

## MO 5: MO Poster 1

Time: Monday 17:00–19:00

Location: Empore Lichthof

MO 5.1 Mon 17:00 Empore Lichthof

**Data fusion for photoelectron spectroscopy @FLASH: a GPU accelerated approach** — ●FABIANO LEVER<sup>1</sup>, DENNIS MAYER<sup>1</sup>, JAN METJE<sup>1</sup>, MARKUS BRAUNE<sup>2</sup>, STEFAN DÜSTERER<sup>2</sup>, and MARKUS GÜHR<sup>1</sup> — <sup>1</sup>University of Potsdam, Germany — <sup>2</sup>Deutsches Elektronen- Synchrotron, Hamburg, Germany

We present a collection of data analysis techniques that are used to extract information from the large amount of data produced at the newly-built URSA-PQ instrument at the free electron laser FLASH. Data fusion procedures are used to combine together information from diverse sources, providing a more unified picture of the physical process under study. Graphical processing units (GPU) accelerated computing is used to increase the efficiency of the data processing algorithms.

MO 5.2 Mon 17:00 Empore Lichthof

**Small waist multimode cavity design for spatially resolved imaging of cold molecules** — ●JANNIS SCHNARS<sup>1</sup>, KAI VOGES<sup>1</sup>, PHILIPP GERSEMA<sup>1</sup>, TORSTEN HARTMANN<sup>1</sup>, ALESSANDRO ZENESINI<sup>1</sup>, KLEMENS HAMMERER<sup>2</sup>, and SILKE OSPELKAUS<sup>1</sup> — <sup>1</sup>Institut für Quantenoptik, Universität Hannover — <sup>2</sup>Institut für Theoretische Physik, Universität Hannover

Ultracold polar molecules offer exciting research perspectives due to strong dipole-dipole interactions. Pathways for the creation of ultracold ground state molecules are nowadays well known, the most common is to cool two atomic species close to quantum degeneracy, to associate atoms into loosely bound Feshbach molecules and transfer the molecular ensemble to the ground state by a stimulated Raman adiabatic passage. However, imaging techniques for atoms cannot be applied to molecules due to their complex internal structure with rotational and vibrational degrees of freedom, which often forbids optical cycling on a closed transition. For imaging, the creation process is therefore often reversed, dissociating molecules into atoms for convenient fluorescence or absorption imaging. This technique is highly destructive. Here we present a technique that allows to directly observe the molecules inside a 2D-optical lattice. The detection scheme relies on a dispersive matter-light interaction in the low saturation regime. The interaction is enhanced by a small-waist cavity. Furthermore the cavity is pursued in the multimode regime facilitating spatial resolution of several lattice sites. We present possible resonator geometries combing both requirements of a small waist and frequency degeneracy.

MO 5.3 Mon 17:00 Empore Lichthof

**Reconstructing Nanoclusters from Single Wide-Angle Scattering Images with Neural Networks** — ●THOMAS STIELOW, THOMAS FENNEL, and STEFAN SCHEEL — Institut für Physik, Universität Rostock, Albert-Einstein-Straße 23, 18059 Rostock

Single-shot diffraction imaging by soft X-ray laser pulses is a valuable tool for structural analyses of unsupported and short-lived nanosystems, although inversion of the scattering patterns still prove challenging [1]. Deep learning, on the other hand, is widely used in data sciences for the extraction of information from images and sees more and more application in various sciences. Recently, several advances have showcased how the predictive power of neural networks can be harnessed for extracting certain features from wide angle X-ray scattering patterns [2, 3]. We aim to solve the full inversion problem of wide-angle X-ray scattering with neural networks. Our approach is based on reconstructing the scatterer's density based on a training set of arbitrary convex bodies. We demonstrate the predictive capability of the trained networks by using real-world experimental data.

[1] I. BARKE et al., Nat. Comm. **6**, 6187 (2015).

