

## MO 20: Poster – Molecular Spectroscopy and Dynamics

Time: Wednesday 17:00–19:00

Location: Tent

MO 20.1 Wed 17:00 Tent

**Auger electron spectroscopy of isothiocyanic acid, HNCS** — ●DOROTHEE SCHAFFNER<sup>1</sup>, MARIUS GERLACH<sup>1</sup>, EMIL KARAEV<sup>1</sup>, JOHN BOZEK<sup>2</sup>, INGO FISCHER<sup>1</sup>, and REINHOLD FINK<sup>3</sup> — <sup>1</sup>University of Würzburg, Germany — <sup>2</sup>Synchrotron SOLEIL, Saint-Aubin, France — <sup>3</sup>University of Tübingen, Germany

Isothiocyanic acid, HNCS, is the simplest isothiocyanate and a molecule of astrochemical interest. In 1979 it was first detected in the interstellar medium towards the molecular cloud Sgr B2(OH).<sup>[1]</sup> The detection of HNCS in space is intriguing due to its composition of biogenic elements. Its oxygen analogue isocyanic acid, HNCO, is a well-known astrochemical molecule for which a prebiotic role was suggested.<sup>[2]</sup> Investigating the interaction of HNCS with X-ray radiation is critical to understanding its fate in space.

Here we present the gas phase Auger electron spectra of the reactive molecule isothiocyanic acid that were recorded at the PLEIADES beamline at the synchrotron SOLEIL. X-ray photoelectron and NEX-AFS spectra were obtained and the normal and resonant Auger-Meitner processes were studied at the N1s, C1s and S2p edge. We compare our spectra to the previously recorded spectra of isocyanic acid as well as to theoretical simulations in order to give further insights into the observed transitions and the influence of heavy atom substitution on Auger electron spectra.

[1] M. A. Frerking *et al.*, *Astrophys. J.* **1979**, 234, L143-L145.

[2] E. Mendoza *et al.*, *Mon. Not. R. Astron. Soc.* **2014**, 445, 151-161.

MO 20.2 Wed 17:00 Tent

**Towards laser spectroscopy of highly excited states of H<sub>3</sub><sup>+</sup>** — ●MARLEEN MAXTON, LUKAS BERGER, FLORIAN GRUSSIE, OLDŘICH NOVOTNÝ, VIVIANE C. SCHMIDT, AIGARS ZNOTINS, and HÖLGER KRECKEL — Max-Planck-Institut für Kernphysik, Heidelberg

The H<sub>3</sub><sup>+</sup> ion is the simplest polyatomic molecule. Apart from being an important benchmark for theoretical calculations, H<sub>3</sub><sup>+</sup> is one of the main drivers of astrochemistry in dilute interstellar clouds. Despite the structural simplicity of H<sub>3</sub><sup>+</sup>, its spectrum at higher excitation remains largely unexplored, with the highest reported transition occurring at around 16 500 cm<sup>-1</sup> with respect to the ground state, less than halfway from the dissociation energy of 35 000 cm<sup>-1</sup>. To extend the reach of laser spectroscopy beyond previous limits, a concept for a multi-color spectroscopy scheme was proposed [1]. In this approach, highly excited states are populated from the lowest ground states via long-lived metastable intermediates in a two-step laser excitation process, followed by UV photodissociation. For such studies, the Cryogenic Storage Ring (CSR) at the Max-Planck-Institut für Kernphysik provides an ideal platform, combining long storage times for intermediate state population with highly sensitive detection of the dissociation products in an almost background free cryogenic environment. A rotationally cold molecular ion beam is produced by a supersonic expansion source, stored in the CSR and probed for extended periods of time. Currently, the first excitation step is being implemented at the CSR, with plans to realize the full spectroscopy scheme in the future.

