

## MO 22: Posters 3: Experimental and Theoretical Techniques and High Resolution Spectroscopy

Time: Thursday 16:15–18:15

Location: Zelt West

MO 22.1 Thu 16:15 Zelt West

**Fast-timing-readout for a micro-calorimeter particle detector** — ●SEBASTIAN SPANIOL<sup>1</sup>, OLDŘICH NOVOTNÝ<sup>1</sup>, STEFFEN ALLGEIER<sup>2</sup>, CHRISTIAN ENSS<sup>2</sup>, ANDREAS FLEISCHMANN<sup>2</sup>, LISA GAMER<sup>2</sup>, DENNIS SCHULZ<sup>2</sup>, and ANDREAS WOLF<sup>1</sup> — <sup>1</sup>Max Planck Institute for Nuclear Physics, Heidelberg, Germany — <sup>2</sup>Kirchhoff Institute for Physics, Heidelberg, Germany

For the Cryogenic Storage Ring (CSR) we are developing the molecule camera MOCCA, a micro-calorimeter based particle detector for mass-resolved detection of electrically neutral molecular fragments, originating from molecular-ion collisions on electrons, photons, etc. 3D imaging will be employed to determine the kinetic energy released in the fragmentation. Here the transverse position sensitivity is provided by the segmentation of the detector into 64 x 64 pixels onto a detection area of 45mm x 45mm. For impact time measurement on a ns scale we are developing a fast-timing-readout of secondary electrons. We discuss simulations of the employed electrostatic transport system, qualitatively approving the proposed concept and leading to a detailed mechanical design.

MO 22.2 Thu 16:15 Zelt West

**Cost effective time-to-digital and high repetition rate boxcar averager for efficient signal processing** — ●DANIEL UHL, LUKAS BRUDER, VLADYSLAV TYZHNEVYI, KAMBIZ MAHBOUBI, and FRANK STIENKEMEIER — Physikalisches Institut, Universität Freiburg, Hermann-Herder Str. 3, 79104 Freiburg

The development in ultrafast spectroscopy generally tends towards higher laser repetition rates (>100kHz), which requires fast signal processing. Many measurement schemes require boxcar averagers to isolate the spectroscopic signatures of interest. Commercially available devices for high repetition rates are, however, expensive. Likewise, digitizing signal traces, e.g. time-of-flight (TOF) traces, require typically fast ( $\geq 1\text{GSa/s}$ ), fairly expensive digitizers. In addition, fully digitized traces often contain redundant information (many zeros) but produce large datasets that are impractical for real-time signal processing. Here, time-to-digital converters (TDC) provide an optimal solution. We are developing a combined cost-effective solution for TDC and boxcar applications implemented in a field programmable gate array (FPGA). Our device provides TDC with high timing precision and multiple hit modulus, as well as a boxcar averager with a high repetition rate and multiple gates.

MO 22.3 Thu 16:15 Zelt West

**An electron UV/VIS-photon coincidence set-up using a magnetic bottle and a position sensitive photon detector** — ●CHRISTIAN OZGA<sup>1</sup>, GREGOR HARTMANN<sup>1</sup>, PHILIPP SCHMIDT<sup>1</sup>, CLEMENS RICHTER<sup>2,3</sup>, ANDREAS HANS<sup>1</sup>, UWE HERGENHAHN<sup>3,4</sup>, ARNO EHRESMANN<sup>1</sup>, and ANDRÉ KNIE<sup>1</sup> — <sup>1</sup>Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — <sup>2</sup>Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>3</sup>Leibniz Institute of Surface Modification (HZB-IOM Joint-Photonic Lab), Permoserstr. 15, 04318 Leipzig, Germany — <sup>4</sup>Max Planck Institute for Plasma Physics, Wendelsteinstr. 1, 17491 Greifswald, Germany

