

MO 6: Poster I

Time: Tuesday 16:30–19:00

Location: Empore Lichthof

MO 6.1 Tue 16:30 Empore Lichthof

Boundary effects in sensory adaptation & interacting sensory systems — ●VANSH KHARBANDA — Cell Biophysics and Statistical Physics, Faculty of Veterinary Medicine, LMU Munich

Sensory adaptation is vital to all living organisms. An adaptive sensory system can be modelled as a stochastic, nonlinear feedback network. Using a generic framework, we study the accuracy of adaptive mechanisms and its energetic cost. Recently, it has been suggested that the steady-state dissipation rate associated to maintenance of an adaptive state increases logarithmically with the adaptation accuracy. We present results that demonstrate that this logarithmic scaling does not hold generally, but appears to be linear when the state of the system is close to the phase-space boundaries. Our numerical results also suggest that boundaries in the phase space of system variables limit the capacity of the system to dissipate. Moreover, we conjecture a new empirical expression relating the steady-state dissipation rate and the strength of the input signal if the state lies in the vicinity of the boundaries. Finally, the combined adaptation accuracy of two linearly coupled systems is studied. We show that a coupling the outputs of the systems deteriorates the overall adaptation accuracy while the associated energy cost is also reduced. In contrast, a coupling of the control elements reduces the dissipation rate without compromising on the adaptation accuracy.

MO 6.2 Tue 16:30 Empore Lichthof

Time-resolved study of the photogeneration of the phenylselenium cation from diphenyl diselenide and subsequent use for covalent activation in organic reactions — ●DANIEL GREYDA¹, ANNA TIEFEL², CARINA ALLACHER¹, ALEXANDER BREDER², and PATRICK NÜRNBERGER¹ — ¹Institute of Physical and Theoretical Chemistry, University of Regensburg, Regensburg — ²Institute of Organic Chemistry, University of Regensburg, Regensburg

Using a pump-probe setup on a μ s-timescale with a streak-camera detector [1], one can investigate light-induced chemical reactions with long-lived intermediates. We apply this technique to organoselenium compounds, which are useful catalysts in organic synthesis due to their stability towards oxygen and their rich radical chemistry [2]. Especially diphenyl diselenide is a versatile precursor for organic synthesis, as it is often used to generate phenylselenium radicals by photolytic cleavage of the selenium-selenium bond [3]. However, we demonstrate that given the right reaction conditions, the phenylselenium cation can be generated in a similar way, which then is utilizable for covalent activation of allylic selenium species [4].

[1] R. J. Kutta *et al.*, *Appl. Phys. B* **111**, 203-216 (2013).[2] A. Breder *et al.*, *Tetrahedron Lett.* **56**, 2843-2852 (2015).[3] O. Ito *et al.*, *J. Am. Chem. Soc.*, **105**, 850-853 (1983).[4] M. Tingoli *et al.*, *J. Org. Chem.* **61**, 7085-7091 (1996).

MO 6.3 Tue 16:30 Empore Lichthof

Photoemission delays in similarly sized molecules — ●MAXIMILIAN FORSTER, CHRISTIAN SCHRÖDER, MAXIMILIAN POLLANKA, PASCAL SCIGALLA, MICHAEL MITTERMAIR, ANDREAS DUENSING, and REINHARD KIENBERGER — Chair for laser and x-ray physics, E11, Technische Universität München, Germany

In the gas phase we measure the relative photoemission delay between the Helium 1s and the Iodine 4d state in Iodobenzene and Iodocyclohexane. This allows us to determine the absolute timing of the Iodine 4d photoelectrons.

Iodine as a substituent was chosen for its giant resonance and therefore high cross section in the I4d state which is expected to be unaffected by its chemical surrounding. Measurements on a variety of different iodoalkanes have shown an unexpected variation of the I4d delay for different molecules, with no clear correlation with the molecular size, showing that the chemical environment may play a role in forming the observed photoemission delay. Therefore performing measurements on molecules with similar size and yet significant differences in their bonding structure yields further information about the possible underlying effects causing the delay.

