

MO 15: Poster 2

Time: Wednesday 16:30–18:30

Location: P

MO 15.1 Wed 16:30 P

Multiple-Quantum Two-Dimensional Fluorescence Spectroscopy of a Squaraine Polymer — ●AJAY JAYACHANDRAN, STEFAN MÜLLER, and TOBIAS BRIXNER — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Molecular aggregates such as squaraine heteropolymers feature a manifold of multiexcitonic states [1]. These multiexcitonic states are a result of numerous electronically coupled heterochromophoric units. However, it is challenging to investigate the correlations and spectral properties of the states of a particular multiexciton manifold using conventional spectroscopic tools due to convolution with spectral signatures of singly excited states. Here we make use of advances in fluorescence-based multidimensional spectroscopy to selectively measure multi-quantum correlations by using phase-cycled pulse sequences in a collinear excitation geometry [2]. Spectrally resolved two-quantum and three-quantum coherence signatures are captured through fourth-order and sixth-order signals which are acquired using a 36-fold phase-cycling scheme of a three-pulse excitation sequence. We also examine the eighth-order signals which can be resolved by using 64-fold phase cycling to observe correlations with four-quantum coherences without signal aliasing.

- [1] S. F. Völker *et al.*, *J. Phys. Chem. C* **118**, 17467 (2014).
 [2] S. Draeger *et al.*, *Opt. Express* **25**, 3259 (2017).

MO 15.2 Wed 16:30 P

Improved mass spectrometer for two-dimensional electronic spectroscopy in the gas phase — ●ARNE MORLOK, ULRICH BANGERT, LUKAS BRUDER, YILIN LI, DANIEL UHL, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

Two-dimensional electronic spectroscopy (2DES) is a very powerful method to study the ultrafast dynamics of matter. In our group, we apply the technique to molecules and cluster beams in the gas phase and combine it with photoion mass-detection [1,2]. To increase the flexibility of the mass spectrometer, we implement a pulsed electron gun for electron impact ionization. This enables beam depletion measurements and cluster beam characterization while avoiding the issue of overcoming the high ionization potentials of most molecules. We will present first characterization results.

- [1] L. Bruder *et al.*, *Nat Commun* **9**, 4823 (2018).
 [2] L. Bruder, U. Bangert, M. Binz, D. Uhl, and F. Stienkemeier, *J. Phys. B: At. Mol. Opt. Phys.* **52**, 183501 (2019)

MO 15.3 Wed 16:30 P

Femtosecond time-resolved pump-probe spectroscopy of benzene isomers — ●LUKAS FASCHINGBAUER¹, TOBIAS PREITSCHOPP¹, LIONEL POISSON², and INGO FISCHER¹ — ¹University of Wuerzburg, Institute for Physical and Theoretical Chemistry, Am Hubland, 97074 Wuerzburg, Germany — ²Universite Paris-Saclay, Institut des Sciences Moléculaires d'Orsay, Rue André Rivière, Bâtiment 520, 91405 Orsay Cedex, France

The excited state dynamics of the benzene isomers 3,4-dimethylenecyclobutene and fulvene were investigated by femtosecond time-resolved pump-probe spectroscopy at ISMO, Paris-Saclay, France. Lifetimes of the excited states were obtained by time-of-flight mass spectrometry, while photoelectron spectroscopy enabled the identification of the states involved in the relaxation processes. Preliminary results are presented.

MO 15.4 Wed 16:30 P

Coherent multidimensional spectroscopy of molecular and cluster beam samples — ●YILIN LI, ARNE MORLOK, ULRICH BANGERT, DANIEL UHL, FRANK STIENKEMEIER, and LUKAS BRUDER — Institute of Physics, University of Freiburg, Germany

Coherent multidimensional spectroscopy is a versatile technique enabling further insight into intra- and inter-molecular couplings on femtosecond time scales. We have recently extended the method to molecular and cluster beam samples in the gas phase [1] and combined it with photoionization probes [2,3]. In preparation for further experiments, we are currently characterizing the optical absorption, fluorescence, and photoelectron/ion yields of various molecular and cluster sam-

ples in the gas phase. We will give an overview of the optical setup and first characterization results.