[2] J. ZIMMERMANN, et al., Phys. Rev. E, 063309 (2019).

[3] T. STIELOW et al., arXiv:1906.06883 (2019).

MO 5.4 Mon 17:00 Empore Lichthof

**Attosecond pulse induced ionization dynamics in a molecular charge-transfer system with correlated electrons** — ●KARL MICHAEL ZIEMS<sup>1,2</sup>, FRIEDRICH GEORG FRÖBEL<sup>1</sup>, STEFANIE GRÄFE<sup>1,2</sup>, and ALEXANDER SCHUBERT<sup>1</sup> — <sup>1</sup>Institute of Physical Chemistry, Friedrich-Schiller-University Jena, Germany — <sup>2</sup>Max Planck School of Photonics, Germany

The attosecond ultrafast ionization dynamics of correlated two- or many-electron systems have, so far, been mainly addressed investigat-

ing atomic systems. In the case of single ionization, it is well known that electron-electron correlation modifies the ionization dynamics and observables beyond the single active electron picture, resulting in effects such as the Auger effect or shake-up and knock up processes. Here, we extend these works by investigating the attosecond ionization of a molecular system involving the correlated two-electron dynamics, as well as the non-adiabatic nuclear dynamics. We demonstrate, employing a charge-transfer molecular model system, how elastic and inelastic correlation-driven processes can be observed. As the model system investigated here involves two differently bound electrons, a stronger and a weaker bound electron, we can distinguish different pathways leading to ionization, be it direct ionization or ionization involving elastic and inelastic electron scattering processes. We find that different pathways result in a difference in the electronic population of the parent molecular ion, which, in turn, involves different subsequent (non-adiabatic) vibrational dynamics.

MO 5.5 Mon 17:00 Empore Lichthof

**PhotoElectron Circular Dichroism (PECD) of Anionic Metal Complexes** — ●JENNY TRIPTOW, GERARD MEIJER, and ANDRÉ FIELICKE — Fritz-Haber-Institut der Max Planck Gesellschaft, Berlin, Deutschland

Experiments on PECD are typically done with neutral chiral molecules and reveal asymmetries in the Photoelectron distribution of up to 10%. To perform these experiments, fs-lasers or synchrotron beamlines have to be used.

In our experiment, the PECD method is performed on anionic chiral molecules where a tabletop ns-laser is sufficient to photo-detach the relatively weakly-bound electron. Since a neutral chiral molecule and an electron are left behind, the missing long range interaction of the Coulomb potential can reveal the influence of short range interactions between the electron and the dipole moments of the molecule on the PECD effect.

Our initial approach to create chiral anions was to bind a neutral chiral molecule to an atomic gold anion. Atomic gold anions are easily produced in a laser ablation source. Our current procedure is deprotonation in a Plasma Entrainment Source followed by a supersonic expansion. Both the production of the chiral molecules bound to gold anions and the deprotonated molecules are verified by a Wiley-McLaren time-of-flight mass spectrometer and a velocity map imaging spectrometer.

MO 5.6 Mon 17:00 Empore Lichthof

**Finding molecules for consecutive photoinduced electron transfer (conPET)** — ●CARINA ALLACHER, PATRICK NUERNBERGER, and BERNHARD DICK — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Germany

In photosynthesis, nature combines the energy of several photons to perform a chemical reaction. In 2014 König et al. [1] proposed the conPET mechanism (consecutive photoinduced electron transfer) in order to combine two photons in a photochemical reaction. The first photon excites a photocatalyst molecule **M** to the excited state **M\*** which extracts an electron from a donor molecule **D**. The resulting radical **M•** is excited by a second photon, and the excited radical **M\*\*** transfers the electron to an acceptor molecule **A** which is reduced and undergoes further chemical reactions. In a search for such photocatalysts we generate the radical **M•** electrochemically. This allows a study of the photophysics of the conPET species **M•** separated from the photochemistry involved in generating the radical. Cyclic voltammetry in combination with fs transient spectroscopy yields the reduction potential of **M•** and the lifetime **M\*\***. First results obtained with the photocatalyst R6G show that the properties and reactivities of the electrochemically generated radical are the same as those of the photochemically generated radical.

