

MO 13: Posters 1: Ultrafast Spectroscopy

Time: Tuesday 16:15–18:15

Location: Orangerie

MO 13.1 Tue 16:15 Orangerie

Multidimensional electronic spectroscopy with mass-resolved ion detection — •HANS-PETER SOLOWAN, TRISTAN FORD, SEBASTIAN ROEDING, and TOBIAS BRIXNER — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We report a new technique, molecular-beam coherent two-dimensional (2D) electronic spectroscopy, enabling multidimensional electronic spectroscopy of gas-phase samples with mass-resolved ion detection. Using time-of-flight mass spectrometry, we have introduced cations as a new observable in coherent 2D spectroscopy.

Using a pulse shaper based on an acousto-optic programmable dispersive filter and rapid scanning [1] we focus a train of four collinear pulses in the visible regime into an interaction region with a molecular beam. Via phase cycling [2] the signals of the time-of-flight mass spectrometer can be disentangled to extract the different contributions, like the photon-echo response. With this new experimental method, the ionization pathway of nitrogen dioxide is investigated and the first ion-selective 2D spectrum of a molecular-beam sample is acquired. By implementation of a supersonic molecular beam with argon as a seed gas, the range of potential samples will be extended.

[1] S. Draeger, S. Roeding, and T. Brixner, *Opt. Express* 25, 3259 (2017)

[2] H.-S. Tan, *J. Chem. Phys.* 129, 124501 (2008).

MO 13.2 Tue 16:15 Orangerie

Setup of a transportable monolithic platform for phase-modulated UV wave-packet interferometry — •LARS-STEPHAN KLEIN, ANDREAS WITUSCHEK, LUKAS BRUDER, and FRANK STIENKEMEIER — Universität Freiburg, Physikalisches Institut, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Coherent time-resolved spectroscopy allows the precise analysis of ultrafast dynamics in complex systems. Using short UV wavelengths would provide new opportunities for studying electronic excitations in molecular systems. However, the practical realization poses high demands on interferometric stability. In our approach, we use acousto-optical (AO) phase-modulation to ease demands on stability and to isolate weak nonlinear signals from huge backgrounds. We present a transportable monolithic platform for the interferometer including high-efficiency AO modulators with large apertures due to high pulse powers. A cw-laser is used as reference tracer which is needed at low repetition rates, as well as transversally driven fused-silica wedges as a delay unit. This makes the setup suitable for seed laser beamlines of free electron lasers where long beam paths to the undulator cannot be avoided.

MO 13.3 Tue 16:15 Orangerie

Broadband rapid-scan coherent 2D fluorescence spectroscopy — STEFAN MÜLLER, •SIMON DRAEGER, XIAONAN MA, MATTHIAS HENSEN, and TOBIAS BRIXNER — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

We developed an all-collinear setup for 2D electronic spectroscopy using fluorescence as an observable. The supercontinuum output of an argon-filled hollow-core fiber is used for broadband excitation in the visible spectral range. The pulse trains are generated and varied by an acousto-optic dispersive filter on a 1 kHz shot-to-shot basis, thus enabling rapid data acquisition. We show that it is possible to obtain 2D spectra within a few seconds, containing various nonlinear contributions such as photon echo and two-quantum coherences. Furthermore, we provide a detailed description of the underlying Liouville pathways that give rise to those nonlinear contributions, and show how to extract them experimentally with three- and four-pulse sequences via phase cycling.

MO 13.4 Tue 16:15 Orangerie

Photophysics of molecular systems studied by THz emission spectroscopy — •PHILIPP KRAUSPE and NATALIE BANERJI — University of Bern Department of Chemistry and Biochemistry, Freiestrasse 3, 3012 Bern

Terahertz Emission Spectroscopy (TES) is a versatile technique to

monitor ultrafast processes in material systems such as Dihalco-genides, Perovskites, Semiconductors or organic semiconductors which are the focus of this work. With TES we can monitor ultrafast electronic processes through the emission of photons in the THz frequency range. Therefore we subject the material system to an external bias field and excite it with an ultrashort light pulse (35 fs).

Electric field sensitive species within the material are accelerated by the bias field and thus create the THz waveform which is subsequently probed with electro-optic sampling (EOS).