MO 6.4 Tue 16:30 Empore Lichthof

Femtosecond Transient Absorption Spectro-Microscopy with

High Spatial Resolution on Dye Microcrystals — ●MAGNUS FRANK, CHRIS REHHAGEN, and STEFAN LOCHBRUNNER — Institute for Physics and Department of Life, Light and Matter, University of Rostock, 18051 Rostock, Germany

Solid organic materials open a promising pathway for further improvement of optoelectronic devices like OLEDs or organic photovoltaics. The interaction of light and matter in such systems is essential for potential applications. For instance, in organic solar cells, excitons need to diffusive to an interface for charge separation - a dynamic process competing with other decay channels on the femto- and picosecond timescale. Femtosecond transient absorption is still the hallmark of dynamics determination in molecular systems, but though a lot of research has been done on the dynamics of organic solids, many fundamental aspects are still unclear. This is because measuring not only dynamics on the femtosecond timescale but also ensuring high spatial and spectral resolution is challenging. In this work, we combine classical transient absorption with microscopy allowing for spectroscopy with both high spatial and time resolution, 2.5 μ m and sub-100fs respectively. We demonstrate the performance by measuring the dynamics of single microcrystals of a perylene dye, a material class known for its outstanding potential in optoelectronics.

MO 6.5 Tue 16:30 Empore Lichthof

Phase-modulated transient-absorption spectroscopy in the liquid phase — ●JAKOB GERLACH, YILIN LI, ARNE MORLOK, ULRICH BANGERT, FRANK STIENKEMEIER, and LUKAS BRUDER — Institute of Physics, University of Freiburg, Germany

In our group a setup for two-dimensional electronic spectroscopy has previously been developed and used to study dynamics of nanosystems trapped in helium nanodroplets [1]. The action-detected spectroscopy is based on phase modulation of the laser pulses [2]. Many processes relevant in the field of photochemistry take place in a liquid environment, which significantly impacts the investigated dynamics. Therefore, a new setup is assembled to allow the examination of a probe in the liquid phase using transient-absorption spectroscopy. We plan to combine this setup with the phase modulation technique in order to improve the signal-to-noise. The design of the setup and a first characterization of its implementation will be presented.

[1] L. Bruder *et al.*, *Nat Commun* **9**, 4823 (2018).[2] P. F. Tekavec, G. A. Lott, and A. H. Marcus, *J. Chem. Phys.* **127**, 214307 (2007).

MO 6.6 Tue 16:30 Empore Lichthof

Dependence of photoelectron circular dichroism on the distance between marker atom and stereocenter in chiral molecules — ●EMILIA HEIKURA¹, FLORIAN TRINTER², LUTZ MARDER¹, CATMARNA KÜSTNER-WETEKAM¹, DANA BLOSS¹, NILS KIEFER¹, JOHANNES VIEHMANN¹, CHRISTINA ZINDEL¹, MARKUS ILCHEN², ANDREAS HANS¹, and ARNO EHRESMANN¹ — ¹Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — ²Deutsches Elektronen-Synchrotron, DESY, Notkestraße 85, 22607 Hamburg, Germany

Photoelectron circular dichroism (PECD) is one of the most powerful methods to investigate molecular chirality in the gas phase. PECD arises from the asymmetry of the angular distribution of photoelectrons (probe electrons) scattered on the chiral backbone of the molecule even from randomly oriented molecules after interaction with circularly polarized light. One still unclear aspect of PECD is, how the distance between the probe electron emitter site and the center of a point-chiral molecule affects the magnitude of the PECD asymmetry. For detection of these forward-backward asymmetries of emitted photoelectrons a velocity map imaging (VMI) electron spectrometer was used. Measurements were performed on sec-butyl trimethylsilylether and its derivatives.

MO 6.7 Tue 16:30 Empore Lichthof

Ultrafast Transient Absorption Spectroscopy of Metal Complexes with 10 fs Probe Pulses — ●MARVIN KRUPP, MORITZ LANG, CHRIS REHHAGEN, and STEFAN LOCHBRUNNER — Institut für Physik, Uni Rostock, Deutschland

Most of the photoactive complexes used in chemical applications are based on rare metals like iridium or ruthenium. Replacing them with

abundant metals e.g. iron is of long-standing interest, but the resulting complexes are currently limited by their photoactive properties. To analyze newly prepared iron complexes femtosecond transient absorption spectroscopy is typically used to determine the dynamics upon photoexcitation with short pump pulses and a few hundred femtoseconds long white light continuum for probing. Increasing the time resolution by reducing the pulse duration of the probe can make it possible to observe extremely fast processes below the current time resolution and give insights into the very first relaxation steps in the metal complexes such as intersystem crossing. In this work a broadband noncollinear optical parametric amplifier (NOPA) is used to generate broadband pulses with a duration below 10 fs. These pulses are used as probe light improving the time resolution in comparison to the usual CaF₂ white light. The setup was characterized with transient grating frequency-resolved optical gating (TG FROG) and first measurements on Fe-complexes are compared with respect to the two probe sources.

