

MO 14: Posters 3: Novelties in Molecular Physics: Theory of Molecular Dynamics, Collisions and Energy Transfer, and Experimental Techniques

Time: Wednesday 16:30–19:00

Location: Empore Lichthof

MO 14.1 Wed 16:30 Empore Lichthof

Quantum dynamics and electronic effects in ion-molecule interactions in cold traps — ●IBROKHIM ISKANDAROV, FABIO CARELLI, FRANCESCO GIANTURCO, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Until a few years ago, studies of cold reactive processes in hybrid-traps have been restricted to atomic ions and neutral atoms. The ion-neutral hybrid-trapping technique has been recently extended to also probe cold reactive collisions of sympathetically cooled molecular ions by their interaction with laser cooled atomic ions [1]. By choosing N_2^+ molecules and Rb atoms as a system, they can reveal very important features about the interaction forces between molecular ions and atoms.

Inelastic collisions with neutral buffer gas have been shown to represent an effective way to cool the internal molecular degrees of freedom and going beyond the translational cooling [2]. This approach rests on the fact that in the framework of the neutral buffer gas cooling scheme, the rotational molecular temperature can be tuned to a value lower than the translational one. We are currently computationally probing this effect in case of interaction of MgH^+ with He as a buffer gas.

[1] F. Hall and S. Willitsch, *Phys. Rev. Lett.* **109**, 233202 (2012).

[2] P.F. Staunum, K. Hojbjerg, P.S. Skyt, A.K. Hansen, M. Drewsen, *Nature Physics* **6**, 271 (2010).

MO 14.2 Wed 16:30 Empore Lichthof

Coupled electron-nuclear dynamics: A comparison of methods — ●THOMAS SCHNAPPINGER, JULIUS ZAULECK, ROBERT SIEMERING, and REGINA DE VIVIE-RIEDLE — Department Chemie, LMU München

The purpose of this work is a first comparison of two methods describing a coupled electron-nuclear dynamics: the purely quantum mechanical ansatz NEMol and the TD-DFT based Ehrenfest dynamics. For this purpose the dynamics of (Z)-3-aminoacrolein in the electronic ground state was analyzed. Using different quantum chemical methods the potential profile of tautomerism was calculated and the critical points of the reaction were identified to set up one-dimensional potential energy surfaces along the reaction. We introduce a novel form of the NEMol ansatz which is formulated for a single electronic state. This modified NEMol ansatz was used to calculate the dynamics of the tautomerism using the one-dimensional potential energy surfaces. The TD-DFT based Ehrenfest dynamics was investigated for a single trajectory. The comparison between the NEMol ansatz and the TD-DFT Ehrenfest dynamics is so far limited due to the difference in dimensionality. Therefore the first steps for a one-dimensional TD-DFT Ehrenfest dynamics are presented. Comparing the TD-DFT Ehrenfest trajectory with a semi classical trajectory shows that the electron dynamics has an influence on the motion of the nuclei even for this very simple reaction in the electronic ground state.

MO 14.3 Wed 16:30 Empore Lichthof

Ab initio calculations of the Ion feature in X-ray Thomson scattering — KAI-UWE PLAGEMANN¹, HANNES RÜTER¹, THOMAS BORNATH¹, ●MOHAMMED SHIHAB^{1,2}, MICHAEL P. DESJARLAIS³, CARSTEN FORTMANN⁴, SIEGFRIED H. GLENZER⁵, and RONALD REDMER¹ — ¹Institut für Physik, Universität Rostock — ²Physics Department, Tanta University, Egypt — ³SNL, Albuquerque, USA — ⁴QuantumWise A/S, 2100 Copenhagen, Denmark — ⁵SLAC, Menlo Park, C 94025, USA