[1] Znotins *et al.*, *J. Mol. Spectrosc.* **378**, 111476 (2021)

MO 20.3 Wed 17:00 Tent

**A new setup for Free Electron Laser based photoelectron spectroscopy** — ●NISHITHA LAKHANPAL, KARIMAN ELSHIMI, BERND VON ISSENDORFF, and FABIAN BÄR — University of Freiburg

The development of intense light sources in the XUV and X-ray ranges opens new avenues for the study of free clusters and nanoparticles. A new setup for photoelectron spectroscopy is currently under construction to investigate size-selected, deeply cold clusters, with a focus on characterizing ultrafast electronic processes. This setup will enable the exploitation of the vast potential of FELs in photoelectron spectroscopy. Several components, such as the magnetic bottle photoelectron spectrometer, cluster source, and specialized ion optics, are already in place. Additional components, including a QMS, deflector, and ion trap, are still under development.

[1] Bär, F. High-resolution photoelectron spectroscopy on cold metal clusters (Albert-Ludwigs-Universität Freiburg, 2023); <https://doi.org/10.6094/UNIFR/237632>

MO 20.4 Wed 17:00 Tent

**Interaction of nitro-compounds with asymmetric ( $\omega/2\omega$ ) fs laser fields** — ●PANAGIOTIS VAMVAKIDIS and CONSTANTINE KOSMIDIS — Department of Physics, University of Ioannina, Ioannina 45110, Greece

The focus of our work is to deepen our understanding and, potentially, control the processes of molecular bond rearrangement using asymmetric femtosecond (fs) laser beams. These processes may lead to isomerization and therefore to a change in molecular properties. The studied nitro-compounds have attracted research interest for many years because they are energetic molecules which contribute significantly to "brown carbon" and are also important in biological, pharmaceutical and pesticide applications [1], [2]. Of particular interest is their isomerization processes from nitro (-NO<sub>2</sub>) to nitrite (-ONO) structure.

The asymmetric  $\omega/2\omega$  fs laser fields are created by spatial and temporal overlapping of the  $\omega$  ( $800 \leq \lambda \leq 2000$  nm) frequency beam with its second harmonic ( $2\omega$ ) ( $400 \leq \lambda \leq 1000$  nm) [3]. Interest in this interaction stems from the presence of charge-transfer electronic states within nitro-compounds. By varying the relative phase of the two pulses we can change the shape of the asymmetric field and thus control the distribution of the electronic cloud on the molecular skeleton which offers the ability to (possibly) manipulate their isomerization.

[1] J. M. Shusterman *et al.* *J. Phys. Chem. A*, (2022)

[2] A. D. Tasker *et al.* *J. Phys. Chem. A*, (2002)

[3] E. Kechaoglou *et al.* *J. Chem. Phys.*, (2021)

MO 20.5 Wed 17:00 Tent

**Investigating Photoinduced Dynamics of a 1,4-Azaborine with Time-Resolved X-ray Spectroscopy** — ●KATHARINA THEIL<sup>1</sup>, INGO FISCHER<sup>1</sup>, JONAS FACKELMAYER<sup>1</sup>, MERLIN HESS<sup>1</sup>, HÖLGER BRAUNSCHWEIG<sup>1</sup>, CONSTANT SCHOUDER<sup>2</sup>, DENNIS MAYER<sup>3</sup>, FABIANO LEVER<sup>3</sup>, XIAOJUN WANG<sup>3</sup>, RUI PAN<sup>3</sup>, ULRIKE FRÜHLING<sup>3</sup>, CHRISTINA PAPADOPOULOU<sup>3</sup>, MARKUS GÜHR<sup>3</sup>, XINCHENG MIAO<sup>1</sup>, SIMONE VEGLIANTI<sup>1</sup>, and ROLAND MITTRIC<sup>1</sup> — <sup>1</sup>University of Würzburg, Germany — <sup>2</sup>ISMO, ParisSaclay University, France — <sup>3</sup>DESY, Hamburg, Germany

Azaborines are molecules containing boron and nitrogen, offering unique electronic properties by replacing carbon bonds in organic compounds. This makes them promising for energy and electronic applications, such as optoelectronics and singlet fission materials. In this study, the ultrafast dynamics of the non-commercial 1,4-di-tert-butyl-azaborine were studied using time-resolved X-ray photoelectron spectroscopy. Experiments at FLASH2 at DESY used a pump-probe setup to investigate boron-specific electronic changes after UV excitation. Key processes, including fast relaxation via a conical intersection and slower long-term dynamics, were observed. Supported by static theoretical calculations and quantum dynamic simulations, the study provided insights into excitation energies, long-lived reaction products, and detailed relaxation pathways. These findings highlight the potential of 1,4-azaborines as versatile building blocks for optoelectronic materials, where understanding ultrafast dynamics is key to optimizing performance.