[1] I. Gosh, T. Gosh, J. I. Bardagi, B. König, *Science* **2014**, 346, 725–728.

MO 5.7 Mon 17:00 Empore Lichthof

**Hydrogen Atom Transfer (HAT) between phenol and phenoxy-radical** — ●UWE FALTERMEIER and BERNHARD DICK — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Germany

Hydrogen Atom Transfer (HAT) reactions involving phenoxy radicals

occur in various biological processes, like the breaking of free-radical chain reactions by tocopherol (Vitamin E). The self-exchange of a hydrogen atom between phenol and its corresponding phenoxy radical is the simplest-case scenario for such reactions. As such, it lends itself as calibration point for theoretical models. Despite its seemingly simple nature, almost no experimental data exists for this reaction. We present a method for determining the rate constant of this exchange and its thermal behavior by looking at the pseudo-self-exchange between phenol and phenol-d5. The radicals are produced by photolysis and the transient absorption of the samples in the  $\mu\text{s}$  range is recorded with a streak camera. Measurements at temperatures ranging from  $-5^\circ\text{C}$  to  $35^\circ\text{C}$  yield rate constants for the exchange of  $\approx 4 \times 10^5 \text{s}^{-1} \text{mol}^{-1}$ . Reversing the direction of the exchange, from phenol to phenoxy-d5, we find the same rate constants. This shows that our system is a good approximation to the phenoxy/phenol self-exchange reaction.

MO 5.8 Mon 17:00 Empore Lichthof

**Study of the photophysics and photochemistry of the phenol-ammonia complex** — ●STEFAN FUCHS and BERNHARD DICK — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Germany

Excited-state hydrogen transfer (ESHT) reactions provide photostability of biomolecules and are applied for the photoprotection of compounds (e.g. plastics) exposed to sunlight. Mechanistic proposals include hydrogen transfer and electron coupled proton transfer (ECPT). Clusters of phenol with ammonia have been used as model systems for the study of the mechanism. Previous studies on the dissociation of such clusters into a neutral phenoxy radical and the neutral hydrated ammonia cluster have considered clusters containing 5 ammonia molecules [1,2]. We use time-of-flight mass spectroscopy in combination with quantum chemical calculations which yields data on the phenol-ammonia(1) cluster.

[1] M. Miyazaki, R. Ohara, K. Daigoku, K. Hashimoto, J. R. Woodward, C. Dedonder, Ch. Jouvét, M. Fujii, *Angew. Chem. Int. Ed.* **2015**, 54, 15089–15093.

[2] M. Miyazaki, R. Ohara, C. Dedonder, Ch. Jouvét, M. Fujii *Chem. Eur. J.* **2018**, 24, 881 – 890.

MO 5.9 Mon 17:00 Empore Lichthof

**Understanding Geometric and Electronic Properties of Small Silicon Oxides Relevant in Interstellar Dust Formation Processes** — ●KAI POLLW, KARIM SAROUKH, ROBERT RADLOFF, LARS DAHLÖF, MARKO FÖRSTEL, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

Interstellar dust is an important ingredient in the formation of solar systems like our own. Some properties of interstellar dust are known, many questions, however, are still unanswered. Molecular SiO can form in the atmospheres of oxygen-rich stars and interstellar dust contains particles made of macroscopic silicates of various compositions. Intermediates have been elusive to observations.

We present fragmentation pathways, geometric structure and optical properties of several possible intermediate species obtained via photodissociation spectroscopy and quantum chemical calculations. Knowledge of these parameters may help to model the complex formation processes and enable an observational search for these intermediate species.