Warm dense matter of solid-like densities and temperatures of several eV is relevant for planetary interiors and inertial confinement fusion experiments. A versatile and reliable tool to probe such extreme states of matter is X-ray Thomson scattering (XRTS) from which information about plasma parameters like electron density, electron temperature and mean ionization state can be inferred directly from the dynamic structure factor [1]. An important contribution to the dynamic structure factor is the ion feature [4] which describes elastic scattering of X-rays off electrons. We apply an ab initio method for the calculation of the form factor of bound electrons, the slope of the screening cloud of free electrons, and the ion-ion structure factor in warm dense beryl-

lium. With the presented method we can calculate the ion feature from first principles [5]. These results will facilitate a better understanding of X-ray scattering in warm dense matter and an accurate measurement of ion temperatures which would allow determining non-equilibrium conditions, e.g., along shock propagation.

MO 14.4 Wed 16:30 Empore Lichthof

Ab initio calculations of the Ion feature in X-ray Thomson scattering — KAI-UWE PLAGEMANN¹, HANNES RÜTER¹, THOMAS BORNATH¹, ●MOHAMMED SHIHAB^{1,2}, MICHAEL P. DESJARLAIS³, CARSTEN FORTMANN⁴, SIEGFRIED H. GLENZER⁵, and RONALD REDMER¹ — ¹Institut für Physik, Universität Rostock, Germany — ²Physics Department, Tanta University, Egypt — ³SNL, Albuquerque, USA — ⁴QuantumWise A/S, 2100 Copenhagen, Denmark — ⁵SLAC, Menlo Park, C 94025, USA

Warm dense matter of solid-like densities and temperatures of several eV is relevant for planetary interiors and inertial confinement fusion experiments. A versatile and reliable tool to probe such extreme states of matter is X-ray Thomson scattering (XRTS) from which information about plasma parameters can be inferred directly from the dynamic structure factor [1]. An important contribution to the dynamic structure factor is the ion feature [2] which describes elastic scattering of X-rays off electrons. We apply an ab initio method for the calculation of the form factor of bound electrons, the slope of the screening cloud of free electrons, and the ion-ion structure factor in warm dense beryllium. With the presented method we can calculate the ion feature from first principles [3]. These results will facilitate a better understanding of X-ray scattering in warm dense matter and an accurate measurement of ion temperatures which would allow determining non-equilibrium conditions, e.g., along shock propagation. [1] Glenzer and Redmer, *Rev. Mod. Phys.*, 81(2009).[2] Chihara, *J. Phys.: Condens. Matter*, 12(2000).[3] K.-U. Plagemann et al., *Phys. Rev. E* 92(2015).

MO 14.5 Wed 16:30 Empore Lichthof

Charge transfer reactions with Ar^+ in its ground state — TIM MICHAELSEN, ●BJÖRN BASTIAN, ATILAY AYASLI, JENNIFER MEYER, EDUARDO CARRASCOA, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

The crossed-beam technique has become the method of choice for the analysis of reaction dynamics [1] as it allows to precisely assess the complete kinematics of both reactants and products. In the last decade, it could be extended from neutral partners to ion neutral reactions [2]. The combination with three-dimensional velocity map imaging has allowed us to obtain energy- and angle-differential cross sections for the $Ar^+ + N_2$ charge transfer reaction [3], opposing previous experimental results and in agreement with theoretical predictions [4]. Recently, a radio-frequency ion trap has been added to our setup that allows to achieve an improved energy resolution of the ion beam and, more notably, quenching of reactant ions to their ground state.

Here, we present the status of experiments that aim for fully state-to-state resolved differential cross sections of the charge transfer reaction involving the Ar^+ ground state into the different vibrational levels of the N_2^+ product. Further, reactions with other neutral partners as O_2 and CO will be considered.

[1] Y. T. Lee. *Science* **236** (4803), 793 (1987). [2] J. Mikosch et al. *Phys. Chem. Chem. Phys.* **8**, 2990 (2006). [3] S. Trippel et al. *Phys. Rev. Lett.* **110**, 163201 (2013). [4] R. Candori et al. *J. Chem. Phys.* **115**, 8888 (2001).