MO 20.6 Wed 17:00 Tent

**Detailed investigation of unexpected photoelectron spectra via angle-resolved spectroscopy of Gold clusters** — ●STEVE TAKOUAN TCHOUNGA, LUCAS WEISE, and BERND VON ISSENDORFF — Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany

Angle-resolved spectroscopy provides an important test of the theoretical description of clusters since these spectra carry more information than the bare electron binding energies. Specifically, the anisotropy of photoelectron spectra depends on the angular momentum state [1]. In the experiment cluster anions are produced in a magnetron sputter source, cooled to 7K, and enter a time-of-flight spectrometer for mass selection. Electrons are then detached by linear polarised laser light and projected onto an MCP detector in a velocity map imaging setup.

The presented analysis utilizes the additional information from angle-resolved spectroscopy to gain a better understanding of the electronic structure of the cluster. For Au<sub>33</sub><sup>-</sup> an electronic shell closing is expected, leading to the opening of a new shell for Au<sub>34</sub><sup>-</sup>. The angular momentum character of this new shell is not in accordance with

a simple shell model. It also differs from the mixed character as observed for Sodium clusters of the same size [2]. Possible influences of the high-lying d-band are discussed.

[1] A. Piechaczek, C. Bartels, C. Hock, J.-M. Rost, and B. v. Issendorff, *Phys. Rev. Lett.* (2021), 126.

[2] C. Bartels, C. Hock, R. Kuhnen, M. Walter, and B. v. Issendorff, *Phys. Rev. A* (2013), 88.

MO 20.7 Wed 17:00 Tent

**Photoelectron spectroscopy study of cold anthracene anions in gas phase** — ●KEVIN SCHWARZ and BERND VON ISSENDORFF — Institute of Physics, University of Freiburg, Hermann- Herder-Str. 3, 79104 Freiburg, Germany

Organic semiconductors like anthracene ( $C_{14}H_{10}$ ) show interesting properties and keep being of interest across science and technology. In modified form they are used, for instance, in organic solar cells. To get a better understanding of these molecules, they are investigated in the gas phase by anion photoelectron spectroscopy (PES), providing insight into the vibrational modes of the electronic ground state and different electronically excited states of the neutral molecule as well as into electronic relaxation processes within the anion. As published previously [1], the photoelectron spectra exhibit strong photon energy-dependent changes in the vibrational excitation of the molecule. These changes result from photoemission via autodetaching excited states of the anion. Seven of eight different identified electronic excitations correspond to resonances of the anthracene anion known from absorption spectroscopy [2]. Recently, a cryogenic radio frequency hexapole ion trap was added to the device, with the goal to study the temperature dependence of the observed ultrafast relaxation processes. New results will be presented.

[1] A. Jalehdoust, B. von Issendorff, *J. Chem. Phys.* 158: 194302 (2023). DOI: <https://doi.org/10.1063/5.0145038>

[2] T. Shida and S. Iwata, *J. Chem. Phys.* 56: 2858-2864 (1972). DOI: <https://doi.org/10.1063/1.1677618>

MO 20.8 Wed 17:00 Tent

**Time-resolved Imaging of CH<sub>4</sub> Fragmentation in Strong Laser Fields** — ●NIKOLAS RAPP, WEIYU ZHANG, THOMAS PFEIFER, and ROBERT MOSHAMMER — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

With a Reaction Microscope (ReMi) [1] the ionization and dissociation dynamics of methane in strong laser fields were studied in a series of pump-probe experiments. For the creation of temporally separated laser pulses and pulse shaping a spatial light modulator (SLM) was used. It allows the control of laser pulses in terms of amplitude, polarization, and phase [2, 3]. By employing the SLM technique, we successfully compressed the laser pulses to below 10 fs and achieved a precise control over the time-delay between the two pulses. Upon strong-field ionization the molecule undergoes fragmentation and Coulomb explosion (CE) and the corresponding charged fragments are collected with the ReMi. For example, in the case of CE the initial inter-nuclear distances can be determined via the measurement of final kinetic energies, and in pump-probe measurements the evolution of the molecular geometry is visualized as function of time. Selected results will be presented and discussed.