- [1] L. Bruder *et al.*, *Nat Commun* **9**, 4823 (2018)
 [2] L. Bruder *et al.*, *J. Phys. B: At. Mol. Opt. Phys.* **52**, 183501 (2019)
 [3] D. Uhl *et al.*, *Optica* **8**, 1316 (2021).

MO 15.5 Wed 16:30 P

Studies on the Photocleavage Mechanism of the Manganese Complex $\text{MnBr}(\text{CO})_3(\text{pytz-CH}_2\text{C}_6\text{H}_5)$ — ●NIKLAS GESSNER¹, ULRICH SCHATZSCHNEIDER², and PATRICK NUERNBERGER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg — ²Institut für Anorganische Chemie, Universität Würzburg, Am Hubland, D-97074 Würzburg

Photoactivatable carbon monoxide (CO) releasing molecules (PhotoCORMs) have promising applications in medicine and biology, e.g. as cancer treatment agents [1]. In a common approach, one or more CO molecules are bound to an inert transition metal complex that comprises a multidentate organic ligand to control its physical and (bio-)chemical properties [2] like photoexcitation energies or the enrichment efficiency in cancerous tissue.

By using UV pump/mid-IR probe ultrafast transient absorption spectroscopy, the PhotoCORM $[\text{MnBr}(\text{CO})_3(\text{pytz-CH}_2\text{C}_6\text{H}_5)]$, pytz being 2-(1,2,3-triazol-4-yl)pyridine, has been investigated in order to identify the ligand that is cleaved off and to elucidate the reaction mechanism and the dynamics after photoexcitation. Results are compared to density functional theory calculations of possible transient intermediates and products, as well as to steady-state absorption measurements. It is found that a ligand is cleaved off after photoexcitation and that the dynamics are finished within 100 ps, so that either the reactant complex is retrieved or a persistent photoproduct is formed.

- [1] J. Niesel *et al.*, *Chem. Commun.* **15**, 1798–1800 (2008).
 [2] M. A. Gonzalez *et al.*, *Inorg. Chem.* **21**, 11930–11940 (2012).

MO 15.6 Wed 16:30 P

Ultrafast dynamics of $[\text{Ru}(\text{bipyridine})_2(\text{nicotinamide})_2]^{2+}$ and photoinduced formation of its water splitting adducts in gas and liquid phase — ●ROUMANS ISRAEL¹, LARS SCHÜSSLER², PATRICK HÜTCHEN¹, WERNER THIEL¹, ROLF DILLER², and CHRISTOPH RIEHN¹ — ¹TU Kaiserslautern, FB Chemie, 52, 54 — ²TU Kaiserslautern, FB Physik, 46

A fundamental understanding of the kinetics of Ru^{II} polypyridyl complexes is essential to exploit their photochemical applicability in areas such as medicine (photoactivatable prodrugs) and material science (photovoltaics/catalysis). In particular, the monodentate ligand nicotinamide in $[\text{Ru}(\text{bpy})_2(\text{na})_2]^{2+}$ (bpy = bipyridine) enables the efficient population of the dissociative triplet metal-centered (³MC) state on a sub-ps time scale, allowing for fast photosolvolytic and subsequent reactions of the complex. Here, the photoactive $[\text{Ru}(\text{bpy})_2(\text{na})_2]^{2+}$, including its related photoproducts such as the penta-coordinate intermediate (PCI, $[\text{Ru}(\text{bpy})_2(\text{na})]^{2+}$) and the monoqua species $[\text{Ru}(\text{bpy})_2(\text{na})(\text{H}_2\text{O})]^{2+}$ were object to transient ion action spectroscopy in gas phase and transient absorption spectroscopy in solution. In gas phase, dynamics ($\tau_1 \sim 0.6$ ps, $\tau_2 \sim 3$ ps) of $[\text{Ru}(\text{bpy})_2(\text{na})_2]^{2+}$ is in line with the liquid phase. However, prominent larger time components (~ 10 ps, 100–400 ps) found in solution, do not appear in gas phase, allowing their unequivocal assignment to intermolecular processes. This study is an important step towards controlling the efficiency and photoactivity of Ru^{II} polypyridyl complexes by tailored ligands design.