MO 14.6 Wed 16:30 Empore Lichthof

Toward ion-neutral collision measurements at the CSR — ●ELISABETH A. GUERIN, FLORIAN GRUSSIE, AODH P. O'CONNOR, and HOLGER KRECKEL — Max-Planck-Institut für Kernphysik, Heidelberg

To date, almost 200 molecules have been detected in the interstellar medium or circumstellar shells, including relatively complex organic molecules. It has become clear that two-body ion-neutral collisions play a critical role in the formation of molecules in the interstellar medium. However, with temperatures in interstellar clouds typically ranging from 10 to 100 K, the exact pathways and time scales of chemical reactions under these conditions are still poorly studied. In par-

ticular, thermal rate coefficients at relevant conditions have not been experimentally established for most ion-neutral reactions.

Simulating such reactions in a laboratory environment is one goal for the Cryogenic Storage Ring (CSR) located at the Max Planck Institute for Nuclear Physics in Heidelberg. Cooled ions (~ 10 K) stored in the ring will be merged with a neutral atomic beam at a tunable center of mass collision energy. Reaction rate coefficients can be determined by measuring particle fluxes, beam overlap and the production rate of reaction products. The storage ring itself has been successfully commissioned in the summer of 2015 with the experimental vacuum chambers reaching temperatures below 10 K. In the neutral beam setup, neutral particles will be created by photodetachment of a negative ion beam (kinetic energy up to 300 keV) which for this purpose is crossed with a continuous wave high-power diode laser (2 kW) operating at 808 nm.

MO 14.7 Wed 16:30 Empore Lichthof

First experiments with the Cologne Chirped Pulse FTMW Spectrometer — ●MARIUS HERMANN¹, CHRISTIAN ENDRES², ALEXEY POTAPOV¹, and STEPHAN SCHLEMMER¹ — ¹I. Physikalisches Institut, Universität zu Köln, Zùlpicher Strasse 77, 50937 Köln, Germany — ²present address: Max Planck Institute for extraterrestrial Physics, Giessenbachstrasse 1, 85748 Garching, Germany

Detection of complex molecules in space strongly relies on the ability to reproduce and precisely measure their spectra in the laboratory [1, 2]. With the recent advancements in semiconductor development and the ability to have fast and high frequency amplifiers and detectors available the chirped pulse Fourier transform microwave techniques has been widely tested and established [3]. Having the ability to polarize a molecular ensemble and study its free induction decay and its collision behaviour within short measuring times promises to improve our understanding of molecular collisions in space.

Here we report and present our set-up of a chirped pulse Fourier transform microwave spectrometer. Utilizing a short waveguide molecular gas cell on a cold head we hope to be able to measure and characterize pure rotational transition data on many complex molecules in the frequency range of 2-26.5 GHz using a 5 GHz arbitrary waveform generator. Preliminary measurements on ammonia as a proof of concept were taken and are presented as a benchmark for sensitivity.

[1] A. Belloche et. al, A&A (2013).

[2] Müller, H. S. P. et. al, A&A (2001)

[3] Brown, G. G., Review of Scientific Instruments (2008)

MO 14.8 Wed 16:30 Empore Lichthof

The low-energy electron cooler for the Cryogenic Storage Ring (CSR) — ●PATRICK WILHELM, KLAUS BLAUM, CLAUDE KRANTZ, JORRIT LION, SVENJA LOHMANN, OLDŘICH NOVOTNÝ, STEPHEN VOGEL, and ANDREAS WOLF — Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Deutschland

In the recently commissioned Cryogenic Storage Ring CSR, molecular ions are stored for hundreds to thousands of seconds in a low temperature radiation field with a mean temperature below 10 K. By this, stored ionic molecules and clusters can undergo radiative relaxation down toward their ro-vibrational ground-state. Measurements probing fundamental molecular and cluster dynamics can be performed with good internal state definition. For phase-space cooling and for high-precision electron-ion reaction experiments, a low-energy velocity-matched merged electron beam device is set up for the cryogenic environment. Cold electrons are produced by a GaAs photocathode setup at 300 K. The merging of the electrons with the stored ion beam is realized by a cryogenic magnetic guiding field created by a set of solenoids, toroids and racetrack coils made from high-temperature superconductors. The CSR electron cooler is designed to achieve an average kinetic electron beam energy of as low as 1 eV at a thermal energy spread of about 1 meV. The manufacturing process of the cooler system is completed; implementation in the storage ring and commissioning are planned for the first half of 2016.