References:

[1] J. Ullrich et al., 2003, *Rep. Prog. Phys.* 66, 1463-1545

[2] Stefanie Kerbstadt, 2016, MA thesis. Universität Oldenburg

[3] T Brixner and G Gerber, 2001, *Opt. Lett.* 26,557-559

MO 20.9 Wed 17:00 Tent

**In search for superconductivity in Niobium clusters** — ●MAZIYAR KAZMEI and BERND VON ISSENDORFF — Physikalisches Institut Universität Freiburg

Among the superconducting materials, Nb stands out due to its high critical temperature and is often used as a model system, to investigate superconductivity-related physics. The question arises at what size Nb clusters will exhibit properties related to superconductivity, namely Cooper pair formation. Some hints for this to happen already at small sizes have been found by de Heer and coworkers [1]. We have measured photoelectron spectroscopy of size -selected Nb clusters in similar size ranges, with temperatures between 3.9-50 K in the gas phase, employing a recently developed photoelectron magnetic bottle spectrometer with a resolution of  $\Delta E/E = 0.2\%$ . Vibrationally resolved spectra have been obtained for several sizes, but no direct evidence for unusual temperature effects yet.

MO 20.10 Wed 17:00 Tent

**Toward understanding ultrafast dynamics of uracil and uraci-water clusters** — ●ADITI PRADHAN<sup>1,2</sup>, IVO S. VINKLÁREK<sup>1</sup>, HUBERTUS BROMBERGER<sup>1</sup>, SEBASTIAN TRIPPEL<sup>1,3</sup>, and JOCHEN KÜPPER<sup>1,2,3</sup> — <sup>1</sup>Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — <sup>2</sup>Department of Chemistry, Universität Hamburg, Germany — <sup>3</sup>The Hamburg Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

The solute-solvent interactions in biomolecule-water clusters remain underexplored at ultrafast timescales with atomic scale precision. Studying solvated clusters at the same level of detail as single isolated molecules is a significant challenge. We propose a bottom-up approach to tackle this. The versatile transportable endstation for controlled molecule (eCOMO) [1] employs the electrostatic deflector in combination with velocity map imaging to study clusters in a size-selected fashion [2]. Examining systems with multiple water molecules attached to the building blocks of life, we aim to advance the understanding of ubiquitous interactions like hydrogen bonding. Preliminary experiments on uracil-water clusters reveal interesting dynamics following strong-field ionization. Further UV-photoinduced dynamics of these important model systems will be studied using short-pulse laser sources as well as short-wavelength facilities.

[1] Jin *et int.* (8 authors), Küpper, arXiv:2406.16491 [physics]

[2] Chang *et int.* (2 authors), Küpper, *Int. Rev. Phys. Chem.*, **34**, 1077838 (2015) arXiv:1505.05632 [physics]

MO 20.11 Wed 17:00 Tent

**Towards Unravelling Solvation Dynamics: From Isolated Molecules to Micro-Hydrated Environments** — ●DEEPAK K. PANDEY<sup>1</sup>, LILIANA M. RAMOS MORENO<sup>1</sup>, CLAUS-PETER SCHULZ<sup>2</sup>, and JOCHEN MIKOSCH<sup>1</sup> — <sup>1</sup>Institut für Physik, Universität Kassel, Kassel, Germany — <sup>2</sup>Max Born Institute (MBI), Berlin, Germany

Exploring the behavior of micro-solvated molecules is vital for bridging our understanding of isolated molecules in bulk-liquid environments. Through the gradual addition of water molecules one at a time, our research explores the effects of solvation on neutral molecules. We employ Photoelectron Photoion Coincidence (PEPICO) spectroscopy to investigate both the static and dynamic effects of solvation. Our experimental setup at the University of Kassel employs a water cluster technique to systematically investigate how micro-hydration affects molecular behavior. Using ultrafast pump-probe experiments, this technique enables us to investigate how solvation affects photochemical processes such as photodissociation and photo-induced isomerization. In the past year, we have achieved coincidence measurements with our PEPICO spectrometer, making significant progress in characterizing our water cluster source. With the goal to gain greater insight into the dynamics of micro-hydrated chiral molecules, we intend to include the time-resolved Photoelectron Circular Dichroism (PECD) investigations in the future. Our poster emphasizes on the experimental methodology, analysis of the water cluster source and spectrometer, and progress made in experimental techniques for investigating the molecular dynamics of chemical processes.