In contrast to optical pump THz probe spectroscopy the time resolution in TES is not limited by the duration of the THz probe pulse but by the gating pulse in the EOS. We use this advantage to resolve the charge generation mechanisms on a sub picosecond timescale.

MO 13.5 Tue 16:15 Orangerie

Transient Absorption Spectroscopy of a Photochromic Coordination Cage — •KEVIN ARTMANN¹, RUJIN LI², SIMON SCHULKE¹, GUIDO H. CLEVER², and PATRICK NUERNBERGER¹ — ¹Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum — ²Anorganische Chemie, Technische Universität Dortmund, 44227 Dortmund

Coordination cages have auspicious applications due to their ability to encapsulate guest compounds selectively. Recently, Han *et al.* established a photochromic coordination cage for which uptake and release of the guest molecule can be triggered by light [1]. The cage is composed of two square-planar-coordinated Pd²⁺ ions and four bismonodentate pyridyl ligands based on a dithienylethene (DTE) photoswitch. UV excitation may initiate a ring-closure of the DTE ligand and traps the guest inside the cage. In this study, we demonstrate that the ultrafast photodynamics of the single ligand in solution are similar to those of a closely related DTE derivative examined by Ern *et al.* [2]. However, the metal-organic coordination cage shows significant differences in its photodynamics compared to the ligand building blocks. Whereas the ground-state bleach almost completely recovers within a few ps after excitation of the closed DTE ligand, it persists for the accessible time range of several ns in the case of the closed coordination cage.

*[1] Han *et al.*, *Angew. Chem. Int. Ed.* 2013, 52, 1319-1323.

*[2] Ern *et al.*, *J. Phys. Chem. A* 2001, 105, 1741-1749.

MO 13.6 Tue 16:15 Orangerie

Quantum Chemical Study of a Super-Photoacid — •NIKLAS SUELZNER and CHRISTOF HÄTTIG — Arbeitsgruppe Quantenchemie, Ruhr-Universität Bochum, 44780 Bochum

Photoacidity, i.e. the increase of acidity upon photo-excitation, is a common feature of aromatic alcohols. Depending on the ring's substituents, the strength of a photoacid may vary significantly which, in turn, initiated the discussion of different mechanism for excited-state proton transfer (ESPT). Frequently mentioned molecular origins of photoacidity include intramolecular charge redistribution (charge transfer), hydrogen bonding and solvent interactions.

Accompanying the experimental work on hydroxypyrenetrtris(hexafluoropropanylsulfonate), we performed a detailed quantum chemical study on this super-photoacid using the wavefunction-based methods ADC(2) and CC2 together with the solvation model COSMO for the treatment of bulk solvation effects. We aimed at gaining insights into the electronic structure and the structural changes occurring upon electronic excitation. The protonated and deprotonated forms were treated separately and in addition, a water complex was investigated. Our results clearly indicate a contribution of charge redistribution in the first excited-state as well as hydrogen bonding to solvent molecules, in accordance with the experimental electronic spectra.

MO 13.7 Tue 16:15 Orangerie

The Effect of Water on the Dynamics of a Superphotoacid in Acetone–Water Mixtures — •NIKLAS SUELZNER¹, BASTIAN GEISSLER¹, JOHANNES KNORR¹, CHRISTIAN SPIES¹, BJÖRN FINKLER², GREGOR JUNG², and PATRICK NUERNBERGER¹ — ¹Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum — ²Biophysikalische Chemie, Universität des Saarlandes, 66123 Saarbrücken

Photoacids exhibit a higher tendency to transfer an acidic proton in their electronically excited state compared to the ground state, which can trigger an excited-state proton transfer (ESPT). Using time-resolved spectroscopy, the ESPT process can be investigated on its actual timescale. Previous studies disclosed that the particularly strong photoacid hydroxypyrene-tris(hexafluoropropanylsulfonate) is capable of performing an ESPT even in the weakly basic solvent acetone. The role of water acting as an impurity in such aprotic, polar solvents remained unsettled though and might have a severe effect.

In this study, the influence of water on the ESPT of this photoacid in acetone–water mixtures was scrutinized by use of time-resolved streak camera fluorescence spectroscopy. Acetoneous samples with linearly increasing amounts of water (0–5%) revealed a significant enhancement of the ESPT rate by nearly one order of magnitude. A further study on the alternating effect of adding water and acidifying the solution demonstrated that the observed ESPT acceleration was partially reversible. We infer that the water molecules act as acceptors facilitating the proton transfer but can be passivated by acidification.