MO 6.8 Tue 16:30 Empore Lichthof
THz-Streaking for Detecting Inner-valence-shell Correlation-induced Time-delays in the Ionization of PAHs. — ●MOHAMED ABDELRASOUL, MARK PRANDOLINI, MAREK WIELAND, and MARKUS DRESCHER — Institute of Experimental Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany.

Photoionization delays (Wigner time delay) in outer molecular shells occur in the range of a few ten attoseconds. This delay increases for inner valence shell photoionization due to strong correlation effects, namely, shake-up/down and knock-up/down processes, leading to markedly longer relaxation times, and raising an interesting question: how long does it take to remove an electron from the molecular inner shell relative to the outermost shell? Most polycyclic aromatic hydrocarbons (PAHs) have relatively high photoelectron emission cross sections in the energy range typically between 15 and 25 eV, and to access both inner and outer photoelectron spectra, an Extreme Ultraviolet (XUV) photon energy in that range is required. A laser-based setup is presented, combining a high harmonic XUV source with THz streaking for measuring the photoelectron emission delay in PAHs of different sizes.

MO 6.9 Tue 16:30 Empore Lichthof
Photodissociation dynamics of CHCl₂ — ●JONAS FACKELMAYER, CHRISTIAN MATTHAEI, and INGO FISCHER — Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Recent studies suggest that the depletion of atmospheric O₃ is not only caused by the banned CFCs and HCFCs but also catalysed by commonly used solvents such as dichloromethane.^[1] Photodissociation of these compounds often results in the release of highly reactive halogen radicals. While the dissociation dynamics of molecular halocarbons have been studied in detail in the past, less is known about their open shell counterparts.

The photofragmentation of the open shell CHCl₂, generated by pyrolysis from the bromide precursor CHCl₂Br, was investigated in a free jet utilising time-of-flight mass-spectrometry and velocity map imaging. Photodissociation was achieved by a pulsed dye laser in the range of 230 - 250 nm mainly producing CHCl and Cl fragments, while ionisation was provided by either a second dye laser (REMPI) or a frequency multiplied solid state laser at 118 nm (SPI). First insights into the involved dissociation mechanisms are discussed.

[1] Hossaini, R. et al., *Nat. Commun.* **2017**, 8, 15962.

MO 6.10 Tue 16:30 Empore Lichthof
Probing conical intersection dynamics in the dissociative photoionization of formaldehyde — ●DAVID CHICHARRO VACAS, WEIYU ZHANG, THOMAS PFEIFER, and ROBERT MOSHAMMER — IMax-Planck-Institute für Kernphysik, Heidelberg, Germany

Conical intersections (CI) between electronic states often govern the photochemistry of molecules and radicals. Their role and characteristics have been largely studied before both theoretically and experimentally. It has been proven that CI are crucial in different photochemical reactions and are characterized by coupled electronic and nuclear dynamics, breaking the Born-Oppenheimer approximation. The neutral photofragmentation of formaldehyde has been widely studied in the past years mainly because of a great interest for the roaming pathway producing H₂. However, the photoionization and dissociative photoionization (DPI) has been less studied. Experimentally, the DPI of formaldehyde has been studied and two main DPI processes were found: The H-atom loss and the molecular channel. More recently, experimental and theoretical findings allowed to predict the mechanism

involved in the DPI of formaldehyde, suggesting the presence of a conical intersection that controls this mechanism. The aim of this work is to directly observe the presence of this conical intersection by using pump-probe schemes along with the reaction microscope. The 3D-ion-electron momentum coincidence measurements in a pump-probe experiment provides enough information to fully understand this process and to directly visualize the presence of the conical intersection in the experimental results.