MO 20.12 Wed 17:00 Tent

**Dynamics of the activation of small molecules by zirconium cations in the gas phase** — ●BORIS HEEB, MARCEL META, and JENNIFER MEYER — RPTU Kaiserslautern-Landau, Fachbereich Chemie und Landesforschungszentrum OPTIMAS, Kaiserslautern, Germany

The reaction of  $Zr^+$  with  $CH_4$  in the gas phase proceeds efficiently to the carbene  $ZrCH_2^+$  at room temperature with a two-state reactivity along the reaction coordinate [1]. To investigate the bond activation of  $CH_4$  by  $Zr^+$ , energy and angle differential cross sections were recorded by crossed-beam velocity map imaging. The product ion velocity distribution is dominated by signatures of indirect dynamics commonly associated to a small impact parameter. Additional scattering events outside the kinematic limits are found, which largely disappear when switching to  $CD_4$ . A comparison with the reactions  $Ta^+ + CH_4$  and  $Ta^+ + CD_4$  show almost identical energy and angular distributions [2]. Continuing experiments with 1-butene show three product channels, whereby a mainly forward-scattered distribution is observed for the loss of  $H_2$ , which supports the considerations.

MO 20.13 Wed 17:00 Tent

**Photofragmentation studies of cold deoxyadenosine monophosphate (dAMP) anions** — ●MIRIAM WESTERMEIER, CHRISTIAN SPRENGER, SAMUEL WHITE, ERIC ENDRES, and ROLAND

WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria

dAMP is a nucleotide which makes up one part of the DNA. It is likely involved in the mutation of genes, if the dAMP is wrongly incorporated into the DNA. Such a mutation could occur when a G to T (guanine to thymine) transversion happens. [1] dAMP consists of a sugar group, a phosphate group and the nucleobase adenine. The phosphate and the sugar form the phosphate-sugar-backbone of a DNA strand. The adenine in this case can form a hydrogen bond with a nucleobase of the second strand. It is possible to fragment the dAMP with ultraviolet light, but the absolute cross-section of this interaction is still unknown. Also the dependence of the fragment branching ratio on the dissociation wavelength is of interest. With our setup, consisting of an electrospray ionization source, an octupole, a quadrupole coupled to a cryogenic 16-pole wire ion-trap and a time-of-flight mass spectrometer, we are studying the absolute cross section of the photofragmentation, and carry out a wavelength scan as well as study the dependence of the fragment yield on the wavelength.

[1] Piette J., Biological consequences associated with DNA oxidation mediated by singlet oxygen. *J. Photochem. Photobiol. B*, 11, 241 (1991)

MO 20.14 Wed 17:00 Tent

**Probing De-excitation and Vibrational Re-Distribution Processes in Jet-Cooled N<sub>2</sub>O Using a Combination of cw-Infrared and Microwave Chirped Pulse Technique** — ●JONAS BOSMANN, FABIAN PETERS, JAN WENSKE, GUIDO FUCHS, and THOMAS GIESEN — Institute of Physics, University of Kassel, Germany

Chirped pulse Fourier transform spectroscopy (CP-FT) is a sensitive and nowadays widely used method for recording gas phase spectra of molecules in the microwave (MW) and millimeter wave (mmW) range. Here, we present CP-FT supersonic beam measurements of N<sub>2</sub>O, state selectively excited by an infrared continuous wave (cw) optical parametric oscillator (OPO). The CP-FT signal of the  $J = 4 \leftarrow 3$  transition around 100 GHz was used to study the relaxation of vibrationally excited N<sub>2</sub>O into different vibrational levels of lower energy. Since this is to our knowledge the first CP-MW study that uses cw-laser excitation, we investigated the strength of the FID signal as a function of the infrared laser power. The collision-induced redistribution of pure rotational levels in vibrationally states and the redistribution of vibrational energy were investigated in two different jet environments, for which a slit nozzle of high collision rates and a pin-hole nozzle of low collision rates in the jet expansion were used.