Here we present a set-up for the detection of photons in the wavelength regime from 200 nm to 680 nm which are measured in coincidence with electrons having kinetic energies as low as 0.5 eV up to a few hundred eV using a magnetic bottle electron spectrometer. While the collection efficiency of the emitted electrons is drastically increased by this type of electron spectrometer it is also possible to use a set of mirrors and lenses to increase the solid angle for the photon collection resulting in a much higher efficiency of the coincidence measurement. Furthermore, the usage of lenses allows to guide the emitted photons which increases the flexibility and versatility of the photon detection. While this set-up can be used for the investigation of liquid samples, we demonstrate the feasibility of the experiment using the well-known Neon 1s photoexcitation as a proof-of-principle.

MO 22.4 Thu 16:15 Zelt West

**A magnetic bottle spectrometer for 2D electronic spectroscopy experiments in the gas phase** — ●MAX JAKOB,

LUKAS BRUDER, MARCEL BINZ, DANIEL UHL, ULRICH BANGERT, and FRANK STIENKEMEIER — Physikalisches Institut, Universität Freiburg, Hermann-Herder Str. 3, 79104 Freiburg

2D electronic spectroscopy (2DES) is a powerful tool to study complex dynamics in real time. While most 2D studies have been conducted in the condensed phase, we have built an apparatus to perform 2DES experiments on molecular and cluster beams in the gas phase. As an advantage, our setup can be combined with energy-resolved photoelectron detection, which basically adds an additional dimension to the 2D spectra. For this purpose, we have constructed a magnetic bottle spectrometer, which provides high collection efficiencies for photoelectrons. Binding energies are deduced from time-of-flight efficiently processed with time-to-digital conversion and combined with lock-in detection to increase the sensitivity.

MO 22.5 Thu 16:15 Zelt West

**New beamlines for molecular pump-probe experiments in the XUV and SXR** — MATTHEW ROBINSON, ●CHRISTIAN MATTHAEI, and MARKUS GÜHR — Institut für Physik und Astronomie, Universität Potsdam

Until recently the only place to perform pump-probe experiments with femtosecond Soft X-Ray (SXR) probe pulses was at the few large X-ray Free Electron Laser (XFEL) facilities, like the Linac Coherent Light Source (LCLS) and the European XFEL. With recent innovations in the field of High Harmonic Generation (HHG) it has become possible to create photons with energies in excess of the carbon K-edge [1,2,3], thus allowing time resolved X-ray probing in a small lab setting.

We are currently constructing such a set-up at Potsdam University, which will be used for the study of small molecules in the gas phase. Extreme UV and SXR pulses are produced using HHG, followed by a set-up for time-resolved atom-specific spectroscopy. In these studies a thorough understanding of nonadiabatic molecular dynamics is our goal.

[1] S. L. Cousin et al., *Optics Letters*, 39, pp. 5383-5386, 2014[2] Y. Pertot et al., *Science*, 355, pp. 264-267, 2017[3] T. Popmintchev et al., *Science*, 336, pp. 1287-1291, 2012

MO 22.6 Thu 16:15 Zelt West

**An ultrafast electron diffraction setup for molecules in aqueous solution** — ●ARNE UNGEHEUER, ARNE SENFTLEBEN, MARLENE ADRIAN, and THOMAS BAUMERT — Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Deutschland

Here we present a scheme for an ultrafast electron diffraction setup for electron diffraction on liquids and particles in aqueous solution. We adapt the idea to use two obliquely colliding single laminar jets for the creation of a leaf-shaped flatjet with sub-micrometer thickness required for electron diffraction in transmission mode. The issue of multiple scattering in these relatively thick samples is addressed by the use of an energy-filter to increase the signal-to-noise ratio. Preliminary measurements of the liquid jet thickness and stability regimes under ambient conditions are shown.