MO 15.7 Wed 16:30 P

Chirp dependence of the Circular Dichroism in ion yield of 3-methylcyclopentanone — ●SAGNIK DAS, JAYANTA GHOSH, SUDHEENDRAN VASUDEVAN, HANGYEOL LEE, NICOLAS LADDA, SIMON RANECKY, TONIO ROSEN, ARNE SENFTLEBEN, THOMAS BAUMERT, and HENDRIKE BRAUN — Institut für Physik, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

One of the methods to differentiate between the two enantiomers of a chiral molecule is Circular Dichroism (CD). It arises due to the difference in absorption of left and right circularly polarised light. The difference in absorption can also be mapped to the difference in ioni-

sation of the enantiomers and is known as CD in ion yield [1,2]. We use our home-built Time of Flight (ToF) mass spectrometer with our recently established twin peak [3] measurement setup to study the effect of linear chirp (GDD) on the anisotropy. The candidate molecule for this experiment is 3-methylcyclopentanone (3-MCP). The experiments are done at 309 nm and 322 nm, where 3-MCP is known to have anisotropies of up to 4% and 1%, respectively, for bandwidth limited pulse. At these wavelengths, a 1+1+1 resonance-enhanced multiphoton ionisation (REMPI) takes place in 3-MCP through the $\pi^* \leftarrow n$ transition. We observe an asymmetric enhancement of anisotropy for chirped pulses, which we compare to bandwidth limited pulses of equal peak intensity.

- [1] U. Boesl and A. Bornschlegl, *ChemPhysChem*, 7, 2085, 2006
 [2] H. G. Breunig et al., *ChemPhysChem*, 10, 1199, 2009
 [3] T. Ring et al., *Rev. Sci. Instrum.*, 92, 033001, 2021

MO 15.8 Wed 16:30 P

Probing vibrational wave packets in the electronic ground state of methyl p-tolyl sulfoxide via time-resolved PECD — ●NICOLAS LADDA¹, MAX WATERS², VÍT SVOBODA², MIKHAIL BELOZERTSOV², SUDHEENDRAN VASUDEVAN¹, SIMON RANECKY¹, TONIO ROSEN¹, SAGNIK DAS¹, JAYANTA GHOSH¹, HANGYEOL LEE¹, HENDRIKE BRAUN¹, THOMAS BAUMERT¹, HANS JAKOB WÖRNER², and ARNE SENFTLEBEN¹ — ¹Institut für Physik, Universität Kassel, 34132 Kassel, Germany — ²Laboratorium für Physikalische Chemie, ETH Zürich, 8093Zürich, Switzerland

The dynamic change of the chiral character upon the laser-induced vibrational motion in the electronic ground state of methyl p-tolyl sulfoxide (MISO) is investigated. For this purpose, the forward/backward asymmetry of the photoelectron angular distribution (PAD) with respect to the propagation direction of ionising circularly polarised light of the randomly oriented chiral molecule, known as photoelectron circular dichroism (PECD), was measured. Geometry dependent ionisation rates of a molecule when interacting with an ultrashort laser pulse causes the formation of a coherent oscillating wave packet in the electronic ground state. The vibrational motion - umbrella motion of the sulfoxide molecule - changes the chiral character of the molecule, which can be studied by probing the time-resolved PECD with a VUV femtosecond laser pulse.

