveable interdigitated double comb mirrors into two collinearly propagating replicas with a variable delay [2,3]. This Michelson-type all-reflective interferometric autocorrelation scheme is used for recording the time-dependend pump-probe signal with simultaneous non-resonant two-photon ionization of krypton as a precise timing-reference. The photoreaction dynamics are probed via one and two VUV photon absorption, enabling different observables for the pump-probe signal which expands intrinsic limitations in observation of the molecular wavepacket. Additional spectral information obtained by the interferometric resolution give access to the involved harmonic orders and the order of nonlinearity.

- [1] Schepp, O. et. al., *Phys Rev. A* **94**, 033411 (2016)  
 [2] Rompotis, D. et. al., *Opt. Lett.* **50** 1675 (2015)  
 [3] Gebert, T., et al., *New J. Phys.* **16** 0170347 (2014)

MO 9.10 Tue 17:00 P OGS

**Experimental set-up for dispersed photon emission spectroscopy of liquid microjets** — ●CHRISTIAN OZGA<sup>1</sup>, ANDREAS HANS<sup>1</sup>, ROBERT SEIDEL<sup>2</sup>, PHILIPP SCHMIDT<sup>1</sup>, XAVER HOLZAPFEL<sup>1</sup>, MARVIN POHL<sup>2</sup>, BERND WINTER<sup>2</sup>, ARNO EHRESMANN<sup>1</sup>, and ANDRÉ KNIE<sup>1</sup> — <sup>1</sup>Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology (CINaT), Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — <sup>2</sup>Helmholtz-Zentrum für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany

With the development of liquid microjets the interest in the investigation of the molecular structure of volatile liquids after X-ray irradiation increased progressively. This structure was probed by different measurement techniques ranging from the detection of charged particles, Raman spectroscopy to X-ray emission spectroscopy and revealed e.g. interatomic coulombic decay processes in liquid water as well as different types of hydrogen bonds in bulk liquid water. However, the low energy photon emission regime, i.e. the wavelength region from 40 nm to 650 nm, remains hitherto unexplored. This spectral range acts as a complementary tool for the other techniques allowing a deeper understanding of the still not fully understood molecular structure of liquids, solvated (bio-)molecules and the interaction of solvents and solutes. Here we present an experimental set-up for the detection of dispersed photons with emission wavelengths from 40 nm to 650 nm. It can be easily adapted for the additional measurement of photoelectrons allowing a direct comparison of photon and electron emission.

MO 9.11 Tue 17:00 P OGS

**From Rare Gas to Hydrogen-bonded clusters: Size distributions of supersonic beams from a pulsed valve using the titration technique** — ●MATTHIAS BOHLEN, AARON LAForge, RUPERT MICHELS, NICOLAS RENDLER, MYKOLA SHCHERBININ, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str.3, D-79104 Freiburg i.B.

Pulsed valves, in general, offer many advantages over continuous beam sources such as higher beam densities and reduced gas load. Recently, we developed a pulsed valve in collaboration with UBC, Vancouver, which produces supersonic gas pulses down to 20 μs duration at repetition rates up to several hundred Hz. Overall, the valve is versatile in the type of clusters which can be produced ranging from rare gas clusters to hydrogen bonded clusters. Additionally, cryogenic cooling of the valve can be utilized to produce helium nanodroplets. To estimate the cluster size distribution, we use the so-called titration technique [1], which has accurately determined cluster sizes of continuous supersonic beams. Here, we report on a systematic study of cluster size distributions by varying expansion parameters. We apply this technique to argon, ammonia, and water clusters.

- [1] L. F. Gomez, E. Loginov, R. Sliter, A. F. Vilesov; *J. Chem. Phys.* **135**, 154201 (2011)

MO 9.12 Tue 17:00 P OGS

**Small metal clusters on porphyrin templates** — ●FREDERIC USSLING<sup>1</sup>, TOBIAS BISCHOFF<sup>1</sup>, ANDRÉ KNECHT<sup>1</sup>, ANDREA MERLI<sup>1</sup>, MERLE I. S. RÖHR<sup>2</sup>, POLINA G. LISINETSKAYA<sup>2</sup>, JENS PETERSEN<sup>2</sup>, ROLAND MITRIĆ<sup>2</sup>, THOMAS MÖLLER<sup>1</sup>, and TORBJÖRN RANDER<sup>1</sup> — <sup>1</sup>Institut für Optik und Atomare Physik, Technische Universität Berlin — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, Universität Würzburg