MO 22.7 Thu 16:15 Zelt West

**Experimental set-up for electron impact induced luminescencespectroscopy of a liquid microjet** — ●DANA BLOSS<sup>1</sup>, ANDREAS HANS<sup>1</sup>, CHRISTIAN OZGA<sup>1</sup>, PHILIPP SCHMIDT<sup>1</sup>, MASATOSHI UKAI<sup>2</sup>, ARNO EHRESMANN<sup>1</sup>, and ANDRÉ KNIE<sup>1</sup> — <sup>1</sup>Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel — <sup>2</sup>Department of Applied Physics, Tokyo University of Agriculture and Technology, Koganei-shi, Tokyo 184-8588, Japan

The liquid microjet technique allows the investigation of a variety of different targets ranging from pure liquids to solutions which mimic biological systems. While most experiments use photon excitation, other methods such as electron impact can offer an additional insight due to a broadband excitation. Here we present an experimental set-up for the measurement of dispersed luminescence of liquid microjets induced by electron impact with keV kinetic energy. These measurements provide a comparison with the photon-induced luminescence spectra. Perspective this set-up can be used to investigate the behaviour and interaction of solvated (bio-) molecules as function of the penetration depth of the primary electron beam.

MO 22.8 Thu 16:15 Zelt West

**TrapRemi - A Device to Investigate the Quantum Dynamics of Molecular Ions** — ●FRANS SCHOTSCH, LUDWIG HOIBL, DENIS DJENDJUR, and ROBERT MOSHAMMER — Max-Planck-Institute for Nuclear Physics

The investigation of quantum few-body dynamics in atoms and molecules is of fundamental interest for physics and chemistry. Enabled by the innovation and development of Reaction Microscopes (REMI) during the last two decades, reactions such as ionization, dissociation and geometrical reformation can be investigated in an angle-resolved and kinematically complete manner. Combined with short-pulse laser systems, these dynamics can be even resolved on attosecond time scale. The TrapRemi extends this development to enable similar investigations in charged systems: atomic and molecular ions of arbitrary charge and mass. These systems are of high interest since they often play key roles in astrochemical reactions as for example the Trihydrogen cation. For this purpose, we designed a new experimental setup: The combination of a linear electrostatic ion trap (Zajfman-Trap) with a REMI. This poster describes the project progress from first ion optics simulations to successful ion storage.

MO 22.9 Thu 16:15 Zelt West

**molecular frame young-type interference in (e, 2e) reactions on hydrogen molecule** — ●ENLIANG WANG<sup>1</sup>, XUEGUANG REN<sup>1</sup>, KHOKON HOSSEN<sup>1</sup>, XINGYU LI<sup>2</sup>, XIANGJUN CHEN<sup>2</sup>, and ALEXANDER DORN<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — <sup>2</sup>Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China

The wave-particle duality is one of the fundamental concepts of quantum mechanism where the wave like behaviors of particles were mostly demonstrate through Young's double-slit experiment in which the coherent superposition of different outgoing amplitudes will present interference patterns. Here we perform a high energy ( $E_0 = 520$  eV) (e, 2e) experiment on  $H_2$  to trace the interference effect using a dedicated reaction microscope. The present experimental results show that a strong dependence to the molecular alignment of the FDOS is observed where two intense areas are observed with molecular alignment at 0 and 180° for 10 eV ejected electrons. The MCDW calculation well reproduce the experimental results while the pure interference description fails completely. This is mainly due to the rather low energy (10 eV) of the ejected electron which does not justify the spherical wave description used in the derivation of the interference factor. Future experiments will consider fast outgoing electrons (up to 80 eV) to trace the interference effect.

MO 22.10 Thu 16:15 Zelt West

**Low-energy electron emission in strong-field photoionization of methane** — ●MARTIN LAUX, NICOLAS CAMUS, YONGHAO MI, LUTZ FECHNER, ROBERT MOSHAMMER, and THOMAS PFEIFER — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

We present results of strong-field ionization of methane measured in a Reaction Microscope (Remi) by 25 fs, 800/400 nm two-color laser pulses. Photoelectron spectra were analyzed separately for different ionization and dissociation channels, which could be identified by the ion fragments detected in coincidence, i.e.  $CH_4^+$ ,  $CH_3^+$ , and  $H^+$ . The spectra differ significantly from each other at kinetic energies below 0.5 eV, in contradiction to the established two-step model of molecular photoionization [1]. However, autoionization of vibrationally excited Rydberg states is found to explain the enhancement of low-energy electrons. Our findings generalize this strong-field excitation and autoionization mechanism, observed recently in molecular hydrogen [2], to more complex systems.