MO 6.11 Tue 16:30 Empore Lichthof
Ultrafast coherent control of single molecules via two-photon excitation at room temperature — ●XINPENG XU¹, ULLRICH SCHERF², and RICHARD HILDNER¹ — ¹Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — ²Institut für Polymertechnologie, Universität Wuppertal, Germany

Quantum coherent control has been a powerful technique to understand and manipulate ultrafast photoinduced processes occurring at the inter-/intra-molecular level for more than twenty years. In a coherent control experiment, one can exploit quantum interference between competing pathways of multiphoton transitions toward the desired outcome by tailoring the spectral phase, amplitude, or polarization of the electromagnetic field of the exciting laser. For larger functional molecules in condensed phase, the influence of the (often disordered) surrounding environment varies between molecules. Hence, ensemble measurements do typically not allow to exert full control over competing pathways. Here, we demonstrate that the two-photon transition of single molecules can be controlled by a sequence of shaped pulses at room temperature. Varying the spectral phase of the pulses, we observe phase-dependent photoluminescence signals corresponding to the two-photon excitation probability. We assign this phase dependence to the combination of quantum photon interference and coherence between the incident laser spectrum and the single molecule absorption spectrum. Notably, cancellation of the transition probability by so-called *dark pulses* is observed in some molecules, which shows the ability to fully coherent control of single molecules in condensed phase.

MO 6.12 Tue 16:30 Empore Lichthof
Attosecond Chronoscopy of organic iodine compounds on Pt111 — ●SVEN PAUL¹, PASCAL SCIGALLA¹, CHRISTIAN SCHRÖDER¹, PETER FEULNER², and REINHARD KIENBERGER¹ — ¹Chair for laser and x-ray physics, E11, Technische Universität München, Germany — ²Surface and Interface Physics, E20, Technische Universität München, Germany

We report on attosecond streaking measurements of the relative photoemission delay between the Iodine 4d state in organic iodine compounds like Iodoethane and -methane adsorbed on a Pt111 surface in respect to the Pt valence band. Iodine was chosen as a substituent in these organic molecules because of its giant dipole resonance in the 4d state, which results in a high cross section that is mostly unaffected by the rest of the molecule. The surface coverage of the organic iodine compounds on the Pt crystal is controlled via thermal programmed desorption. This is important because the orientation, i.e. horizontal and vertical configuration, of these adsorbents on the surface depends on the surface coverage. By using those two effects, we can ensure whether the detected photoelectrons have been perturbed by the whole organic chain or only by parts of it. A change in photoemission delay between both configurations is expected, as suggested by previous measurements for Iodoethane. Similar measurements are now made for Iodomethane as part of my master thesis, as we want to study the correlation of the photoemission delay with the length of the organic chain.

MO 6.13 Tue 16:30 Empore Lichthof
Lamellar and amorphous Alucones as Nanoscaffolds for Cellular Response; A Route for Building Nature-Inspired Materials. — ●MABEL MORENO¹, ANGÉLICA ZACARIAS², SIMÓN GUERRERO¹, LUIS VELASQUEZ¹, YUSSER OLGUIN^{3,4}, and EBERHARD GROSS⁵ — ¹Universidad SEK, Instituto de Investigación Interdisciplinar en Ciencias Biomédicas SEK (I3CBSEK). — ²Max Planck Institute of Microstructure Physics, Weinberg 2, D 06120, Halle, Germany, and ETSF. — ³Universidad Técnica Federico Santa María, Centro de Biotecnología, Avenida España 1680, Valparaíso, Chile. — ⁴Universidad Técnica Federico Santa María, Departamento de Física, Avenida España 1680, Valparaíso, Chile — ⁵Fritz Haber Research Center for Molecular Dynamics and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, ISRAEL.

We present our study of the growth of alucone thin films (AIO-T

and AIO-A, T: terephthalate and A: adipate) by atomic layer deposition (ALD) and molecular layer deposition (MLD). Stoichiometric thin films with large area uniformity were obtained in both cases, as shown in SEM/Focus Ion Beam (FIB), transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray reflectometry (XRR), Atomic force microscopy (AFM), reflectance diffuse by UV-Visible, and attenuated total reflectance (ATR) data. Quantum information (QI), C2C12 cells cultured test and antibacterial activity were performed to prove the QI and biocompatibility concepts on such thin films, making them possible candidates for bioinspired-quantum devices.