MO 20.15 Wed 17:00 Tent

**3D Time Resolved Photoelectron Spectroscopy on Carbondisulfide** — ●MARVIN KRUPP<sup>1</sup>, SCOTT GOUDREAU<sup>2</sup>, ANDREY BOGUSLAVSKIY<sup>2</sup>, JEAN-LUC BÉGIN<sup>2</sup>, and ALBERT STOLOW<sup>2</sup> — <sup>1</sup>Institute of Physics, University of Rostock, 18059 Rostock, Germany — <sup>2</sup>Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada

Time-resolved photoelectron spectroscopy (TRPES) is a versatile probe of ultrafast dynamics in molecules and has been widely used in recent years to study non-adiabatic dynamics in numerous systems. Here, the 2D photoelectron velocity map imaging (VMI) technique is commonly employed in gas-phase molecular spectroscopy and dynamics investigations due to its ability to efficiently extract photoelectron spectra and angular distributions in a single experiment. However, the standard technique is limited to specific light-source polarization geometries. This has led to significant interest in the development of 3D VMI techniques, which are capable of measuring individual electron positions and arrival times, obtaining the full 3D distribution without the need for inversion, forward-convolution, or tomographic reconstruction approaches. Time resolved photoelectron spectra of the  $^1B_2(^1\Sigma_u^+)$ -state of CS<sub>2</sub> at pump wavelengths in the region of 200 nm have been previously studied and indicate that the lifetime of the decay is dependent on the relative laser polarisation geometry. In this work, we present the first results employing the new 3D VMI technique on CS<sub>2</sub> and comparing it with the previous 2D VMI study.

MO 20.16 Wed 17:00 Tent

**Imaging thermal-energy chemical dynamics of a solvated (bio)molecular complex system** — ●MUKHTAR SINGH<sup>1,2,3</sup>, MATTHEW SCOTT ROBINSON<sup>1,2,3</sup>, HUBERTUS BROMBERGER<sup>1,2</sup>, SEBASTIAN TRIPPEL<sup>1,2</sup>, and JOCHEN KÜPPER<sup>1,2,3</sup> — <sup>1</sup>Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — <sup>2</sup>Center for Ultrafast Imaging, Universität Ham-

burg — <sup>3</sup>Department of Physics, Universität Hamburg

We present the imaging of ultrafast thermal-energy-induced chemical dynamics of a micro-solvated indole-water molecular complex probed with a time-dependent strong field ionization and ion mass spectrometry [1]. We produce a pure gas-phase indole-water sample using a combination of a cold molecular beam and the electrostatic deflector [2]. Employing a 2.9 μm mid-IR pump to excite the N-H and C-H vibrational modes induced dynamics between the indole and water moieties.[3]. The dissociation of the micro-solvated system was monitored using strong-field multi-photon ionization by 1.3 μm wavelength light from a femtosecond pulsed laser, tracking the time-dependent ion signals of the intact indole-water cluster as well as the individual indole and water ionic products.

[1] J. Onvlee, *et al.*, *Nat. Commun.* **13**, 7462 (2022).

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

[3] M.S. Robinson, *et al.*, *Phys. Chem. Chem. Phys.* (2023).

MO 20.17 Wed 17:00 Tent

**UV photo-induced dissociation dynamics of solvated (bio)molecular complex system** — ●MUKHTAR SINGH<sup>1,2,3</sup>, MATTHEW SCOTT ROBINSON<sup>1,2,3</sup>, HUBERTUS BROMBERGER<sup>1,2</sup>, SEBASTIAN TRIPPEL<sup>1,2</sup>, and JOCHEN KÜPPER<sup>1,2,3</sup> — <sup>1</sup>Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg — <sup>2</sup>Center for Ultrafast Imaging, Universität Hamburg — <sup>3</sup>Department of Physics, Universität Hamburg