[1] M.F. Kling *et al.*, Science **312**, 246 (2006)[2] Y. Mi *et al.*, Phys. Rev. Lett. **118**, 183201 (2017)

MO 22.11 Thu 16:15 Zelt West

**Fragmentation pathways of protonated nucleic acid building blocks** — ●MARTIN PITZER<sup>1,2</sup>, CHRISTIAN OZGA<sup>1</sup>, CATMARN KÜSTNER-WETEKAM<sup>1</sup>, PHILIPP REISS<sup>1</sup>, ALEXANDRE GIULIANI<sup>3</sup>, and LAURENT NAHON<sup>3</sup> — <sup>1</sup>Institut für Physik und CiNSAT, Universität Kassel, Germany — <sup>2</sup>Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel — <sup>3</sup>Synchrotron SOLEIL, Gif-sur-Yvette, France

Ultraviolet radiation is known to have large absorption cross sections in biologically relevant molecules. Due to the complexity of these molecules, many destructive and non-destructive pathways for deexcitation exist. Which pathways are chosen is extremely relevant for the resulting radiation damage in biological tissue. Although not performed in a natural environment, experimental studies on isolated molecules are essential to understand the interplay between photoexcitation and fragmentation.

By combining an Electrospray Ionization source (ESI) with tunable photoexcitation in the VUV range and a tandem mass spectrometer, the appearance energies of fragments can be determined in dependence of various parameters such as hydration or charge state [1]. Our contribution shows recent results for the RNA components uracil and uridine which exhibit a rich fragmentation behaviour in the region of 4-12 eV photon energy. We compare for various fragments how the yield depends on the exciting photon energy and are thus able to test theoretically predicted fragmentation pathways and dissociation thresholds.

[1] A. Milosavljevic *et al.*, J. Synchrotron Rad. **19**, 174-178 (2012)

MO 22.12 Thu 16:15 Zelt West

**Laser Induced Electron Diffraction on strongly aligned OCS molecules** — ●PHILIPP M. STAMMER<sup>1</sup>, EVANGELOS THOMAS KARAMATSKOS<sup>2,3</sup>, SEBASTIAN RAABE<sup>1</sup>, GILDAS GOLDSZTEJN<sup>1</sup>, ANDREA TRABATTONI<sup>2</sup>, TERENCE MULLINS<sup>2</sup>, SEBASTIAN TRIPPEL<sup>2,4</sup>, ARNAUD ROUZÉE<sup>1</sup>, and JOCHEN KÜPPER<sup>2,3,4</sup> — <sup>1</sup>Max Born Institute, Berlin, Germany — <sup>2</sup>DESY, Hamburg, Germany — <sup>3</sup>Universität Hamburg, Germany — <sup>4</sup>CUI, Hamburg, Germany

Strong Field Ionization of an atom or molecule is often described in a simple semi-classical picture: an electron is tunnel ionized by the intense laser field, accelerated away from the atom before to be driven back to the parent ion by the oscillating laser field. Elastic recollision with the parent ion is responsible for the apparition of a second plateau in the photoelectron angular distribution that contains diffraction features from which one can extract direct information about the molecular geometry. This effect is used in a technique called Laser Induced Electron Diffraction (LIED).

To image ultrafast molecular dynamics Laser Induced Electron Diffraction has recently emerged as a powerful tool. We performed LIED experiments in strongly aligned OCS molecules and obtain photoelectron distributions for different angles of the laser polarizations with respect to the molecular orientation. The observed large modifications of the well-known holographic and fork structure with the alignment axis orientation will be discussed.