MO 15.9 Wed 16:30 P

Spectroscopic investigation of the light-induced rearrangement of a Xanthine derivative — ●KARINA HEILMEIER¹, THOMAS RITZNER¹, RAFAEL E. RODRÍGUEZ-LUGO², ROBERT WOLF², and PATRICK NUERNBERGER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg — ²Institut für Anorganische Chemie, Universität Regensburg, 93040 Regensburg

The Xanthine derivative 7-(4-methoxyphenyl)-1,3-dimethyl-8-(pyridin-2-yl)-3,7,8,9-tetrahydro-1*H*-purine-2,6-dione possesses a characteristic purine skeleton additionally modified with pyridine and anisole moieties bound to the five-membered ring. Our studies reveal that ultraviolet light induces the migration of the anisole group from the 7-nitrogen of the purine skeleton to the nitrogen of the pyridine moiety. The isomer emerging as rearrangement product could even be isolated, and the structure was determined by single-crystal X-ray diffraction.

For obtaining a comprehensive picture of the light-induced mechanism leading to the rearrangement, results from stationary measurements are compared to those from ultrafast transient absorption and fluorescence upconversion spectroscopy. In addition, we contrast the photodynamics of the in-situ generated isomer with that of the synthetically isolated one. In further systematic studies, we explore whether photoinduced back-isomerization is achievable as well, and address the role of the solvent's polarity on the rearrangement.

MO 15.10 Wed 16:30 P

Low dispersive phase modulation scheme for interferometric XUV experiments — ●FABIAN RICHTER, SARANG DEV GANESHAMANDIRAM, IANINA KOSSE, RONAK SHAH, GIUSEPPE SANSONE, FRANK STIENKEMEIER, and LUKAS BRUDER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Quantum interference spectroscopy schemes are well established in the visible range to control and resolve the static properties and dynamics of quantum systems. Recently these principles got extended into the XUV regime [1,2]. Here acousto-optical modulators are used to achieve interferometric measurements supported by a phase cycling

scheme. However, in this setup a significant amount of material is introduced in the optical beam path at the fundamental frequency which prohibits using ultrashort pulses and high laser intensities. We present a new approach to achieve phase cycling while minimizing the amount of material dispersion by an order of magnitude. We will present the basic concept of this approach and first characterization results.

[1] Wituschek, A., Bruder, L., Allaria, E. et al. Tracking attosecond electronic coherences using phase-manipulated extreme ultraviolet pulses. *Nature Communications* 11, 883 (2020).

[2] Wituschek, A., Kornilov, O., Witting, T., et al. Phase Cycling of Extreme Ultraviolet Pulse Sequences Generated in Rare Gases. *New Journal of Physics* 22, Nr. 9 (September 2020): 092001.

MO 15.11 Wed 16:30 P

A setup for extreme ultraviolet wave packet interferometry using tabletop high harmonic generation — ●SARANG DEV GANESHAMANDIRAM, FABIAN RICHTER, IANINA KOSSE, RONAK SHAH, LUKAS BRUDER, GIUSEPPE SANSONE, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Quantum interference techniques such as wave packet interferometry (WPI) in the extreme ultraviolet (XUV) regime set the basis for advanced nonlinear spectroscopy methods, such as multidimensional spectroscopy. These methods are however very difficult to implement at short wavelengths due to the required high phase stability and sensitivity. Recently, we have overcome these difficulties and have introduced a concept to implement such experiments with XUV free-electron lasers [1]. We are now developing a new setup optimized for seeding tabletop high-harmonic generation sources which is based on acousto-optic modulation of intense near infrared pulses. In the initial experiments, photons around 30 eV (19th harmonic) are generated and the effect of temporal and spatial dispersion were studied. Here, we will present the concept of the setup along with first characterization results. 1. A. Wituschek et al., Tracking attosecond electronic coherences using phase-manipulated extreme ultraviolet pulses, *Nature Communications*, 11:883 (2020).