MO 14.9 Wed 16:30 Empore Lichthof

Mesophase Behaviour of Binary Mixtures of Symmetric Ester-Type Banana-Shaped Compounds — ●MIROSLAV CVETINOV¹, MAJA STOJANOVIĆ¹, DUŠANKA OBADOVIĆ², ANIKO VAJDA³, KATALIN FODOR-CSORBA³, NANDOR EBER³, NEMANJA TRIŠOVIĆ⁴, and JELENA ANTANASIEVIĆ⁴ — ¹University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Serbia — ²University of Novi Sad, Faculty of Education, Sombor, Serbia, — ³Institute for Solid State Physics and Optics, Wigner Research Centre

for Physics, Hungarian Academy of Sciences, Budapest, Hungary — ⁴University of Belgrade, Faculty of Chemistry, Belgrade

We have investigated three binary mixtures composed of two symmetric ester-type banana-shaped compounds. Compound I is 2,6-bis[2-(4-ethanoyloxyphenyl)ethenyl]pyridine, which is banana-shaped mesogen expressing banana B1 mesophase at high temperature range. Compound II, 1,3-phenylene-bis[4'-(9-decenyloxy)benzoyloxy] benzoate, doesn't exhibit any mesophase in cooling down to its crystallization temperature. The occurring mesophases have been identified by their optical textures and by the means of X-Ray diffraction. Molecular models were prepared using RM1 model of semi-empirical quantum chemistry. At the concentration of 27wt% of compound II, there is apparent lowering of B1 mesophase temperature range in respect to the pure compound I. Yet, at the concentration of 36wt% of compound II, the mixture lost its mesogenic character. Hence, mixing two classic banana-shaped compounds is viable way to attain mesophase range closer to the room temperature.

MO 14.10 Wed 16:30 Empore Lichthof

High-resolution spectroscopy on the hyperfine structure of small aluminum bearing molecules — ●BJÖRN WASSMUTH¹, ALEXANDER BREIER¹, THOMAS F. GIESEN¹, and JÜRGEN GAUSS² — ¹Institut für Physik, Universität Kassel, 34132 Kassel, Germany — ²Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany

An advanced method of producing metal-containing small molecules in the gas phase is based on laser ablation technique. The vaporized gas phase products can be investigated by means of millimeter/submillimeter-wave spectroscopy or by using high-resolution spectrometers in the visible frequency range. The experimental investigation is guided by high-level quantum chemical calculations performed at Mainz.

These experimental methods have been applied to measure AlO and AlS produced by laser ablation of solid aluminum and a dilution of N₂O (2%) or H₂S (7%) in helium. The adiabatically expanding gas mixture is probed by monochromatic radiation in the frequency range up to 400 GHz. Measurements reveal the hyperfine structure of both linear molecules to follow Hund's case *b*_{FS} coupling due to the nuclear spin of aluminum. With the present measurements new highly accurate line positions for future observations and more accurate molecular parameters are available.

MO 14.11 Wed 16:30 Empore Lichthof

Laserbasierte XUV Quelle mit Monochromator für zeitaufgelöste Molekülspektroskopie — ●MARKUS PFAU, MARTIN RANKE, FAWAD KARIMI, ANASTASIOS DIMITRIOU und ULRIKE FRÜHLING — Institut für Experimentalphysik, Universität Hamburg

Für die Untersuchung der Elektronendynamik in Molekülen sind Femtosekunden Lichtpulse mit Photonenergien im Spektralbereich von Vakuumultraviolett bis hin zum weichen Röntgenbereich notwendig. Eine Möglichkeit zur Erzeugung dieser Photonen ist die Nutzung der höheren Harmonischen eines Laserstrahls. Da die Harmonischen kollinear über einen breiten Spektralbereich emittiert werden, ist eine spektrale Trennung nötig.