MO 22.13 Thu 16:15 Zelt West

**Vibrationally resolved electron-nuclear energy sharing in above-threshold multiphoton dissociation of CO** — ●XUFEI SUN — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

We study the photon energy sharing between the photoelectron and the nuclei in the process of above-threshold multiphoton dissociative ionization of CO molecules by measuring the joint energy spectra. The experimental observation shows that the electron-nuclear energy sharing strongly depends on the vibrational state. The experimental observation shows that both the energy deposited to the nuclei of  $CO^+$  and the emitted photoelectron decrease with increasing the vibrational level. Through studying the vibrationally resolved nuclear kinetic energy release and photoelectron energy spectra at different laser intensities, for each vibrational level of  $CO^+$ , the nuclei always tend to take the same amount of energy in every vibrational level regardless of the laser intensity, while the energy deposited to the photoelectron varies with respect to the laser intensity because of the ponderomotive shifted energy and the distinct dissociative ionization mechanisms.

MO 22.14 Thu 16:15 Zelt West

**Improved virtual orbitals for charge transfer excitations in time dependent DFT** — ●ROLF WÜRDEMANN<sup>1</sup> and MICHAEL WALTER<sup>2,3</sup> — <sup>1</sup>FMF, Universität Freiburg, Freiburg, Germany — <sup>2</sup>FIT, Universität Freiburg, Freiburg, Germany — <sup>3</sup>IWM, Freiburg, Germany

Charge transfer excitations (CTE) are of high importance in photo-volatics, organic electronics and molecular and organic magnetism. Range separated functionals (RSF) can be used to correctly determine the energetics of CTEs within linear response time dependent density functional theory (TDDFT).

TDDFT becomes numerically very demanding on grids if hybrid or

RSF are used due to the inclusion of exact exchange derived from Hartree-Fock theory.

We present the implementation of RSF on real space grids and discuss a way to circumvent the problem mentioned above by utilizing Huzinagas improved virtual orbitals (IVOs) that form an improved basis for this type of calculations. The CTE energetics may be even obtained by means of DFT ground-state calculations using IVOs.

MO 22.15 Thu 16:15 Zelt West

**Predicting para-ortho conversion in ammonia** — •GUANG YANG<sup>1</sup>, INGMAR HARTL<sup>2</sup>, ANDREY YACHMENEV<sup>1,3</sup>, and JOCHEN KÜPPER<sup>1,3,4</sup> — <sup>1</sup>Center for Free-Electron Laser Science, DESY, Notkestrasse 85, Hamburg — <sup>2</sup>DESY, Notkestrasse 85, Hamburg — <sup>3</sup>The Hamburg Center for Ultrafast Imaging, Luruper Chaussee 149, Hamburg — <sup>4</sup>Department of Physics, University of Hamburg, Luruper Chaussee 149, Hamburg

We present a theoretical study of the hyperfine-resolved spectrum of ammonia and its deuterated isotopologues in preparation of corresponding experiments. The calculations have been performed using variational approach TROVE, a new spectroscopically determined potential energy surface, and ab initio quadrupole, spin-spin, and spin-rotation coupling surfaces. The computed spectroscopic line lists cover transitions between levels with rotational excitations up to  $J = 20$  and vibrational band centers up to 8000 cm<sup>-1</sup> above zero point energy. Comparisons with experimental data confirm the high accuracy of the computed results. The perspectives of spectroscopic observation of the para-ortho interconversion, for instance using infrared frequency comb spectroscopy, and its modulation by external electric field are discussed.