MO 5.10 Mon 17:00 Empore Lichthof

**Optical Properties of Diamondoid Cations and Their Astrochemical Relevance** — ●PARKER CRANDALL, DAVID MÜLLER, PETER MEINHOLD, MARKO FÖRSTEL, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany

Diamondoids, also known as nanodiamonds, are a class of highly stable, aliphatic cycloalkanes arranged into cage-like structures by the  $\text{sp}^3$  hybridization of the carbon atoms. Members of the astrochemical community have demonstrated similarities between the IR spectra of diamondoids and unidentified infrared emission bands seen in the spectra of young stars with circumstellar disks. A ubiquitous presence of diamondoids is hypothesized, which could account for more than 5 % of cosmic and 40 % of tertiary carbon in interstellar environments. Due to their low ionization energy, it is also suggested that the radical cations of these molecules, which are predicted to absorb in the IR-UV/VIS range, are also present in high abundances and might be responsible for features in the well-known diffuse interstellar bands. However, optical spectra of these cations have not previously been reported. In this contribution, we present the first optical spectra via

laser spectroscopy of the simplest diamondoid cation, the adamantane radical cation, by ion trapping in a cryogenic 22-pole trap. Fragmentation channels of the parent ion were also investigated by reflectron time-of-flight mass spectrometry. The astrophysical implications and future work are also described.

MO 5.11 Mon 17:00 Empore Lichthof

**IR Photodissociation spectra of  $\text{Si}_x\text{H}_{4x-4}^+$  ( $x=4-8$ ): Evidence for Si-H-Si proton bridges** — ●MARTIN ANDREAS ROBERT GEORGE and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany

Silicon hydride clusters ( $\text{Si}_x\text{H}_y^+$ ) play a significant role in plasma chemistry and astrochemistry. Despite this importance their structural and energetic properties are largely unexplored. Building upon our previous investigations of  $\text{Si}_2\text{H}_6^+$  [1],  $\text{Si}_2\text{H}_7^+$  [2],  $\text{Si}_3\text{H}_8^+$  [3], we present infrared photodissociation (IRPD) spectra of previously unknown  $\text{Si}_x\text{H}_y^+$  ions of the form  $\text{Si}_x\text{H}_{4x-4}^+$  with  $x=4-8$  ( $\text{Si}_4\text{H}_{12}^+$ ,  $\text{Si}_8\text{H}_{24}^+$ ) [4]. Our spectral analysis, supported by dispersion-corrected density functional calculations, reveals that all  $\text{Si}_x\text{H}_{4x-4}^+$  ions have at least one Si-H-Si bridge. The characteristic fingerprint of these three-center two-electron (3c-2e) bonds is the strongly IR active anti-symmetric stretch fundamental of the Si-H-Si bridge. The frequency of this vibration depends strongly on the structural and energetic details of the Si-H-Si bridge. Our investigations reveal the correlations between the properties of the various Si-H-Si bridges (bond distances, bond angles, binding energies, stretch frequencies). The bond strength varies from strong symmetric 3c-2e chemical bonds to weak hydrogen or van der Waals bonds. [1] M. Savoca et al. (2013), *Phys. Chem. Chem. Phys.*, 15, 2774 [2] M. Savoca et al., *Angew. Chem. Int. Ed.* (2013), 52, 1568 [3] M.A.R. George et al., *Chem. Eur. J.* (2013), 19, 15315-15328 [4] M.A.R. George, O. Dopfer (2019), *Int. J. Mass Spectrom.* (2019), 435, 51