We present the investigation of ultrafast chemical dynamics induced by UV excitation in a micro-solvated indole-water-complex system probed by time-dependent strong-field ionization and ion mass spectroscopy [1]. Indole-water is important due to indole's role as the chromophore of tryptophan, the strongest near UV absorber in proteins. The experimental setup contains a molecular beam and the electrostatic deflector to produce a pure gas-phase sample of indole-water [2]. We conducted a UV-IR pump-probe experiment, which excited the system to the electronic excited state using 270 nm light. The dissociation dynamics of the system was monitored using strong-field multiphoton ionization by 1.3 μm wavelength light from a femtosecond laser, tracking the time-dependent ion signals of the indole and indole-water ions and electrons.

[1] J. Onvlee, *et al.*, *Nat. Commun.* **13**, 7462 (2022).

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

MO 20.18 Wed 17:00 Tent

**Simplifying rotational spectra: A broadband double resonance approach in millimeter wave spectroscopy** — ●PRACHI MISRA, LUIS BONAH, MARIYAM FATIMA, and STEPHAN SCHLEMMER — I. Physikalisches Institut, Universität zu Köln, Köln, Germany

Rotational spectroscopy is an important technique for understanding molecular structures, as rotational constants are directly linked to the molecular mass distribution and interatomic distances. In Cologne, high-resolution rotational spectra are measured using Chirped-Pulse Fourier Transform (CP-FT) spectroscopy<sup>1</sup> in gas phase.

Analyzing rotational spectra for complex molecules is often complicated by weak features arising from low-lying vibrationally excited states, hyperfine splitting, and internal rotation. To address these challenges, the well-established technique double-resonance spectroscopy is employed. This method uses a probe radiation source to record spectra while a pump source modifies specific transitions due to the Autler-Townes effect. By identifying the connected transitions we can piece together the energy term diagram experimentally. This technique has previously been implemented using absorption spectroscopy<sup>2</sup>, and is now adapted for use with CP-FT spectroscopy allowing for broadband coverage, eliminating the need for frequency-by-frequency scanning of both the pump and probe radiation sources. Proof-of-concept experiments conducted in the 75-110 GHz range using a new signal generation and acquisition board on the CP-FT spectrometer<sup>3</sup> are presented.

1. Park,G.B.(2016)*J.Chem.Phys.*,144(20) 2. Zingsheim,O.(2021)*J. Mol.Spectrosc.*,381,111519 3. Hermanns,M.,(2023)*Rev.Sci.Inst.*,94(3)

MO 20.19 Wed 17:00 Tent

**Investigation of the interaction between organic dopants and a helium nanodroplet environment with time-resolved photoelectron spectroscopy** — ●LEONIE WERNER, ULRICH BANGERT, SEBASTIAN HARTWEG, YILIN LI, ARNE MORLOK, FELIX RIEDEL, FRANK STIENKEMEIER, and LUKAS BRÜDER — University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg im Breisgau, Germany

Embedding molecules in ultracold helium nanodroplets allows us to study molecular processes in a superfluid environment [1]. Here, we apply time-resolved photoelectron spectroscopy to study the dynamics of dopants embedded in helium nanodroplets. Droplet size-dependent photoelectron spectra [2] have been established as an appropriate technique for studying interactions between organic dopants and the helium environment. Probing helium droplets doped with selected organic molecules, we present a systematic study of the evaporation and ejection dynamics upon laser excitation. Both phenomena have been observed previously in helium nanodroplets for different dopants [1,3,4]. First results will be presented, in particular on ultrafast internal conversion in tetracene.

[1] Toennies, J.P. and Vilesov, A. F. (2004), *Angew. Chem.*

In. Ed. 43(20): 2622-2648

[2] Loginov, E. et al. (2005), *Phys. Rev. Lett.* 95(16): 163401

[3] Thaler, B. et al. (2018), *Nat. Commun.* 9(1): 4006

[4] Meyer, M. et al. (2019), *EPJ Web Conf.* 205: 06005

MO 20.20 Wed 17:00 Tent

**Photodissociation dynamics of the bromomethyl radical** —

•LILITH WOHLFART, CHRISTIAN MATTHAEI, and INGO FISCHER — JMU Würzburg, Germany

Bromomethyl belongs to the class of organic halogen radicals. Therefore, it can potentially influence the atmosphere by reacting with the ozone layer and causing its depletion similar to HCFCs. The photoionization of bromomethyl was already investigated by several groups, including Steinbauer and coworkers. They determined the ionization energy and structure with VUV synchrotron radiation and investigated the dissociative photoionization. To obtain further insights into the dissociation of bromomethyl, we analyzed the fragments of the radical using velocity map imaging (VMI).