MO 22.16 Thu 16:15 Zelt West

**Coupling of the  $2^2\Sigma^+$  and  $1^2\Pi$  of LiSr** — •ERIK SCHWANKE, JULIA GERSCHMANN, HORST KNÖCKEL, SILKE OSPELKAUS, and EBERHARD TIEMANN — QUEST und Inst. f. Quantenopik, Leibniz Universität Hannover

Building on our spectroscopic study of the  $2^2\Sigma^+ - 1^2\Sigma^+$  system of LiSr, we modeled perturbations in the thermal emission spectrum as coupling between the  $F_1$  and  $F_2$  levels of the  $2^2\Sigma^+$  state and the  $1^2\Pi_{1/2}$  and  $1^2\Pi_{3/2}$  states. The rotational and vibrational constants of the  $2^2\Sigma^+$  state were derived from the thermal emission spectrum and laser-induced fluorescence in the near infrared.

Several large perturbations of the rotational ladders of  $v' = 0$  and  $v' = 1$  allow to estimate the rotational and vibrational constants of the  $2^2\Pi$  state, while accompanying smaller perturbations hint at its spin-orbit coupling constant. A preliminary deperturbation of one of the larger instances led to more refined values for the rotational and vibrational constants of  $1^2\Pi$ , as well as a first estimate the coupling strength and the spin-rotation coupling in  $2^2\Sigma^+$ . Adding further perturbed states, a more global picture of the coupling constants and the  $1^2\Pi$  state will be derived.

We will report on the status of the investigations.

MO 22.17 Thu 16:15 Zelt West

**High-resolution spectroscopy of tritiated water and analysis of the  $2\nu_1$  mode of HTO** — •JOHANNES MÜLLER<sup>1</sup>, MAGNUS SCHLÖSSER<sup>1</sup>, FRANK HASE<sup>2</sup>, NICOLAS ZIEGLER<sup>1</sup>, ROBIN GRÖSSLE<sup>1</sup>, DAVID HILLESHEIMER<sup>1</sup>, and JOHANNES ORPHAL<sup>2</sup> — <sup>1</sup>Institute for Technical Physics, Tritium Laboratory Karlsruhe (TLK), Karlsruhe Institute of Technology, Germany — <sup>2</sup>Institute for Meteorology and Climate Research (IMK-ASF), Karlsruhe Institute of Technology, Germany

By measuring vibrational and rotational states of tritiated water using high-resolution FTIR spectroscopy, one can obtain data to validate or restrict quantum mechanical models of small molecules at high precision, such as water. Whereas spectroscopy of the H<sub>2</sub>O, HDO and D<sub>2</sub>O isotopologues is easily feasible at high accuracy as there are no restrictions on the sample amount, tritiated water is much harder to grasp. Due to its radiotoxicity and radiochemical activity, handling of tritiated water and gaseous tritium is only possible in a handful facilities worldwide. Therefore, a joint venture between the TLK, providing the tritium and experience in handling it, and the IMK-ASF, providing the expertise in high-resolution FTIR spectroscopy, was formed. We will describe how tritiated water is produced in a tritium compatible optical cell and how the high-resolution spectrometry is performed. We focus on the analysis the  $2\nu_1$  mode in the ro-vibrational spectrum of HTO which has never been measured before. We present rotational and centrifugal distortion constants of HTO, which allow us to access

the fundamental structure and dynamic of this fascinating molecule.

MO 22.18 Thu 16:15 Zelt West

**Absorption spectroscopy on KCa** — •JULIA GERSCHMANN<sup>1</sup>, ERIK SCHWANKE<sup>1</sup>, HORST KNÖCKEL<sup>1</sup>, SILKE OSPELKAUS<sup>1</sup>, ASEN PASHOV<sup>2</sup>, and EBERHARD TIEMANN<sup>1</sup> — <sup>1</sup>QUEST und Inst. f. Quantenopik, Leibniz Universität Hannover — <sup>2</sup>Sofia Universität "St. Kliment Ohridski", Bulgarien

The combination of an alkaline and an alkaline earth atom leads to molecules with permanent electric and magnetic dipole moments and thus offer manipulation of their states by external fields. Several ab initio calculations have been published on various combinations of a group IA and a group IIA atom. Experimentally, not so much is known about the molecular electronic states.