The size- and structure-dependent optical properties of metal clusters have been studied for many years. In the smallest size regime, every single atom is known to have a high impact on both the cluster geometry and optical properties [1]. Several years ago, first studies on the collective optical characteristics and interactions between multiple clusters, and the influence of their orientation were carried out [2]. Recently, it has been predicted that porphyrin templates may be used to produce well defined arrangements of small metal clusters [3]. However, so far, no experimental verification exists. We investigated the possibility to combine cationic Cu<sub>3</sub> clusters with single porphyrins in a collision cell. This represents a first step towards investigating metal clusters on porphyrin templates in the gas phase.

- [1] K. L. Kelly et. al., *J. Phys. Chem. B* **107**, 668 (2003)  
 [2] P. G. Lisinetskaya et. al., *Phys. Rev. B* **89**, 035433 (2014)  
 [3] M. Röhr et. al., *J. Phys. Chem. A* **120**, 4465 (2016)

MO 9.13 Tue 17:00 P OGS

**Untangling the far-infrared/fingerprint region of the absorption spectrum of small water clusters using helium**

**droplet spectroscopy** — ●RAFFAEL SCHWAN<sup>1</sup>, DEVENDRA MANI<sup>1</sup>, NITISH PAL<sup>1</sup>, GERHARD SCHWAAB<sup>1</sup>, BRITTA REDLICH<sup>2</sup>, LEX VAN DER MEER<sup>2</sup>, and MARTINA HAVENITH<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, Ruhr-Universität Bochum — <sup>2</sup>Institute for Molecules and Materials (IMM), Radboud University Nijmegen

The molecular understanding of water-water interactions has been subject of numerous experimental and theoretical studies. The intramolecular modes of water clusters (H<sub>2</sub>O)<sub>n</sub> with  $n \leq 6$  are well investigated in the mid-infrared and in the fingerprint region while there are only few experimental studies treating the far-infrared region. This region is mainly dominated by intermolecular motions. The most prominent one is the librational band ranging from 300 to 1000 cm<sup>-1</sup> in H<sub>2</sub>O.

Recently, we have combined our helium droplet spectrometer with the free electron laser at the FELIX facility, Radboud University Nijmegen. Helium droplets provide a soft matrix suited well for spectroscopic investigations. They enable the step-wise formation and stabilization of weakly bound aggregates at low temperatures of 0.37 K. In combination with mass selective and pressure dependent measurements, helium droplet spectroscopy becomes a powerful tool for assigning spectral signals to distinct aggregates. Here, we show the absorption spectra of small water clusters in the frequency range of the FELIX radiation source and their assignment based on pressure dependent measurements and accompanying calculations.

MO 9.14 Tue 17:00 P OGs

**The role of dispersion interactions on the microsolvation of aromatic ethers** — ●FABIAN DIETRICH, DOMINIC BERNHARD, MARKUS BURKHART, MAXIMILIAN LUCZAK, and MARKUS GERHARDS — TU Kaiserslautern & Research Center Optimas, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern

Aromatic ethers offer different hydrogen bond acceptor sites for the interaction with polar solvent molecules like alcohols or water. Depending on the aromatic group and the second moiety the preference switches from an OH-O hydrogen bonded structure to an OH- $\pi$  structure which is a consequence of dispersion interactions. We investigated the diphenyl ether (DPE) aggregated with one and two water molecules as well as phenyl vinyl ether (PVE) with methanol. This work is a comparison of different quantum chemical methods (DFT-D3, SCS-CC2) with combined IR/UV spectroscopy in the electronic ground state and first excited state inside the priority program SPP 1807.

For DPE complexes with one water the investigation of the OH-stretching vibration leads to the conclusion that the OH- $\pi$  motif (compared to the OH-O motif) is dominant, as also predicted by theory. The cluster with two water contains both motifs as well as a hydrogen bond between both water molecules. For the PVE/methanol cluster three structures are predicted: one with an OH- $\pi$  bond to the phenyl group, a further one with an OH-O arrangement and one isomer with an OH- $\pi$  bond to the ethenyl moiety. All three structures are observed spectroscopically. In the excited state of the PVE/methanol complex a structural rearrangement is expected.