MO 13.8 Tue 16:15 Orangerie

Ultrafast relaxation dynamics of [Fe(CN)₆]-3 studied by means of transient absorption and XUV photoemission spectroscopy — ●AZHR ABDULZAHRAA RAHEEM^{1,2}, NATALIJA KUZKOVA^{1,2}, CHRISTOPH MERSCHJANN^{1,2}, and IGOR KIYAN^{1,2} — ¹Institute of Methods for Material Development, Helmholtz-zentrum Berlin, Albert-Einstein-Str. 15 12489 Berlin Germany — ²Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195, Berlin, Germany

We investigate light-induced structural changes and relaxation dynamics of ferricyanide, [Fe(CN)₆]-3, in aqueous solution using ultrafast transient photoelectron and absorption spectroscopy. The relaxation mechanism of [Fe(CN)₆]-3 has recently received contradictory interpretations. With the use of transient XUV photoemission spectroscopy [1], a two-step ultrafast relaxation following the initial optical ligand-to-metal charge-transfer was revealed. Another study reported on monoexponential ultrafast decay followed by an additional long-lived signal [2]. We performed experiments with two configurations, where we applied perpendicular and magic-angle polarization orientations. Our results confirm the ultrafast double-exponential decay of the excited electron population, as well as the presence of a long-lived state. [1] N. Engel, S. I. Bokarev, A. Moguilevski, A. A. Raheem, R. Al-Obaidi, T. Möhle, G. Grell, K. R. Siefertmann, B. Abel, S. G. Aziz, O. Kühn, M. Borgwardt, I. Yu. Kiyann and E. F. Aziz, *Phys.Chem.Chem.Phys.*, 2017, 19, 14248. [2] J. Ojeda, C. A. Arrell, L. Longetti, M. Chergui and J. Helbing, *Phys.Chem.Chem.Phys.*, 2017, 19, 17052.

MO 13.9 Tue 16:15 Orangerie

Disentangling the different time scales in the photodynamics of the molecular rotor molecule Thioflavin T — ●BASTIAN GEISSLER, KEVIN ARTMANN, and PATRICK NUERNBERGER — *Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum*

In the dye Thioflavin T (ThT), a benzothiazole (BTA) cation is linked to N,N-dimethylaniline (DMA) via a freely rotatable bond. When excited, this rotation can lead to ultrafast deactivation, while the fluorescence yield strongly increases if this rotation is hindered, which is why ThT is a popular marker for protein aggregation and amyloid fibril formation. Moreover, the fluorescence lifetime of ThT can also vary from ps up to ns depending on the excitation wavelength, as a consequence of the pre-rotation angle between the BTA and DMA moieties in the ground state. An initially planar ThT molecule deactivates within ps because of excited-state twisting, whereas an initially pre-twisted ThT molecule shows no excited-state rotational motion and is thus long-lived. Previous work disclosed that the long-lived fluorescence originates from the BTA moiety of the dye. In this study, we performed ultrafast spectroscopy via fluorescence streaking and transient absorption in the UV spectral range for ThT and its building blocks DMA and BTA in various solvents and with different pH values. While the pre-twisted and planar ThT configurations can be selectively excited below and above 400 nm, respectively, leading to pronounced differences in the photodynamics, deep-UV excitation below 300 nm leads to no selectivity. The long-lived emission of ThT can be associated with the ns lifetime observed for BTA.

MO 13.10 Tue 16:15 Orangerie

Towards understanding the mechanism of water splitting on TiO₂ — SAMAN HOSSEINPOUR, SIMON J. SCHLEGEL, MISCHA BONN, and ●ELLEN H.G. BACKUS — *Max Planck Institute for Polymer Re-*

search, Mainz, Germany

Finding a clean and renewable energy source to replace fossil fuels has attracted much attention, the past few decades, as a requirement for the sustainable development of societies. Direct hydrogen generation on TiO₂ by photocatalytic dissociation of water using sunlight was first proposed over 40 years ago. However, despite extensive work in this area, the fundamentals of the process remain ill-understood, mainly due to the lack of a proper tool to specifically explore the interface between water and TiO₂. Sum frequency generation spectroscopy (SFG), is an inherently surface sensitive tool, allowing the study of the water-TiO₂ interface. We show time-resolved SFG data after excitation of TiO₂ with a femtosecond UV pump pulse, which mimics the sunlight. Preliminary data show that both the surface and the interfacial water molecules undergo changes on ultrafast timescales upon excitation. These UV-pump SFG-probe data illustrate the first steps towards following the photo-induced dissociation of water at the TiO₂ interface in real-time.