Wir berichten hier über ein Experiment zur Erzeugung intensiver hoher Harmonischer im XUV Bereich und einem Gittermonochromator zur Trennung der Harmonischen, welcher zum Einen eine hohe Transmission aufweist und zum Anderen die Pulslänge von ca. 35 fs nicht wesentlich vergrößert. Außerdem wird ein experimenteller Aufbau zur zeitaufgelösten Molekülspektroskopie vorgestellt.

MO 14.12 Wed 16:30 Empore Lichthof

Laser absorption spectroscopy of iodine: 915 nm to 985 nm in a single scan — ●CHRISTIAN NÖLLEKE, STEPHAN FALKE, CHRISTOPH RAAB, and RUDOLF NEUHAUS — TOPTICA Photonics AG, Lochhamer Schlag 19, Gräfelfing/München, Germany

Iodine gas cells serve as frequency reference for lasers thanks to the good understanding of their rich molecular spectrum. This is particularly true for the wavelength range 500 nm to 900 nm, where the theoretical model of the B-X system and experimental findings agree on a level of a few MHz. Hence, iodine cells provide frequency references with a line spacing of typically a few GHz only.

In order to extend this knowledge towards longer wavelengths, a deeper understanding of the A-X system of iodine is required. Recent developments in laser technology enable high-resolution spectroscopy

with unprecedented ease. In this work, we record absorption spectra with a 75 cm long iodine cell, in which vapor pressure and temperature of the molecular gas is controlled independently. We utilize the vast mode-hop-free tuning range of the DLC CTL developed within our company to investigate the distribution of observable molecular lines as well as their signal-to-noise ratio in the range 915 nm to 985 nm. Moreover, for selected lines, we perform at saturation absorption spectroscopy using the fine-tuning of the laser. This experiment is an important step towards a detailed theoretical model of the A-X system and hence a good frequency reference in this range.

MO 14.13 Wed 16:30 Empore Lichthof

Detection system for dissociative recombination studies at the Cryogenic Storage Ring — ●SUNNY SAURABH¹, ARNO BECKER¹, CLAUDE KRANTZ¹, OLDŘICH NOVOTNÝ¹, STEFAN SCHIPPERS², KAIJA SPRUCK², XAVIER URBAIN³, STEPHEN VOGEL¹, and ANDREAS WOLF¹ — ¹Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany — ²Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — ³Université Catholique de Louvain B-1348 Louvain-la-Neuve, Belgium

Dissociative recombination (DR) is an important destruction and neutralization process in plasma environments, such as the interstellar medium. DR reaction rates, product channels and product excitation states are important parameters for describing such environments. Based on this DR reaction dynamics can be understood as well. We are planning to perform DR experiments in cold environment below 10 K for the first time in our newly commissioned Cryogenic Storage Ring at MPIK. In a configuration of merged electron and ion beams, neutral products form and leave the ion beam orbit. To collect these products a large-area, MCP-based neutral particle detector is used. The detector provides relative temporal information on neutral products in \sim ns time scale. A fast \sim 1 kHz frame-rate CMOS camera viewing the phosphor screen anode will allow us to correlate this temporal information with the product impact positions on the detector surface on event-to-event basis. For this purpose, a new data acquisition system to control the detector, the timing, and the collision energy between the electron and ion beams for DR rate measurements is under development.