MO 9.15 Tue 17:00 P OGs

**Dissociative electron attachment in small clusters of ammonia and formic acid** — ●MARVIN WEYLAND<sup>1</sup>, ALEXANDER DORN<sup>1</sup>, XUEGUANG REN<sup>1</sup>, HANS RABUS<sup>2</sup>, and WOON YONG BAEK<sup>2</sup> — <sup>1</sup>Max Planck Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg, Germany — <sup>2</sup>Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Dissociative electron attachment (DEA) has been identified as a possible process for radiation damage. In short, DEA is a resonant two-step process in which first a low-energetic electron is captured by a molecule. The created negative ion can subsequently dissociate while the captured electron stays attached to one of the fragments. Most experiments however have been carried out on isolated gas phase molecules. We show the influence of clustering on the dissociation resonance energies and the fragmentation channels, thereby recreating effects which occur in the liquid phase.

Our experiments are carried out in a COLTRIMS type negative ion spectrometer and the electron beam is created using a photo-emission electron source, yielding a good combination of energy resolution and current. In ammonia cluster fragments of up to 17 molecules we observe an increase of the dissociation energy of up to 0.3 eV compared to the isolated molecule. In formic acid dimers and trimers on the other hand the impact energy for the highest dissociation yield is lowered with increasing fragment size, with impact energy for production of the fragments differing by up to 1 eV. We propose different effects which influence the dissociation path to explain our observations.

MO 9.16 Tue 17:00 P OGs

**BerlinTrap: A novel cryogenic 22-pole tandem mass spectrometer** — ●PABLO NIETO, ALAN GÜNTHER, DAVID MÜLLER, ALEX SHELDRICK, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We present the design and first applications of a new tandem mass spectrometer (BerlinTrap) combining an electrospray ion source, a quadrupole mass spectrometer, a cryogenic 22-pole ion trap (4-300 K), and an orthogonal reflectron time-of-flight mass spectrometer [1]. The trapped ions are cooled by helium buffer gas cooling. The formation and solvation shell structure of weakly-bound He<sub>n</sub>H<sub>3</sub>O<sup>+</sup> complexes and the electronic photodissociation spectrum of the protonated amino acid tyrosine are used to calibrate the setup for cooling, tagging, and spectroscopic capabilities. A vibrational temperature below 20 K is inferred for protonated tyrosine. The electronic spectrum of isolated protonated lumichrome, the smallest protonated flavin, is recorded in the visible range and assigned to the most stable N5 isomer by comparison with quantum chemical calculations. These results demonstrate the suitability of the BerlinTrap apparatus for spectroscopy and reactivity studies of small and large (bio-)molecular ions and their clusters.

[1] A. Günther, P. Nieto, D. Müller, A. Sheldrick, D. Gerlich, and O. Dopfer, *J. Mol. Spectrosc.*, in press, DOI:10.1016/j.jms.2016.08.017

MO 9.17 Tue 17:00 P OGs

**Towards high resolution spectroscopy of biomolecular ions in a cryogenic multipole ion trap** — ●FELIX DUENSING, STEFFEN SPIELER, LENA REMMERS, MORITZ FISCHER, KATHARINA GEISTLINGER, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Österreich

High resolution spectroscopy is a versatile method to study molecular structures [1]. At room temperature many close lying rovibrational states are populated, which can make the interpretation difficult. Several biomolecular ionic complexes have already been investigated in combination with buffer gas cooling [2,3]. Our approach combines spectroscopy of charged biomolecular systems and weakly bound clusters with high resolution far-infrared techniques in a radio frequency ion trap setup similar to Ref. [4]. With quadrupole guides and filters we are able to load ions mass selectively in a 16-pole wiretrap cooled to below 4 K. Buffer gas is used to cool the rovibrational states and a reflectron type time of flight mass spectrometer detects the ions. Action spectroscopy on the trapped and cooled ions can be performed perpendicular to the trap axis by means of narrow band infrared lasers and THz radiation. The latest status on vibrational spectroscopy of amino acids and water clusters will be presented.

[1] Spaun, B., et al., *Nature*, 533, 2016, 517.

[2] Boyarkin, O. V., et al., *J. Am. Chem. Soc.*, 128, 2006, 2816.