MO 6.14 Tue 16:30 Empore Lichthof

Long-lasting XUV-induced ignition of avalanche ionization of helium nanodroplets — ●C. MEDIA¹, A. Ø. LAEGDSMAND², L. BEN LTAIEF², Z HOQUE³, A. H. ROOS³, M. JURKOVIC³, O. HORT³, O. FINKE³, M. ALBRECHT³, J. NEJDL³, F. STIENKEMEIER¹, E. KLIMESOVA³, M. KRIVONOVA³, A. HEIDENREICH⁴, and M. MUDRICH² — ¹Institute of Physics, University of Freiburg, Freiburg, Germany — ²Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — ³ELI Beamlines Centre, FZU- Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 21 Prague, Czechia — ⁴IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

We study the dynamics of avalanche ionization of pure helium nanodroplets activated by a weak extreme-ultraviolet (XUV) pulse and driven by an intense near-infrared (NIR) pulse. In addition to a transient enhancement of the droplet ignition probability at short delay times ~ 200 fs, long-term activation of the nanodroplets lasting up to a few nanoseconds is observed. Molecular dynamics simulations suggest that the short-term activation is caused by the injection of seed electrons into the droplets by XUV photoemission. Long-term activation is due to electrons remaining loosely bound to photoions which form stable ‘snowball’ structures in the droplets. Thus, we show that XUV irradiation can induce long-lasting changes of the strong-field optical properties of nanoparticles, potentially opening new routes to controlling avalanche-ionization phenomena in nanostructures and condensed-phase systems.

MO 6.15 Tue 16:30 Empore Lichthof

Bidirectional photorearrangement reaction of a xanthine derivative — ●THOMAS RITTNER¹, KARINA HEILMEIER¹, RAFAEL E. RODRÍGUEZ-LUGO², SIMON DIETZMANN², SVENJA WORTMANN¹, ROGER JAN KUTTA¹, ROBERT WOLF², and PATRICK NUERNBERGER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93053 Regensburg — ²Institut für Anorganische Chemie, Universität Regensburg, 93053 Regensburg

7-Aryl-8-pyridyl substituted theophyllines exhibit a remarkable photoreaction. Our studies show that upon excitation with ultraviolet light, the anisyl substituted 7-(4-methoxyphenyl)-1,3-dimethyl-8-(pyridin-2-yl)-3,7,8,9-tetrahydro-1H-purine-2,6-dione undergoes a rearrangement. The anisyl moiety migrates from the 7-nitrogen on the purine skeleton of the theophylline to the 1'-nitrogen of the pyridine, yielding a zwitterionic isomer. Both isomers could be isolated and subsequently characterized by NMR spectroscopy and single-crystal X-ray scattering. Time-resolved and steady-state absorption and emission spectroscopies in the visible spectral range were used to investigate the photorearrangement mechanism. Together with quantum-chemical calculations a detailed picture on a molecular level could be obtained. We further demonstrate that also a photo-induced back-isomerization is feasible, enabling in principle a general design for photo-switchable molecular structures.

MO 6.16 Tue 16:30 Empore Lichthof

Coverage-dependent agglomeration in molecular films on atomically flat surfaces — ●ERIK VON DER OELSNITZ, TIM VÖLZER, JULIAN SCHRÖER, RICO SCHWARTZ, TOBIAS KORN, and STEFAN LOCHBRUNNER — Institute of Physics, Albert-Einstein-Straße 23-25, 18059 Rostock, Germany

The deposition of a thin, monomeric molecular layer on an atomically flat surface, as it is provided by Van-der-Waals crystals, is crucial to the functionalization of such layered materials and the fabrication of corresponding hybrid structures. In this work, Perylene Orange (PO) molecules were coated onto a thin exfoliated hexagonal boron nitride layer using thermal vapor deposition (TVD) at various evaporation temperatures. The resulting hybrid structures were examined by a fluorescence lifetime imaging microscope, revealing a biexponential fluorescence decay, as well as by micro-photoluminescence spectroscopy, proving for low evaporation temperatures the monomeric nature of

the PO layer. Upon increasing the temperature, the fluorescence intensity rises and at the same time the fast decay component becomes dominant and a low-energy band emerges in the emission spectrum. Interestingly, the slow decay time remains pretty constant. Therefore, this slow component can be assigned to the fluorescence decay of PO monomers, whereas the fast decay component can be attributed to agglomerates that form at higher coverage and provide additional decay channels such as the relaxation into excimer states. From these findings, an optimum for the vaporization temperature can be determined, which will be used in future applications.

MO 6.17 Tue 16:30 Empore Lichthof

Effect of vibropolariton formation on ground-state reactivity of Diels-Alder cycloaddition reaction — ●BERNA ARSLANOGLU, THOMAS SCHNAPPINGER, and MARKUS KOWALEWSKI — Stockholm University, Sweden

It has been experimentally demonstrated that ground-state reaction mechanisms can be modified by an optical cavity at room temperature. It has been shown by Thomas et al. [1], that coupling a Si-C bond resonantly to a quantized field mode can change the chemical reaction rate of the silyl bond cleavage reaction.