MO 14.14 Wed 16:30 Empore Lichthof

Investigation of 1-Phenylethanol with Circular Dichroism - Resonance-enhanced Multiphoton Ionization (CD-REMPI) in the Gas Phase — ●JÖRN LEPELMEIER, ARAS KARTOUZIAN, ULRICH BOESL, and ULRICH HEIZ — Lehrstuhl für Physikalische Chemie, Technische Universität München, Germany

The Circular Dichroism - Resonance-enhanced Multiphoton Ionization (CD-REMPI) provides a three dimensional discrimination method for the investigation of chiral molecules in the gas phase. Beside the already two dimensional combination of mass selectivity given by a Time Of Flight - Mass Spectrometer (TOF-MS) together with wavelength selectivity due to Resonance-enhanced Multiphoton Ionization (REMPI), an enantioselective component is added by utilizing the Circular Dichroism (CD) effect. Therefore, within the REMPI process the resonance excitation of the studied molecules is initialized by circularly instead of linearly polarized light. Thus, CD-REMPI allows fast enantiosensitive gas phase studies of chiral molecules without the requirement of previous sample preparation. These are ideal conditions e.g. for the detection of product species coming from stereoselective catalysis reactions.

With our contribution we want to demonstrate the sensitivity of the CD-REMPI technique with enantiomeric excess measurements regarding the asymmetry factor g of 1-Phenylethanol by using the Twin-Peak method [1].

[1] C. Logé and U. Boesl, ChemPhysChem, 12 (2011) 1940-1947

MO 14.15 Wed 16:30 Empore Lichthof

ion-ion coincidence imaging using an in-vacuum pixel detector — ●JINGMING LONG¹, FEDERICO FURCH¹, JUDITH DURÁ¹, ANTON TREMSIN², CLAU-PETER SCHULZ¹, ARNAUD ROUZÉE¹, and MARC VRAKING¹ — ¹Max Born Institute for Nonlinear Optics and Short Pulses Spectroscopy, Max Born Straße 2A, 12353, Berlin, Germany — ²Space Sciences Laboratory, University of California at Berkeley, Berkeley CA 94720, USA

The ionization and fragmentation of molecules by intense laser fields has been the subject of intense research for decades. Two main experimental techniques developed to record the momentum distribution of the charged particles generated from strong field ionization are widely used: the velocity map imaging and the 3D coincidence imaging. The

full 3D momentum vectors of all participating fragments can be measured in coincidence using a reaction microscope (REMI) or a cold target recoil ion momentum spectrometer (COLTRIMS).

Recently, we have implemented a new in vacuum pixel detector, the so-called Timepix, as a replacement of traditional delay line anodes. This new 3D detector has been tested for ion-ion coincidence experiments showing the possibility to reach sub-pixel spatial resolution ($<55 \mu\text{m}$) and a 25 ps temporal resolution, at a 1 kHz frame readout rate. Combined with a high repetition rate (400 kHz) laser, our ion-ion coincidence imaging spectrometer can achieve an event rate faster than 10^4 ion events per second, and can be a powerful tool in studies of ultrafast nuclear dynamics in strong laser fields.

MO 14.16 Wed 16:30 Empore Lichthof

A novel technique to study time-resolved structural imaging of transition state dynamics — ●KATRIN REININGER, FRIEDRICH FREYSE, and JOCHEN MIKOSCH — Max-Born-Institute, Berlin

Progress in time-resolving transition state dynamics of bimolecular chemical reactions has been very limited due to the start-time dilemma and the absence of a significant probe mechanism, which gives insight into the structural dynamics.

We are developing a novel probe that images, one molecule at a time, the time-dependent spatial structure of individual transition states. For this we combine two modern techniques of molecular physics: (i) Reaction precursors are prepared as small clusters of ions and neutral molecules which serve as starting point for inducing transition state dynamics by photodissociation of a chromophore. The relative collision energy is tunable by varying the photodissociation wavelength. (ii) Coulomb Explosion Imaging, induced by short and intense infrared laser pulses combined with full coincidence detection of the resulting positively charged fragments will then be used to follow the dynamics and ultimately to reconstruct the evolving spatial molecular structure.