MO 15.12 Wed 16:30 P

EUV absorption and recombination dynamics in atmospheric gas species — ●STEFFEN WOLTER¹, ERIK SCHMÖLTER², JENS BERDERMANN², and STEFAN LOCHBRUNNER¹ — ¹Institute of Physics, University of Rostock, 18051 Rostock, Germany — ²Department for Space Weather Impact, Institute for Solar-Terrestrial Physics, Kalkhorstweg 53, 17235 Neustrelitz, Germany

Ground- and space-based measurements show that the extreme ultraviolet (EUV) part of the solar spectrum changes continuously and can be very dynamic, especially during solar flares. The ionospheric plasma in the upper atmosphere is created by the absorption of this radiation and affected by the related variations. Therefore, exact knowledge of the ionization and recombination rates of the atmospheric gas species, mainly oxygen, nitrogen and their ions, is needed to model the ionospheric response to the EUV variations.

To this end, a high harmonic generation (HHG) setup driven by a femtosecond laser combined with an EUV spectrometer is applied to investigate the ionization cross-sections. The setup and first results for different gas species as well as the approach to measure recombination rates are presented in this contribution.

MO 15.13 Wed 16:30 P

Isosteric molecules in the time-domain — ●MAXIMILIAN POLLANKA, CHRISTIAN SCHRÖDER, PASCAL SCIGALLA, ANDREAS DUENSING, MICHAEL MITTERMAIR, and REINHARD KIENBERGER — Chair for laser and x-ray physics E11, Technische Universität München, Germany

In this work, we report on photoemission timing measurements performed on small isosteric molecules in the gas phase. By comparing the photoemission time delay between the respective σ and π orbitals in the valence band of CO₂ and N₂O we expect to find deeper insight in the characteristics of isosterism in the time-domain. Furthermore, the isoelectronicity of CO and N₂ is investigated in detail as a complementary study. Due to the similarities in molecular structure (isostericity) and electronic configurations (isoelectronicity), the pure effect of the specific element's characteristics is expected to be probed. The results regarding similarities and differences in photoemission dynamics in these molecules can serve as a stepping stone for gaining deeper insight into isosteric characteristics in these molecules and may bear the potential to draw conclusions from these simple systems to unknown

or unexplored isosteric molecular bonds in general.

Scattering calculations help us to gain a greater understanding of the correlations between molecular geometry and photoemission time and therefore the isosteric influence, with the focus on assessing the differences between modeling and experimental findings.

MO 15.14 Wed 16:30 P

Probing well aligned molecular environments on surfaces in the time-domain — ●PASCAL SCIGALLA, CHRISTIAN SCHRÖDER, PETER FEULNER, and REINHARD KIENBERGER — Chair for laser and x-ray physics, E11, Technische Universität München, Germany

We report on the photoemission timing measurements of well-aligned ethyl iodine molecules on a platinum crystal surface. The 4d photoemission of iodine is clocked against the Pt5p photoemission, allowing the extraction of an relative photemission delay. As the iodines photoemission in the chosen energy region stems from a giant resonance in the $I4d \rightarrow \epsilon f$ transition its photoemission time is mostly unaffected by its chemical environment. Thus any observed change in the photoemission delay can be attributed to changes in the traversed potential landscape of the molecule.

By carefully selecting the detection angle and coverage of the crystal we can reliably change which parts of the molecular potential landscape were traversed by the detected photoelectron wavepackets.

Complementary scattering simulations are then used in order to gain deeper insight into the observations in order to establish photoemission timing experiments as an efficient and accurate means to study molecular environments on surfaces.