MO 13.11 Tue 16:15 Orangerie

Ultrafast processes in luminescent mono- and dinuclear copper(I)-complexes — ●MERTEN GRUPE¹, FLORIAN BÄPPLER¹, MANUEL ZIMMER², STEFAN BRÄSE³, MARKUS GERHARDS², and ROLF DILLER¹ — ¹Dept. of Physics, TU Kaiserslautern, 67663 Kaiserslautern — ²Dept. of Chem., TU Kaiserslautern, 67663 Kaiserslautern — ³Dept. of Org. Chem., KIT, 76131 Karlsruhe

Copper(I)-complexes play a crucial role for the design of efficient and sustainable light emitters. To get a profound understanding of luminescence, controlled by photoinduced intra- and intermolecular processes, such as molecular flattening, intersystem crossing, solvation etc. we employed femtosecond UV/Vis transient absorption (TA) on mono^[1]- and dinuclear^{[2][3][4]} copper(I)-complexes. The results allow a rigorous comparison of the respective ultrafast dynamics in solution and solid phase, possibly controlled by metal-metal cooperativity. For the elucidation of molecular flattening we employed femtosecond mid-IR TA on a heteroleptic mononuclear copper(I)-complex.

[1] L. Bergmann et al. *Chem. Commun.*, 2013, 49 6501

[2] F. Bäßler et al. *PCCP*, 2017

[3] D. Volz et al. *Chem. Mater.*, 2013

[4] Wallesch et al. *Chem. Eur. J.*, 2016

MO 13.12 Tue 16:15 Orangerie

Excitonic Coupling and Energy Transfer in the LH2 Complex of Allochromatium Vinosum — ●MARCO SCHRÖTER¹, MARCELO ALCOCCER², OLIVER KÜHN¹, and DONATAS ZIGMANTAS² — ¹Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock, Germany — ²Chemical Physics, Lund University, Box 124, 22100 Lund, Sweden

Bacterial photosynthesis is one of the most adaptable and robust energy harvesting processes in nature, with light-harvesting complexes playing a crucial role. The peripheral light-harvesting complex (LH2) of the purple bacterium *Allochromatium vinosum* is particularly distinct as it shows a double peak structure in the B800 absorption band. Two hypotheses concerning the origin of this splitting have been proposed; either two distinct B800 bacteriochlorophyll site energies [1], or an excitonic dimerization of bacteriochlorophylls within the B800 ring [2]. Through the use of two-dimensional electronic spectroscopy, we present unambiguous evidence that the peak splitting is due to the latter. Furthermore, we identify and characterize all energy transfer pathways within this complex by using a refined global fitting procedure [3]. Our approach demonstrates how the combination of two-dimensional spectral resolution and self-consistent fitting allows for the extraction of information on light-harvesting processes, which would otherwise be inaccessible due to signal congestion.

[1] D. M. Niedzwiedzki et al., *Biochim. Biophys. Acta* 1817, 1576 (2012) [2] A. Löhner et al., *Photosynth. Res.* 123, 23 (2015) [3] J. Dostal et al., *J. Chem. Phys.* 145, 124312 (2016)

MO 13.13 Tue 16:15 Orangerie

Ultrafast Transient Reflectivity on Metal Complexes — ●FLORIAN BÄPPLER¹, MERTEN GRUPE¹, LARS SCHÜSSLER¹, CHRISTOPH RIEHN^{1,2}, and ROLF DILLER¹ — ¹TU Kaiserslautern, 67663 Kaiserslautern, Germany — ²Forschungszentrum OPTIMAS, 67663 Kaiserslautern, Germany

Photophysical properties can be drastically altered by the sample parameters, e.g. packing density, solid state, gas phase, solvent and temperature. Therefore, in order to optimize device efficiency and

functionality, it is critical to investigate the sample in the same environment as in the application. Femtosecond transient absorption (fs-TA) in transmission is a well established method to study ultrafast photophysical processes in molecules. This method is limited to transparent samples.