We present ab initio simulations of the ground state Diels-Alder reaction in the presence of an optical cavity field. The vibrational modes of the reactants are strongly coupled to the light field. The change of the reaction barrier in the presence of the field is studied for varying vacuum field strengths as well as for different resonance conditions. Additionally, we study how the dipole self-energy term influences stationary points of the reaction.

[1] A.Thomas et al., Science 363, 615 (2019)

MO 6.18 Tue 16:30 Empore Lichthof

Classification of noisy spectra using machine learning — ●ARITRA MISHRA and ALEXANDER EISFELD — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A general problem in quantum mechanics is to obtain information of the eigenstates from the experimental measured data which consists inherent noises. In particular, we consider molecular aggregates, where information about excitonic eigenstates is vitally important to understand their optical and transport properties [1,2]. It has been shown that it is possible to reconstruct the underlying delocalised aggregate eigenfunctions from near-field spectra using convolution neural networks [3].

In this work, we also use a convolution neural network but ask a question related to the eigenstate based classification of the spectra in the presence of noise. Given that each eigenstate correspond to a distinct spectrum, we can assign a class to each of the eigenstate. We add a random noise to these spectra and build a network that can classify the spectra into these classes, in the presence of the noise. We find that the network is also able to classify the spectra of different noise strengths along with the one it has been trained for.

- [1] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018)
 [2] S. Nayak, F. Zheng and A. Eisfeld, J. Chem. Phys. 155, 134701 (2021)
 [3] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019)

MO 6.19 Tue 16:30 Empore Lichthof

Photoelectron Circular Dichroism for Chiral Helium — ●MAREC HEGER, MANEL MONDELO-MARTELL, and DANIEL REICH — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

Chiral molecules, i.e. molecules that cannot be superimposed by its mirror image by rotations and translations, show different reactions to other chiral systems depending on their handedness. A prominent example is the interaction of chiral molecules with left and right-circularly polarized light which leads to differences in the photoelectron angular emission spectrum. This difference is called photoelectron circular dichroism (PECD) which can be used as a tool to detect and distinguish chiral signatures of molecules in the gas phase.

Understanding the precise origin and the relationship between the chiral molecular scaffold and the PECD signal is still an ongoing theoretical challenge, particularly when it comes to the role of electron correlation. Numerical simulations for large molecules are particularly challenging in this context. For this reason we perform ab initio simulations for an elementary system - helium with an artificial external chiral potential - and investigate the relationship between PECD and

the chiral potential. Finally, by considering theoretical simulations involving various degrees of electron correlation - from single-active electron approaches to full configuration interaction - we also aim to elucidate the role of electron correlation systematically.

MO 6.20 Tue 16:30 Empore Lichthof

Towards understanding the enhancement of the circular dichroism in the ion yield of 3-methylcyclopentanone via tailored femtosecond laser pulses — ●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 ionisation of the enantiomers and is known as CD in ion yield [1]. We use our home-built Time of Flight (ToF) mass spectrometer with twin peak [2] measurement setup to study the effect of linear chirp (GDD) on the anisotropy. The candidate molecule for this experiment is 3-methylcyclopentanone (3-MCP). We perform all the experiments at 309 nm, where 3-MCP shows enhancement of anisotropy, upto 10%. At this wavelength, a 1+1+1 resonance-enhanced multi-photon ionisation (REMPI) takes place in 3-MCP through the $\pi^* \leftarrow n$ transition. We observed enhancement of anisotropy for chirped pulses, which we have compared to bandwidth limited pulses of equal peak intensity. Furthermore, we perform a pump-probe experiment to investigate the intermediate state dynamics.