MO 5.12 Mon 17:00 Empore Lichthof

**High-resolution infrared study of carbon-rich clusters  $\text{C}_3\text{X}$  and  $\text{XC}_3\text{X}$  ( $X = \text{Se}, \text{Te}$ )** — SVEN THORWIRTH<sup>1</sup>, ●THOMAS SALOMON<sup>1</sup>, JOHN B. DUDEK<sup>2</sup>, YURY CHERNYAK<sup>2</sup>, SOPHIA BURGER<sup>3</sup>, JÜRGEN GAUSS<sup>3</sup>, and STEPHAN SCHLEMMER<sup>1</sup> — <sup>1</sup>I. Physikalisches Institut, Universität zu Köln, Köln, Germany — <sup>2</sup>Department of Chemistry, Hartwick College, Oneonta, NY, U.S.A. — <sup>3</sup>Department Chemie, Johannes Gutenberg-Universität Mainz, Mainz, Germany

To date, carbon-rich clusters harboring heavy elements have received little attention from both experiment and quantum chemistry. Recent high-resolution infrared survey scans of laser ablation products from carbon-selenium and carbon-tellurium targets in the  $5\mu\text{m}$  wavelength regime have revealed several vibration-rotation bands not observed previously. On the basis of comparison with results from density-functional theory (DFT) calculations and high-level quantum-chemical calculations performed at the CCSD(T) level of theory these bands are attributed to new linear chains of the form  $\text{C}_3\text{X}$  and  $\text{XC}_3\text{X}$  with  $X$  being either Se or Te.

MO 5.13 Mon 17:00 Empore Lichthof

**High-resolution infrared and millimeter-wave spectroscopy of  $\text{CNH}_n^+$  ( $n = 0, 4, 6$ ) ions** — ●SVEN THORWIRTH<sup>1</sup>, OSKAR ASVANY<sup>1</sup>, CHARLIE MARKUS<sup>2</sup>, JOSE DOMENECH<sup>3</sup>, THOMAS SALOMON<sup>1</sup>, PHILIPP SCHMID<sup>1</sup>, MATTHIAS TÖPFER<sup>1</sup>, PHILIP SCHREIER<sup>1</sup>, and STEPHAN SCHLEMMER<sup>1</sup> — <sup>1</sup>I. Physikalisches Institut, Universität zu Köln — <sup>2</sup>Department of Chemistry, University of Illinois, Urbana, IL, U.S.A. — <sup>3</sup>Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Molecular ions play crucial roles in the astrochemistry associated with star formation and planetary atmospheres. In this project, we have studied three fundamental cations  $\text{CNH}_n^+$  ( $n = 0, 4, 6$ ) using action spectroscopic techniques in a 22-pole ion trap at a nominal temperature of 4K [1]. The fundamental diatomic  $\text{CN}^+$  [2] as well as protonated methylene imine,  $\text{H}_2\text{C}=\text{NH}_2^+$ , and protonated methyl amine,  $\text{H}_3\text{C}=\text{NH}_3^+$ , were all studied by their pure rotational spectra in the millimeter-wave region employing the method of rotational state-selective He-attachment [3].  $\text{CN}^+$  and  $\text{H}_2\text{C}=\text{NH}_2^+$  were also studied at high spectral resolution in the infrared using LIICG (Laser Induced Inhibition of Complex Growth) [1,4].

[1] O. Asvany, S. Brünken, L. Kluge, and S. Schlemmer 2014, *Appl. Phys. B* 114, 203 [2] S. Thorwirth, P. Schreier, T. Salomon, S. Schlemmer, and O. Asvany 2019, *Astrophys. J. Lett.* 882, L6 [3] S. Brünken, L. Kluge, A. Stoffels, J. Peres-Rios, and S. Schlemmer 2017, *J. Mol. Spectrosc.* 322, 67 [4] S. Chakrabarty, M. Holz, E. K. Campbell, A. Banerjee, D. Gerlich, and J. P. Maier 2013, *J. Phys. Chem. Lett.* 4,

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MO 5.14 Mon 17:00 Empore Lichthof  
**phase transitions of nanoconfined water in self-assembled L,L-diphenylalanine peptides studied by vibrational spectroscopy** — ●ABUZER ORKUN AYDIN<sup>1</sup>, FERID SALEHLI<sup>1</sup>, SVITLANA KOPYL<sup>2</sup>, and ANDREI KHOLKIN<sup>2</sup> — <sup>1</sup>Physics Department, Istanbul Technical University, Istanbul, Turkey — <sup>2</sup>Physics Department and CICECO, Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal

Self-assembly of diphenylalanine (FF) molecules results in highly organised tubular nanostructures. Water molecules are confined in FF rings with diameter about 1nm along these nanocavities. This work is a fresh look into phase behavior of nanoconfined water in natural synthetic biomacromolecule.