However, for non-transparent samples such as crystals and pressed pellets, femtosecond transient reflectivity (fs-TR) can give unique insights into the ultrafast dynamics upon photoexcitation. Here, we present a recent study comparing photophysical dynamics of the binuclear OLED-emitter $\text{Cu}_2\text{I}_2\text{MePyrPHOS}^{[1]}$ in solution, film and as pressed neat pellet, using both fs-TA alongside with fs-TR. A perspective on how fs-TR as a tool to investigate metal complexes can be applied and improved is given.

[1] F. Bappler et al. PCCP, 2017

MO 13.14 Tue 16:15 Orangerie

Multi-state Photoelectron Circular Dichroism in Femtosecond Multiphoton Ionization — ALEXANDER KASTNER¹, TOM RING¹, ●ROXANA SAVULEA¹, BASTIAN C. KRUGER², G. BARRATT PARK², TIM SCHAFER², ARNE SENFTLEBEN¹, and THOMAS BAUMERT¹ — ¹Universitat Kassel, Institut fur Physik und CINSaT, D-34132 Kassel, Germany — ²Institut fur Physikalische Chemie, Georg-August-Universitat Gottingen, D-37077 Gottingen, Germany

The asymmetry of photoelectron angular distributions (PADs) from randomly oriented enantiomers of chiral molecules in the ionization with circularly polarized light arises in forward/backward direction with respect to the light propagation. This effect was termed Photoelectron Circular Dichroism (PECD) and so far investigated using synchrotron radiation [1, 2]. Due to the multi-photon ionization, we observed highly structured asymmetries with a magnitude in the range of $\pm 10\%$ on bicyclic Ketones [3, 4]. By scanning the laser excitation wavelength, up to three electronically distinct resonances can be simultaneously populated. The intermediate state and the excitation wavelength define the photoelectron energy. We report on the dependence of magnitude and sign of PECD on photoelectron energy [5].

[1] I. Powis, Adv. Chem. Phys. 138, 267-329, (2008)

[2] L. Nahon et al., J. El. Spectr. 204, 322-334, (2015)

[3] C. Lux et al., Chem. Phys. Chem. 16, 115-137, (2015)

[4] A. Kastner et al., Chem. Phys. Chem. 17, 1119-1122, (2016)

[5] A. Kastner et al., J. Chem. Phys. 147, 013926, (2017)

MO 13.15 Tue 16:15 Orangerie

Time-resolved photoelectron circular dichroism in solution — ●JANINA LEBENDIG-KUHILA, HANS-HERMANN RITZE, and ANDREA LUBCKE — Max-Born-Institut fur Nichtlineare Optik und Kurzzeitspektroskopie, Berlin

The phenomenon of chirality is a widely spread characteristic of molecules, especially in biological systems. This property is accompanied by circular dichroism, the effect of a chiral molecule interacting differently with circularly polarized light of different handedness. We combine time-resolved photoelectron circular dichroism (TR-PECD) measurements with the liquid jet technique to investigate the excited state dynamics of chiral molecules in solution. This method implies the generation of ultrashort circularly polarized UV-pulses as well as a detection scheme compatible with the liquid jet environment. We will present our experimental approach and show first results.

MO 13.16 Tue 16:15 Orangerie

Generating laser-pulse enantiomers — ANDREAS STEINBACHER^{1,2}, ●HEIKO HILDENBRAND¹, SEBASTIAN SCHOTT¹, JOHANNES BUBACK¹, MARCO SCHMID¹, PATRICK NUERNBERGER³, and TOBIAS BRIXNER¹ — ¹Institut fur Physikalische und Theoretische Chemie, Universitat Wurzburg, Am Hubland, 97074 Wurzburg — ²Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA — ³Physikalische Chemie II, Ruhr-Universitat Bochum, 44780 Bochum

We developed an optical setup capable of mirroring an arbitrary, potentially time-varying, polarization state of an ultrashort broadband laser pulse [1]. This is achieved by splitting up the incident beam in two separate beams of which one is mirrored by reflection off a mirror in normal incidence. Afterwards, both beams are recombined in time and space such that two collinearly propagating ultrashort laser pulses with mutually mirrored polarization, i.e., laser-pulse enantiomers, leave the setup. Via this approach, wave plates are not needed and broadband pulses in a large wavelength range can be processed.