In the past we were able to describe potential energy curves for the first two  $2^2\Sigma^+$  states via high resolution Fourier transform spectroscopy. We have used laser induced fluorescence to assign the quantum numbers up to  $N = 179$  of transitions from  $v' \leq 7$  to  $v'' \leq 10$ . The rovibrational spectrum can be described by fitted potential energy curves and the spin-rotation coupling.

Currently, based on ab initio calculations, we set up a laser absorption experiment in the visible region around 17000 cm<sup>-1</sup> to address higher  $2^2\Sigma^+$  and  $2^2\Pi$  states from the known ground state. There we expect low density of K<sub>2</sub> lines. Lines thus identified as belonging to KCa can then be used for further laser induced fluorescence experiments.

We will report on the status of the investigations.

MO 22.19 Thu 16:15 Zelt West

**Electronic structure investigations on mono- and binuclear transition metal complexes** — •TATJANA WALL<sup>1</sup>, LOUIS OBERWEIS<sup>1</sup>, MARKO LEIST<sup>2</sup>, WERNER THIEL<sup>2</sup>, and MARKUS GERHARDS<sup>1</sup> — <sup>1</sup>TU Kaiserslautern, Physical Chemistry & Research Center Optimas, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern, Germany — <sup>2</sup>TU Kaiserslautern, Inorganic Chemistry, Erwin-Schrödinger-Str. 54, 67663 Kaiserslautern, Germany

Binuclear heterometallic complexes are of great interest in synthesis due to their catalytical activity e.g. for transfer hydrogenation or cross-coupling. Absorption and emission spectra of mono- and binuclear transition metal complexes based on bispyrimidine in solution are recorded to investigate their electronic structure. Furthermore the lifetimes of the excited states are determined by using the time correlated single photon counting (TCSPC) method. The results are compared with the pure bispyrimidine ligand and additionally a comparison with DFT calculations is performed. Here we represent the results for mono- and binuclear Ir and Pd containing complexes. For both types of complexes MLCT (Metal to Ligand Charge Transfer) and ligand centered transitions are observed. Lifetime determinations show multiple exponential decays for all emission bands, whereas the emission band of the pure ligand has a mono-exponential decay. The average lifetimes of the ligand centered bands are similar to the lifetime of the pure ligand. The photophysics of complexes with respect to lifetimes, coordination sites and characters of electronically excited states are discussed.

MO 22.20 Thu 16:15 Zelt West

**Ionization Loss/Gain Stimulated Raman Spectroscopy of isolated molecules in the gas phase: diphenyl ether and bisphe-nyldiamantane** — •DOMINIQUE MAUE<sup>1</sup>, ANKE STAMM<sup>1</sup>, DOMINIC BERNHARD<sup>1</sup>, ANDREY FOKIN<sup>2</sup>, PETER SCHREINER<sup>2</sup> und MARKUS GERHARDS<sup>1</sup> — <sup>1</sup>TU Kaiserslautern, Department of Chemistry, Physical Chemistry, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern, Germany — <sup>2</sup>Universität Gießen, Department of Chemistry, Organic Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

Ionization Loss/Gain Stimulated Raman Spectroscopy (ILSRS/ILGRS) is a powerful tool for the structural investigation of isolated molecules and clusters in the gas phase. With these methods, it is possible to investigate structurally relevant Raman active vibrations as well as the spectral range below 800 cm<sup>-1</sup>, which is difficult to access with table top IR lasers in molecular beam experiments. Here, we present the first examinations with the newly installed ILSRS/ILGRS setup investigating diphenyl ether (DPE) and bisphe-nyldiamantane (BPA) in the gas phase. This is the first application of the stimulated Raman technique on the class of diadamantanes, which is of great importance because of the extraordinary length of the connective C-C bond. In combination with dispersion-corrected DFT calculations we are able to receive a structural agreement of experiment and theory.