We obtained MIR spectra in the temperature range between 90K and 330 K. Five OH-stretching modes were identified in absorbance spectra as tetrahedral water in different confinements in FF rings, consequently ( $k_1=3105\text{ cm}^{-1}$ ,  $k_2=3150\text{ cm}^{-1}$ ,  $k_3=3200\text{ cm}^{-1}$ ,  $k_4=3275\text{ cm}^{-1}$ ) and non-completed tetrahedral water molecules between rings ( $k_5=3375\text{ cm}^{-1}$ ). We found that these modes exhibit pronounced integral anomalies in the region of 195 K and 230 K, red shift and blue shift around  $20\text{ cm}^{-1}$ , consequently. First anomaly indicates the onset of long-range tetrahedral water order, whereas the second anomaly signifies the mentioned order. Three OH-bending modes at  $1520\text{ cm}^{-1}$ ,  $1515\text{ cm}^{-1}$  and  $1620\text{ cm}^{-1}$  demonstrate redshift about  $5\text{ cm}^{-1}$  around 230 K confirming the phase transition.

MO 5.15 Mon 17:00 Empore Lichthof  
**URSA-PQ@FLASH: A mobile, highly flexible endstation for pump-probe electron spectroscopy at the FLASH free electron laser** — ●JAN METJE<sup>1</sup>, DENNIS MAYER<sup>1</sup>, FABIANO LEVER<sup>1</sup>, MARIO NIEBUHR<sup>1</sup>, MATTHEW ROBINSON<sup>1</sup>, AXEL HEUER<sup>1</sup>, RICHARD SQUIBB<sup>2</sup>, RAIMUND FEIFEL<sup>2</sup>, STEFAN DÜSTERER<sup>3</sup>, and MARKUS GÜHR<sup>1</sup> — <sup>1</sup>University of Potsdam, Potsdam, Germany — <sup>2</sup>University of Gothenburg, Gothenburg, Sweden — <sup>3</sup>DESY, Hamburg, Germany

We designed and built a mobile, highly flexible endstation designated for users at the free electron laser FLASH called URSA-PQ (Ultraschnelle Röntgenspektroskopie zur Abfrage der Photoenergiekonversion in Quantensystemen). The main instrument consists of a vacuum chamber with molecular capillary oven, a magnetic bottle time-of-flight electron spectrometer, and various tools to perform pump-probe experiments with optical laser pulses and x-ray pulses. The main chamber body adheres to CAMP-standards and thus many different compatible instruments may be incorporated.

We present the design of the vacuum apparatus and its mobile frame together with the control system of the experiment. The performance of the instrument was evaluated from commissioning at the beamline FL24. We present static as well as time resolved data to show various characteristics of the instrument.

MO 5.16 Mon 17:00 Empore Lichthof  
**Electron imaging of noble gases clusters under MIR laser-fields** — ●CRISTIAN MEDINA<sup>1</sup>, DOMINIK SCHOMAS<sup>1</sup>, MARKUS DEBATIN<sup>1</sup>, LTAIF LTAIF<sup>2</sup>, ROBERT MOSHAMMER<sup>3</sup>, THOMAS PFEIFER<sup>3</sup>, FRANK STIENKEMEIER<sup>1</sup>, and MARCEL MUDRICH<sup>2</sup> — <sup>1</sup>Albert-Ludwigs-Universität, Freiburg — <sup>2</sup>Aarhus University, Aarhus — <sup>3</sup>Max-Planck-Institut für Kernphysik, Heidelberg