We will present the experimental setup and its characterisation. First experiments on controlling vibrations in a diatomic molecule will be shown. To increase the repetition rate, the implementation of an Electrostatic Ion Beam Trap to recycle the ion target is investigated.

MO 14.17 Wed 16:30 Empore Lichthof

Multiplex Detection of Homodyne Nonlinear Time-Resolved Signals for Multimodal Spectroscopy — ●ANDREAS LUDWIG, TAKESHI MIKI, TIAGO BUCKUP, and MARCUS MOTZKUS — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität, D-69120 Heidelberg, Germany

The goal of Multimodal Time-Resolved Spectroscopy is the combination of multiple time-resolved signals to understand complex molecular dynamics. Spectral resolution of such signals is a fundamental aspect because signal contributions in different techniques appear at different detection wavelengths. While detection at kHz rates of (self-) heterodyne signals, like those of transient absorption, is nowadays straightforward, the same is not true for weak homodyne signals. In this work, we have implemented a detection setup based on a spectrometer and kHz CCD. The setup covers the spectral range from 450 to 700nm with a resolution of about 1nm. Readout rates of up to 1.5kHz can be achieved. Synchronizing the CCD detector readout to the laser as well as to the scanning of optical delay stages enables shot-to-shot detection. The setup is benchmarked by detecting spectrally resolved third- and fifth-order techniques like degenerate four-wave mixing, pump-four wave mixing and 2D Raman at 1kHz readout rates. Dephasing of vibrational coherence in the excited state and coupling between different modes is demonstrated for different organic molecules in solution.

MO 14.18 Wed 16:30 Empore Lichthof

Spectral focusing with flexible shaped laser pulses for chemical imaging — ●LUKAS BRÜCKNER, TIAGO BUCKUP, and MARCUS MOTZKUS — Physikalisch-Chemisches Institut, Universität Heidelberg, Germany

Due to the high degree of control, the implementation of spectral focusing into a single-beam CARS setup containing a pulse shaper has several advantages over usual multi-beam setups and opens up new possibilities. We show in simulation and experiment how the flexible adjustment of the spectral focusing phase makes it possible to address and optimize multiple important parameters for imaging and microspectroscopy. The effect of the applied chirp on the spectral resolution and the possibility of dividing the spectrum into pump, Stokes and probe frequencies in order to allow for time-delaying the probe for background-free imaging are shown. In addition, their amplitudes can be independently adjusted and certain spectral regions completely

suppressed to prevent biological samples from photo damage. The possibility of using a transform-limited probe also greatly increases the signal levels of simultaneously detected SHG and TPEF-signals in multimodal imaging. Furthermore, the applicability of the concept to a broad spectral range from the fingerprint region to the CH-vibrations around 3000 wavenumbers is shown

[1] J. Rehbinder, L. Brückner, A. Wipfler, T. Buckup, and M. Motzkus, *Opt. Express* **22**, 28790 (2014)

[2] L. Brückner, T. Buckup and M. Motzkus, *Opt. Lett.* **22**, 5204-5207 (2015)

MO 14.19 Wed 16:30 Empore Lichthof

Unique inherent property of seawater promotes the SERS detection in femtomolar range — RAHSHA HASSANEIN, ●PATRICE DONFACK, BERND VON DER KAMMER, and ARNULF MATERNY — Physics and Earth Sciences, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Surface-enhanced Raman spectroscopy (SERS) has been used extensively in order to overcome the inherent weakness of the Raman signal when detecting substances at very low concentrations. Underwater sensing is becoming an emerging and yet rather challenging field. Since often only traces of substances have to be detected, SERS is the only way to obtain vibrational data. Complex SERS substrates have been tested for this application. In this contribution, we will demonstrate that colloidal SERS substrates in solution when added to sea water yields extremely high enhancement factors. Using such a straightforward approach leads to the enhancement of the Raman signal of crystal violet in sea water, which enabled us to detect concentrations as low as femtomolar.