MO 15.15 Wed 16:30 P

Strong-field effects on singly excited vibronic resonances in the hydrogen molecule — ●PAULA BARBER BELDA¹, GERGANA D. BORISOVA¹, DANIEL FAN¹, SHUYUAN HU¹, MAXIMILIAN HARTMANN¹, PAUL BIRK¹, ALEJANDRO SAENZ², CHRISTIAN OTT¹, and THOMAS PFEIFER¹ — ¹Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Studies of the hydrogen molecule and its interaction with ultrashort light pulses allow for the understanding of many quantum molecular phenomena in the simplest possible case of a molecule with only two nuclei and two electrons. In a transient absorption experiment with H₂ in the spectral range 13-17eV we drive transitions from the molecular ground state to the electronically excited B, C and D states. The included energy levels of the eigenstates of H₂ are calculated numerically, as well as the dipole matrix elements for the considered transitions. We observe intensity-dependent changes in the XUV absorption spectrum in the presence of moderately strong NIR field, coupling different excited states. In a few-level simulation, where we can consciously include and exclude states in the model system, we use numerically calculated energy levels of the eigenstates of H₂, as well as dipole matrix elements for the considered transitions. We aim to understand with it the importance of different couplings to the changing absorption lines and the corresponding time-dependent dipole we reconstruct from the measurement.

MO 15.16 Wed 16:30 P

Channel-Resolved Laser-Driven Electron Rescattering in the Molecular-Frame — ●FEDERICO BRANCHI¹, FELIX SCHELL¹, TILMANN EHRlich¹, MARK MERO¹, HORST ROTTKER¹, SERGUEI PATCHKOVSKII¹, VARUN MAKHJA², MARC J.J. VRAKING¹, and JOCHEN MIKOSCH¹ — ¹Max-Born-Institut, Berlin, Germany — ²University of Mary Washington, Fredericksburg, USA

A series of reaction microscope experiments on strong-field ionization and laser-driven electron rescattering of the asymmetric top molecule 1,3-butadiene is presented. Importantly, by virtue of the ion-electron coincidence detection, these experiments separate the ground-state (D₀) and first excited state (D₁) ionization channel. By analyzing coherent rotational wavepacket evolution we extract the polar and azimuthal angle-resolved molecular frame ionization and rescattering probability. By extracting the differential scattering cross section (DCS) for near- to mid-infrared wavelengths we explore the role of different continuum wavepackets for molecular structure determination. By measuring the ellipticity dependence of the return-energy dependent rescattering probability we explore the role of short versus long trajectories. A multi-faceted picture of molecular effects in strong-field ionization and laser-induced electron diffraction ensues.

MO 15.17 Wed 16:30 P

Experimental study of the laser-induced ionization of heavy metal and metalloid ions: Au⁺ and Si²⁺ — ●BO YING^{1,2,3}, FRANK MACHALETT^{1,2,3}, VANESSA HUTH¹, MATTHIAS KÜBEL^{1,2}, A MAX SAYLER^{1,2,4}, THOMAS STÖHLKER^{1,2,3}, GERHARD G PAULUS^{1,2,3}, and PHILIPP WUSTELT^{1,2} — ¹Institute of Optics and Quantum Electronics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany — ²Helmholtz Institute Jena, Fröbelstieg 3, 07743 Jena, Germany — ³GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany — ⁴Benedictine College, Atchison, KS 66002, USA

We implement a liquid metal ion source in a 3D coincidence momentum spectroscopy setup for studying the interaction of ionic targets with intense laser pulses. Laser intensities of up to 4×10^{16} W cm⁻² allow for the observation of up to ten-fold ionization of Au⁺-ions and double ionization of Si²⁺-ions. Further, by utilizing two-color sculpted laser fields to control the ionization process on the attosecond time scale, we demonstrate the capability to resolve the recoil ion momenta of heavy metal atoms. Simulations based on a semiclassical model assuming purely sequential ionization reproduce the experimental data well. This work opens up the use of a range of metallic and metalloid ions, which have hardly been investigated in strong-field laser physics so far.