[1] U. Boesl and A. Bornschlegl, ChemPhysChem, 7, 2085, 2006

[2] T. Ring et al., Rev. Sci. Instrum., 92, 033001, 2021

MO 6.21 Tue 16:30 Empore Lichthof

Excited-state dynamics of aqueous aminoazobenzene Metanil Yellow studied by time-resolved transient absorption spectroscopy — ●ALINA KHODKO^{1,5}, MATTHEW MGBUKWU⁴, CAMILO GRANADOS^{1,4}, EVGENII TITOV^{2,3}, STEFAN HAACKE⁴, OLEG KORNILOV¹, and JÉRÉMIE LÉONARD⁴ — ¹Max Born Institute, Max-Born-Straße 2A, 12489 Berlin, Germany — ²Institute of Physical and Theoretical Chemistry, University of Würzburg, Germany — ³Institute of Chemistry, University of Potsdam, Germany — ⁴Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, Strasbourg, France — ⁵Institute of Physics NAS of Ukraine, Nauky Ave, 46, 03028, Kyiv, Ukraine

The excited-state dynamics of the aminoazobenzene Metanil Yellow in aqueous solutions was studied using ultrafast time-resolved transient absorption spectroscopy in both the UV-visible and the NIR regions. The different solutions were studied with different excitation wavelengths to investigate the protonated and non-protonated forms of the molecule and reveal differences in the corresponding dynamics. The relaxation dynamics of the non-protonated form was previously studied by time-resolved photoelectron spectroscopy and TDDFT calculations and revealed transitions from the bright S2 to the ground state S0 via

the dark S1 state. As a first interpretation, the present results for the protonated form could be explained by direct excitation of S1 followed by the proton ejection during the first 0.5-1.0 ps. After 1 ps the excited state absorption looks similar for both forms and reflects the internal conversion to the trans ground state along the torsional coordinate.

MO 6.22 Tue 16:30 Empore Lichthof

Ultrafast dynamics and reversible switching of azobenzene-copper complexes — ●MARCEL J. P. SCHMITT¹, JUSTIN HORNBOGEN², RAPHAEL I. PETRIKAT¹, SABINE BECKER¹, ROLF DILLER², and CHRISTOPH RIEHN^{1,3} — ¹Dept. of Chemistry, RPTU Kaiserslautern — ²Dept. of Physics, RPTU Kaiserslautern — ³Forschungszentrum OPTIMAS, 67663 Kaiserslautern (Germany)

Azobenzenes and their derivatives are known for their reversible *E-Z*-photoisomerization around the N=N bond.[1,2] Their usage as photoswitchable ligands in metal complexation has also been explored.[3] We present preliminary spectroscopic and ultrafast dynamic results in solution and gas phase of a newly synthesized cyclic [Cu₂L₂]²⁺ complex, comprised of two pyridyl-substituted azobenzene ligands (L) in conjunction with Cu(I). We focus on the photoswitching dynamics and possible cooperative effects involving the ligands and metal cores. Therefore, we have examined the dynamics in parallel in solution by transient absorption and in gas phase by femtosecond transient photodissociation using an electropray ionization mass spectrometer. The resulting ultrafast dynamic spectra reveal multiexponential electronic decay with lifetimes in the sub-ps and ps time ranges for both *E* and *Z* configurations. For comparison with UV/Vis and mIR spectra, the binding situation of the copper centers (tetrahedral vs. planar) in the (*E,E*), (*E,Z*) and (*Z,Z*) complexes was quantum chemically modelled by RI-DFT/TD-DFT calculations.

[1] Nat. Rev. Chem. 2019, 3, 133. [2] Chem. Soc. Rev. 2012, 41, 18091825. [3] J. Phys. Chem. Lett. 2019, 10, 6048.

MO 6.23 Tue 16:30 Empore Lichthof

Femtosecond Spectroscopy of a highly strained benzene isomer — ●LUKAS FASCHINGBAUER¹, TOBIAS PREITSCHOPF¹, JENS PETERSEN¹, LOU BARREAU², LIONEL POISSON², ROLAND MITRIC¹, and INGO FISCHER¹ — ¹Institut für Physikalische und Theoretische Chemie, Würzburg, Germany — ²Institut des Sciences Moléculaires d'Orsay, Orsay, France

As a highly strained benzene isomer, 3,4-dimethylenecyclobutene (DMCB) forms an intriguing system to study the dynamics of its excited states, both from an experimental and a theoretical point of view. The formally Woodward-Hoffmann allowed electrocyclic ring opening to 1,2,4,5-hexatetraene is not observed, in contrast to the thermal counterpart, which has been observed in pathways to benzene in flames. Nevertheless, as indicated by a very broad and diffuse gas-phase UV/VIS absorption spectrum, ultrafast non-radiative decay is observed by femtosecond time-resolved photoelectron and time-of-flight mass spectrometry. To explore the underlying mechanism, ab initio calculations and mixed quantum-classical surface hopping molecular dynamics simulations have been performed.