MO 14.20 Wed 16:30 Empore Lichthof

Raman Spectroscopy for the Characterization of Milk Properties — ●MAXIMILIAN SCHALLWIG¹, PATRICE DONFACK¹, FAEZEH MOHAGHEGH¹, RALF ZINK², NADINE GEBERS², and ARNULF MATERNY¹ — ¹Physics and Earth Sciences, Jacobs University Bremen, Campus Ring 1, 28759 Bremen — ²DMK Deutsches Milchkontor GmbH, Flughafental 17, 28199 Bremen

Raman spectroscopy yields molecular fingerprints in form of unique vibrational spectra. Therefore, it is a useful technique also for analytical purposes. Raman spectra obtained from systems like natural food of plant or animal origin are rather complex due to the superposition of spectra from different components. Still the spectra can be used to extract information about essential nutrients, but also contaminations, adulterations and deterioration. In the present study, we have used Raman spectroscopy in combination with statistical evaluation techniques like principal component analysis and linear regression in order to analyse milk and milk products. We show that different important parameters can be determined like fat contents, saturation degree etc.

Raman spectroscopy has proven to be a valuable tool for the fast and non-invasive characterization of these samples.

MO 14.21 Wed 16:30 Empore Lichthof

Polarization Rotation IMPACT-FT-MW Spectrometer — ●DENNIS WACHSMUTH and JENS-UWE GRABOW — Institut für Physikalische Chemie, Leibniz Universität Hannover, Callinstr. 3A, Hannover, Deutschland

As has been previously shown, the in-phase/quadrature phase modulation passage-acquired coherence technique (IMPACT) Fourier-transform microwave (FT-MW) spectrometer delivers broadband capabilities at highest spectral resolution.

Nevertheless due to specific details in the electronic setup the applicable maximum polarization power was limited. Hence less polar molecules were difficult to measure.

In a novel approach this disadvantage could be circumvented by use of the polarization direction of the microwave radiation. The setup prevails the high spectral resolution but increases the sensitivity dramatically while allowing the utilisation of very high power tube amplifiers. In this contribution we present the novel apparatus in detail as well as experimental results obtained with the modified spectrometer.

MO 14.22 Wed 16:30 Empore Lichthof

Optical focusing of isolated particles for diffractive imaging experiments — ●SALAH AWEL^{1,2}, RICK KIRIAN⁴, JOCHEN KÜPPER^{1,2,3} und HENRY CHAPMAN^{1,2,3} — ¹Center for Free-Electron Laser Science, DESY — ²The Hamburg Center for Ultrafast Imaging, University of Hamburg, — ³Department of Physics, University of Hamburg — ⁴Arizona State University, Tempe

The short, intense, and coherent x-ray pulses produced by x-ray free-electron lasers (XFELs) have led to major advances in macromolecular structure determination. Single-particle imaging is among the new paradigm to emerge consists of directing a stream of randomly oriented bioparticles across the focus of the XFEL beam so that high-resolution 3D structure can be constructed from diffraction patterns of multiple identical particles. Presently, the difficulty of efficiently delivering bioparticles to a sub-micrometer x-ray focus is a limiting factor. For a 100 nm x-ray focus, current sample delivery efficiencies (fraction of particles intercepted by an x-ray pulse) are on the order of 10^{-7} on average, and hit fractions (fraction of x-ray pulses intercepting a particle) are below 0.1%. In order to mitigate this problem, we are developing techniques for guiding aerosolized nanoparticles to the X-ray focus with specially shaped laser illumination [1]. Our current experiments aim at transversely confining streams of aerosolized particles as they exit an aerosol injector with a counter-propagating "hollow" quasi-Bessel beam, using radiation pressure and thermal (photophoretic) forces [2].

[1] Eckerskorn et al., *Opt. Exp.* **21**, 30492-30499 (2013).

[2] Eckerskorn et al., *Phys. Rev. Applied* (accepted 29 Oct. 2015).