MO 15.18 Wed 16:30 P

Design and implementation of XUV setup for time resolved photoelectron spectrometry — ●MARTA LUISA MURILLO-SÁNCHEZ, CONSTANTIN WALZ, DENNIS MAYER, and MARKUS GÜHR — Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Straße 24/25, 14476 Potsdam-Golm Germany

To investigate photoinduced ultrafast relaxation processes in gas phase isolated molecules, a tabletop setup for time-resolved photoelectron spectroscopy employing ultrashort extreme ultraviolet pulses (XUV) is currently under construction in the laboratory of the Experimental Quantum Physics group at Potsdam University. High-energy XUV pulses obtained by high order generation are achieved by focusing a fraction of the output pulses from an amplified laser system into a cell filled with a rare gas, under proper phase matching conditions. The odd frequency comb constituted by several harmonics is two-step filtered by a silicon wafer and an aluminium bandpass metallic filter to remove the residual infrared radiation. Afterwards, the beam is sent to a toroidal mirror to focus the beam. The different harmonics are spatially separated by a diffraction grating allowing to individually select them by means of a slit. This system for obtaining monochromatic XUV pulses is perhaps the simplest possible nevertheless compromising the optimum temporal duration of the pulses. Focused XUV laser pulses interact with an evaporated sample by an oven in the interaction region of a magnetic bottle spectrometer through which photoelectrons are detected with increased efficiency. XUV pulses can also be recombined with UV pulses in order to perform pump-probe experiments.

MO 15.19 Wed 16:30 P

Development of a glass based supersonic molecular beam source for organic molecules — ●BRENDAN WOUTERLOOD, SEBASTIAN HARTWEG, LUKAS BRUDER, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

Two-dimensional electronic spectroscopy (2DES) is a powerful spectroscopic tool which allows for the probing of atomic and molecular dynamics on ultra-fast timescales [1]. Application of this spectroscopic technique to polycyclic aromatic hydrocarbons (PAHs), such as acenes and porphyrins, promises a detailed understanding of their electronic structure and excited state dynamics. These electronic properties make some of these molecules interesting candidates for application in organic photovoltaics and motivate much past and present research [2]. One challenge of these studies has been the generation of high gas-phase target densities of these molecules due to their low vapour pressure and thermal decomposition by excessive heating.

In order to provide large target densities, since these molecules have relatively low vapour pressures, the supersonic nozzle will need to be heated to around 500°C. A quartz glass nozzle system will thus be developed in order to allow us to heat the molecules to these high temperatures while minimising the risk of thermal decomposition of the sample that can be catalysed by hot metal surfaces. We will present the nozzle design and initial characterisation results.

[1] L. Bruder et al., Nat Commun 9, 4823 (2018).

[2] O. Ostroverkhova, Chemical Reviews 116 (22), 13279-13412 (2016).

MO 15.20 Wed 16:30 P

Setup Of A Spectrometer To Detect Raman Optical Activity — •KLAUS HOFMANN — Universität Würzburg, Institut für Physikalische und Theoretische Chemie

A custom-built Raman spectrometer was modified to detect Raman optical activity (ROA), a type of vibrational circular dichroism. A modulation scheme was implemented to repeatedly convert linear to right and left circular polarized light for excitation. Python was used to automate the experiment, data acquisition and post-processing. Experimental challenges and their influences on the resulting ROA signal as well as the margins of error are presented. The recorded ROA spectrum of (-)- α -pinene was acquired by subtracting the spectra of both enantiomers and shows good agreement with literature.