Since the two beams travel separately through the optical system, shot-to-shot chopping and detection schemes can be applied.

These capabilities are desired, e.g., for circular dichroism, ellipsometry, anisotropy or chiral quantum control experiments. As an application example, the latest progress on time-resolved circular dichroism and transient absorption spectroscopy on the early photochemistry of oxygenated myoglobin is presented.

[1] Steinbacher et al., Opt. Express 25, 21736 (2017)

MO 13.17 Tue 16:15 Orangerie

First results of XUV transient absorption spectroscopy in the ionization continuum of molecular hydrogen — ●GERGANA D. BORISOVA, PAUL BIRK, VEIT STOOSS, MAXIMILIAN HARTMANN, ALEXANDER BLATTERMANN, NIKOLA MOLLOV, ROBERT MOSHAMMER, CHRISTIAN OTT, and THOMAS PFEIFER — Max-Planck-Institut fur Kernphysik, Heidelberg

In studies of the ionization dynamics in atoms and molecules after light-matter interaction, usually electrons and/or ions are detected, as they are the natural products of the ionization process. Investigating ionization dynamics in molecular hydrogen is therefore predominantly done by measuring charged particles [1]. Here, we experimentally consider the complementary approach of attosecond transient-absorption spectroscopy (ATAS) and aim at the energy region around the Qn doubly excited resonances. First results of this technically challenging experiment will be presented, with emphasis on a systematic study of various obstacles that arise when searching for weak and broadband spectral signatures in an ATAS experiment.

[1] Palacios et al., J. Phys. B: At. Mol. Opt. Phys. 48, (2015) 242001

MO 13.18 Tue 16:15 Orangerie

pump-probe experiments with molecules at FLASH — ●YIFAN LIU¹, KIRSTEN SCHNORR¹, GEORG SCHMID¹, SVEN AUGUSTIN¹, SEVERIN MEISTER¹, HANNES LINDENBLATT¹, THOMAS DING¹, YUHAI JIANG², ROLF TREUSCH³, STEFAN DUSTERER³, MATHIEU GISSELBRECHT⁴, CHRISTIAN BURGER⁵, MATTHIAS KUEBEL⁵, MATTHIAS KLING⁵, ARTEM RUDENKO⁶, CLAUDIUS DIETER SCHROETER¹, THOMAS PFEIFER¹, and ROBERT MOSHAMMER¹ — ¹Max-Planck-Institut fur Kernphysik, Saupfercheckweg 1, Heidelberg, 69117, Germany — ²Shanghai Advanced Research Institute, Zhangjiang, Shanghai, 201210, China — ³Deutsches Elektronen-Synchrotron, Notkestrasse 85, 22607, Hamburg, Germany — ⁴Lund University, Lund, Post Box 118, 22100, Sweden — ⁵Max Planck Institute of Quantum Optics, Hans-Kopfermann-Strae 1, D-85748 Garching, Germany — ⁶J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas, 66506, USA

With a pump-probe experimental scheme, the ultrafast temporal resolution molecular dynamics of N₂ and O₂ were investigated at the Free-Electron-LASer in Hamburg (FLASH). Firstly, IR-assisted XUV multiphoton experiment of N₂ was performed at FLASH in combination with a synchronized femtosecond optical laser. The fragmentation and multiple ionization dynamics of N₂ have been investigated using a Reaction-Microscope (ReMi). We find the sequential ionization is to be the dominant and efficient process for molecules in X-ray regime. The second experiment is that we use the THz electric field to trace the autoionization process happening in molecular oxygen.

MO 13.19 Tue 16:15 Orangerie

Studies of atomic and molecular dynamics with few-femtosecond XUV and IR fields — LORENZ DRESCHER, GEERT REITSMA, TOBIAS WITTING, MARC VRAKKING, and ●JOCHEN MIKOSCH — Max-Born-Institute, Max-Born-Strasse 2A, 12489 Berlin

Atomic and molecular dynamics on attosecond and few-femtosecond timescales can be studied using a number of different protocols involving few-cycle infrared (IR) pulses and extreme ultraviolet (XUV) pulses from High Harmonic Generation.

Here we showcase the results from three different experiments performed with the same versatile experimental apparatus:

(1) The few-femtosecond passage of conical intersections in benzene was studied with time-resolved photofragment spectroscopy. The dynamics represent one of the fastest internal conversion processes in a molecule studied to date and allow for a detailed comparison with multi-configurational time-dependent Hartree calculations [1].