In this project, we studied the behavior of the nanoplasma explosion of helium (He) and neon (Ne) droplets exposed to a strong and short mid-infrared laser field. The nanoplasma is initiated by strong-

field ionization of the cluster or dopant atoms, creating an impact-ionization avalanche in the cluster and ending in a Coulomb explosion of the nanoplasma. Clusters provide a large variety of additional effects compared to strong-field ionization in single atoms, such as enhanced ionization due to electron impact ionization, or collective oscillations of quasi-free electrons. He droplets are particularly interesting, due to their extremely high ionization potential. Additionally, they offer unique doping properties, which allows us to investigate the effect of the dopant species and to design an optimal doping system to ignite the process. The large number of charged particles emitted from a single nanoplasma explosion allows us to collect both full electron energy distributions (VMI) and ion mass-over-charge distributions (TOF) from a single hit. We can measure correlated single shot-single hit spectra and we can assign features in the photoelectron spectra to certain charge states of the cluster. We discuss the impact of doping with various species (Xe and Ca) to trigger the nanoplasma formation.

MO 5.17 Mon 17:00 Empore Lichthof  
**Photoelectron circular dichroism using 1+1 resonance-enhanced multi-photon ionization with UV laser pulses** — ●NICOLAS LADDA, CONSTANTIN WITTE, TOM RING, SIMON RANNECKY, SUDHEENDRAN VASUDEVAN, ALEXANDER KASTNER, HANGYEOL LEE, CHRISTIAN SARPE, HENDRIKE BRAUN, ARNE SENTLEBEN, and THOMAS BAUMERT — Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

The forward/backward asymmetry of the photoelectron angular distribution (PAD) with respect to the propagation direction of ionizing circularly polarized light of a randomly orientated chiral molecule is known as photoelectron circular dichroism (PECD). The measurement of the PAD asymmetry can be performed using velocity-map imaging (VMI) technique, where the gas phase provides a nearly collision and interaction free environment. UV fs pulses from fourth harmonic generation (196 nm, 6.3 eV) of our Ti:Sa laser enable a 1+1 resonance-enhanced multi-photon ionization (REMPI) process via energetically higher lying intermediate states of molecules such as fenchone or camphor. In the future, these pulses could also be used to invert the handedness of a chiral molecule by pump-dump-probe experiment, where the UV pulses are required to access an achiral excited state.

MO 5.18 Mon 17:00 Empore Lichthof  
**High Repetition Rate Studies of Laser-Driven Electron Rescattering in Spatially Aligned Molecules** — ●FEDERICO BRANCHI, HORST ROTTKE, MARK MERO, MARC J.J. VRAKING, and JOCHEN MIKOSCH — Max-Born-Institut, Berlin, Germany

In Laser-Induced Electron Diffraction (LIED), a valence electron in an atom or molecule tunnels through the Coulomb potential dressed by a strong laser field, is accelerated by the oscillating field of the laser and driven back to its parent, from which it can elastically rescatter. Structural information can be extracted from measured scattering angle distributions. In particular for mid-infrared lasers the energy of the returning electron can be sufficient to determine bond angles and lengths with LIED. Importantly, since LIED is phase locked to the cycle of the driving laser field, it has inherent time resolution and is hence a promising probe for molecular dynamics studies.

We have recently combined a high repetition-rate (100kHz), mid-IR (1550/3100nm), ultrashort (50fs pulse duration) laser system based on optical parametrical chirped pulse amplification (OPCPA) with a reaction microscope to investigate laser-driven electron rescattering in polyatomic molecules. Current results on laser-aligned 1,3-butadiene molecules are presented, for which coincidence measurements of electron and ion momenta allow to obtain ionization-channel resolved molecular frame information.