MO 15.21 Wed 16:30 P

Towards laser ionisation of H-atoms for kinematically complete coincidence imaging of ion-molecule reactions — •FLORIAN TRUMMER, DASARATH SWARAJ, TIM MICHAELSEN, ARNAB KHAN, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria

Crossed-beam velocity map imaging (VMI) has proven to be a powerful tool to gain insight into atomistic reaction mechanisms [1-3]. Here we will present concepts and simulations for a new experimental setup that uses coincidence detection of reaction products for a kinematically complete VMI study of certain reaction types, involving neutral hydrogen products. Instead of solely detecting the charged initial product of the reactive encounter, a high power and high repetition rate Lyman-alpha source in combination with a UV laser will be used to ionise the neutral H-atoms, which are a product of the chemical reactions under study (e.g., $O^- + H_2 \rightarrow OH^- + H$). We will present the planned laser setup for our upcoming project which is currently under construction. The search for quantum resonances in vibrational state-resolved spectroscopic studies of ion-neutral reactions is among the goals that shall be explored in the future.

[1] R. Wester, *Phys. Chem. Chem. Phys.* 16, 396 (2014)

[2] M. Stei *et al.*, *Nature Chemistry* 8.2, 151-156 (2016)

[3] T. Michaelsen *et al.*, *J. Phys. Chem. Lett.* 11.11, 4331-4336 (2020)

MO 15.22 Wed 16:30 P

eCOMO - A new endstation for controlled molecule experiments — •WUWEI JIN¹, SEBASTIAN TRIPPEL^{1,3}, HUBERTUS BROMBERGER^{1,3}, TOBIAS RÖHLING¹, KAROL DLUGOLECKI¹, SERGEY

RYABCHUK¹, ERIK MÄNSSON¹, ANDREA TRABATTONI¹, VINCENT WANIE¹, IVO VINKLÁREK⁴, FRANCESCA CALEGARI¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg — ²Department of Physics, Universität Hamburg — ³Center for Ultrafast Imaging, Universität Hamburg — ⁴Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

We present details on our newly established transportable endstation eCOMO (Endstation for Controlled Molecules) for investigating the dynamics of small molecules in the gas phase [1]. The endstation consists of three main parts: 1) An Even-Lavie-valve-based gas source. 2) An electrostatic deflector for the generation of pure molecular samples [2-3]. 3) A double-sided VMI spectrometer coupled with two time- and position-sensitive Timepix3 cameras and the PymePix software [4-5]. We found a novel damped oscillation dynamics in the UV-IR (pulse duration are both 6 fs) ionization dynamics of carbonyl sulfide (OCS).

[1] M. Johny, J. Onvlee, *et al.*, *Chem. Phys. Lett.*, **721**, 149 (2019)

[2] S. Trippel, M. Johny, *et al.*, *Rev. Sci. Instrum.*, **89**, 096110 (2018)

[3] Y. P. Chang, D. A. Horke, *et al.*, *Int. Rev. Phys. Chem.*, **557**, 34 (2015)

[4] A. F. Al-Refaie, M. Johny, *et al.*, *J. Instrum.*, **14**, P10003 (2019)

[5] A. Zhao, M. van Beuzekom, *et al.*, *Rev. Sci. Instrum.*, **88**, 113104 (2017)

MO 15.23 Wed 16:30 P

Optical Imaging and Tracking of Single Molecules in Ultrahigh Vacuum — •TIANYU FANG, FLORIAN ELSÉN, NICK VOGELÉY, and DAQING WANG — Institute of Physics, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Molecule-surface interaction is key to many physical and chemical processes at interfaces. Here, we show that the dynamics of single molecules on a surface under ultrahigh vacuum can be resolved using fluorescence imaging. By adapting oil-immersion microscopy to a thin vacuum window, we measure the surface adsorption and translational and rotational diffusion of single perylene molecules on a fused silica surface with high spatial and temporal resolutions. Time-dependent measurements of the fluorescence signal allow us to deduce two characteristic decay time scales, which can be explained through a simplified model involving two adsorption states and five energy levels. The system presented in this work combines fluorescence imaging with essential ingredients for surface science and promises a platform for probing single-molecule-surface interactions in highly defined conditions.