(2) We analyze the XUV-IR induced excitation of neutral states in helium by UV photoelectron spectroscopy. The observed oscillation of the 1s3p population with the XUV-IR phase is assigned to the superposition of two independent two-color two-pathway interferences, which are out-of-phase.

(3) Finally, we present results from attosecond transient absorption

spectroscopy of CH₃I molecules in the core-to-valence and core-to-Rydberg transition region. Our results show the sub-cycle dependent light-induced coupling of these states due to the AC Stark effect.

[1] Galbraith et al., Nature Comm. **8**, 1018 (2017)

MO 13.20 Tue 16:15 Orangerie

All-XUV transient-absorption spectroscopy on the ultrafast dissociation of small molecules — ●MARC REBHOLZ¹, THOMAS DING¹, LENNART AUFLEGER¹, MAXIMILIAN HARTMANN¹, ALEXANDER MAGUNIA¹, DAVID WACHS¹, KRISTINA MEYER¹, VEIT STOOSS¹, PAUL BIRK¹, GERGANA BORISOVA¹, CARINA DA COSTA CASTANHEIRA¹, PATRICK RUPPRECHT¹, ANDREW ATTAR², ZHI HENG LOH³, THOMAS GAUMNITZ⁴, SEBASTIAN ROLING⁵, MARCO BUTZ⁵, HELMUT ZACHARIAS⁵, STEFAN DÜSTERER⁶, ROLF TREUSCH⁶, VICTOR DESPRÉ⁷, ALEXANDER KULEFF⁷, CHRISTIAN OTT¹, and THOMAS PFEIFER¹ — ¹Max-Planck Institut für Kernphysik, Heidelberg, Germany — ²University of California Berkeley, Berkeley, USA — ³Nanyang Technological University Singapore, Singapore — ⁴Eidgenössische Technische Hochschule Zürich, Zürich, Switzerland — ⁵Westfälische Wilhelms-Universität Münster, Münster, Germany — ⁶Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — ⁷Universität Heidelberg, Heidelberg, Germany

We present first results of a transient-absorption experiment using only extreme ultraviolet (XUV) light. The XUV laser pulses with photon energies near 50 eV and pulse durations of ~ 50 fs are provided by the free-electron laser FLASH. This allows us to pump a core-electron transition ($4d \rightarrow \sigma^*$) in the target molecules methyl iodide (MEI) and diiodomethane (DIM) with high-intensity (estimated 10^{14} W/cm²) XUV

light. We investigate the subsequent ultrafast dissociation by tracing changes in the absorption spectrum of an identical XUV probe pulse.

MO 13.21 Tue 16:15 Orangerie

Ultrafast electronic delay of core excited HCl molecules measured with THz streaking — ●KATHARINA WENIG¹, MAREK WIELAND¹, SOPHIE WALTHER¹, ARNE BAUMANN¹, ANATASIOS DIMITRIOU¹, MARK PRANDOLINI¹, OLIVER SCHEPP¹, IVETTE BERMÚDEZ MACHIAS², MALTE SUMFLETH¹, NIKOLA STOJANOVIC², STEFAN DÜSTERER², JULIANE RÖNTSCH-SCHULENBURG², MARKUS DRESCHER¹, and ULRIKE FRÜHLING¹ — ¹Institut für Experimentalphysik, Universität Hamburg, Deutschland — ²Deutsches Elektronen-Synchrotron DESY, Hamburg, Deutschland

We have resonantly excited $2p_{3/2}$ core electrons from HCl molecules to the antibonding σ^* orbital using femtosecond soft-x-ray pulses from the free-electron laser in Hamburg (FLASH). After the excitation the molecules dissociate and the electronic excitation relaxes via the emission of an Auger-electron. Both processes compete on similar ultra-short femtosecond time scales. In order to follow the evolution of this coupled electronic and nuclear dynamics, we equipped x-ray electron spectroscopy with time resolution.

In our experiment the exciting soft-x-ray pulses were collinearly superimposed with intense THz pulses from the FLASH THz undulator. Electrons emitted from the molecules are accelerated (streaked) by the THz electric field whereby the resulting momentum change depends on the THz phase at the instant of ionization. The experimental setup and first experimental results will be presented.