[3] Kamrath, M. Z., et al., *J. Am. Chem. Soc.*, 133, 2011, 6440.

[4] Günther, A., et al., *J. Mol. Spec.*, 2016.

MO 9.18 Tue 17:00 P OGs

**Spectroscopy on cold molecules using a chirped pulse microwave spectrometer** — ●PASCAL STAHL<sup>1</sup>, THOMAS GIESEN<sup>1</sup>, GUIDO FUCHS<sup>1</sup>, and JOHANNA CHANTZOS<sup>2</sup> — <sup>1</sup>Institut für Physik, Universität Kassel, 34132 Kassel, Germany — <sup>2</sup>Max-Planck-Institut für extraterrestrische Physik, 85741 Garching bei München, Germany

We present a novel technique to investigate molecules in the gas phase in the K- and W-band. The new experimental setup comprises an absorption spectrometer in combination with a supersonic jet.

The purpose of the setup is to detect short-living and small molecules at low temperatures. For this a twin-channel arbitrary waveform generator (AWG) with 400 MS/s sample rate and 145 MHz analog bandwidth emits a (linear) chirp both in phase and as quadrature signal (I/Q-signal). Using a single sideband upconverter this signal is mixed with a carrier signal in the GHz regime that has been produced by a synthesizer. The resulting (mixed) signal is amplified and sent into a coaxial waveguide adapter and horn antenna to be broadcasted into a vacuum chamber. There the radiation interacts with molecules and in case of an absorption the reduced signal is detected via a horn-antenna-detector device (zero bias shottky diode). The signal is then digitized and sent to a computer.

We have measured ammonia, nitrous oxide as well as acetonitrile. In combination with a discharge nozzle the spectrometer allows to produce and detect a variety of volatile molecules that are of astrophysical and astrochemical interest.

MO 9.19 Tue 17:00 P OGs

**Sympathetic cooling of anions in a hybrid atom-ion trap**

— •TOBIAS HELDT<sup>1</sup>, HENRY LOPEZ<sup>1</sup>, BASTIAN HÖLTKEMEIER<sup>1</sup>, JONAS TAUCH<sup>1</sup>, ERIC ENDRES<sup>2</sup>, ROLAND WESTER<sup>2</sup>, and MATTHIAS WEIDEMÜLLER<sup>1</sup> — <sup>1</sup>Physikalisches Institut Heidelberg, INF 226, 69120 Heidelberg — <sup>2</sup>Institut für Ionenphysik und Angewandte Physik, Technikerstraße 25/3, 6020 Innsbruck

In our experimental setup  $\text{OH}^-$  ions are confined in an octupole radio-frequency trap, where they can be superimposed by laser-cooled rubidium atoms in a dark spontaneous-force optical trap. By localising the atom cloud to the centre of the trap sympathetic cooling of the anions can be achieved even for atom-to-ion mass ratios bigger than unity. The differences between our two experimental approaches of probing the ion distribution, namely photodetachment tomography and time-of-flight analysis, will be discussed in particular.

MO 9.20 Tue 17:00 P OGS

**Controlling Cold Atom-ion Collisions Using Rydberg States**

— •LIMEI WANG, MARKUS DEISS, and JOHANNES HECKER DEN-SCHLAG — Inst. f. Quantenmaterie, Universität Ulm

We propose a scheme where the cold collision between an ultracold Rb atom and a trapped single  $\text{Ba}^+$  ion will be controlled by a 'blue shielding laser'. During the collision, the laser excites the Rb atom to a repulsive electronically excited molecular state formed by the Rydberg atom and ion once the atom approaches to a certain internuclear distance. In this way the ion is effectively surrounded by a hard potential wall that the atom cannot cross. Once the atom leaves the interaction area, it is de-excited back in an adiabatic way to its original level. By controlling the laser power and the laser frequency, as well as by addressing different Rydberg states, the properties of this 'shielding' can be widely tuned. Long-range shielding effects are expected to be realized with higher  $n$  Rydberg states.

An important application of the collision control is to suppress unwanted chemical reactions between atoms and ion, such as charge exchange or three-body recombination. The suppression of inelastic collisions is an essential tool required for the young developing field of cold atom-ion hybrid systems where in general only elastic collisions are desired.