$\text{CH}_2\text{Br-NO}_2$  was used as a precursor for the halogenated methyl radical, because the weaker C- $\text{NO}_2$  bond can be cleaved through pyrolysis. Subsequently, laser light in the UV region was deployed to dissociate the formed  $\text{CH}_2\text{Br}$  radical. The major dissociation pathway gave the methylene and bromine fragments which were detected with SPI and REMPI respectively. With velocity map ion imaging, the translational kinetic energy distribution of the photofragments was determined. The recorded images of the bromine and methylene photofragments showed an anisotropic distribution, implying a direct dissociation.

MO 20.21 Wed 17:00 Tent

**Generation of long-lived triplet-triplet multiexciton in Pentacene-(Tetracene)2-Pentacene intramolecular singlet fission compound - the theoretical perspective.** — •ARIFA NAZIR<sup>1</sup>, ALOK SHUKLA<sup>2</sup>, and SUMIT MAZUMDAR<sup>3</sup> — <sup>1</sup>Indian Institute of Technology Bombay — <sup>2</sup>Indian Institute of Technology Bombay —

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Singlet fission (SF) is a spin-allowed conversion of the optical singlet exciton of an organic semiconductor to the optically dark triplet-triplet  $^1(\text{T}_1\text{T}_1)$ . In chromophores with small triplet-triplet binding energy  $^1(\text{T}_1\text{T}_1)$  can separate into two free triplets  $\text{T}_1$ , each of which can donate an electron to an acceptor, thereby doubling the photoconductivity of an organic solar cell. Successful implementation of SF requires both ultrafast generation of the  $^1(\text{T}_1\text{T}_1)$  and rapid dissociation into free triplets, which is a challenge, as the former requires strong coupling between the triplets, which implies strong  $^1(\text{T}_1\text{T}_1)$  binding energy. Pun et al. synthesized a series of oligomers Pentacene-(Tetracene) $n$ -Pentacene, P $n$ T $n$ P, in which rapid generation of pentacene-tetracene triplet-triplet  $^1(\text{T}_{1[\text{P}]}\text{T}_{1[\text{T}]})$  is followed by rapid triplet separation to long-lived pentacene-pentacene triplet-triplet  $^1(\text{T}_{1[\text{P}]}\text{T}_{1[\text{P}]})$  [1]. We present the results of many-body investigations of the electronic structures of the optical singlet and low-energy triplet-triplets in PT2P that find distinct  $^1(\text{T}_{1[\text{P}]}\text{T}_{1[\text{T}]})$  and  $^1(\text{T}_{1[\text{P}]}\text{T}_{1[\text{P}]})$ . We also report the ground and excited state absorptions that clarify triplet-triplet generation and triplet separation mechanisms. [1] A. B. Pun et al., *Nat. Chem.* 11, 821 (2019).

MO 20.22 Wed 17:00 Tent

**Coulomb explosion imaging of molecular photoswitches** —

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We present an X-ray Coulomb explosion imaging (CEI) investigation into the photofragmentation and photochemistry of trans-4,4'-difluoroazobenzene (DFAB) using the COLTRIMS Reaction Microscope at the SQS station of the European XFEL. We show a systematic analysis of X-ray-induced fragmentation in DFAB, employing covariance techniques to explore fragmentation dynamics. We then report time-resolved measurements of DFAB excited to its first electronic excited state ( $S_1$ ) under varying visible pump excitation conditions. Our findings highlight the limited propensity of trans-DFAB to undergo trans-to-cis isomerization following  $S_1$  excitation and reveal the emergence of a dissociative ionization process leading to photodissociation.